Full wwPDB EM Validation Report (i)

Jul 15, 2025 – 12:16 PM EDT

PDB ID	:	8VOQ / pdb_00008voq
EMDB ID	:	EMD-43389
Title	:	Escherichia coli transcription-translation loosely coupled complex (TTC-LC) containing mRNA with a 39 nt long spacer, NusG, NusA, and fMet-tRNAs in E-site and P-site
Authors	:	Molodtsov, V.; Wang, C.; Ebright, R.H.
Deposited on	:	2024-01-15
Resolution	:	9.30 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 (i) symbol.

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

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

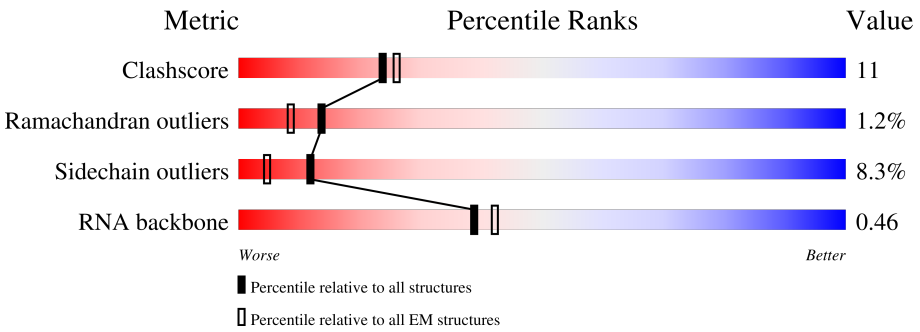
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 9.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	103	11%, 84%, 15%, •
2	1	110	5%, 75%, 25%
3	2	100	9%, 86%, 7%, •, 6%
4	3	104	12%, 84%, 14%, ••
5	4	94	11%, 97%, •
6	5	36	31%, 28%, 36%, 36%
7	6	36	25%, 36%, 39%, 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	7	56	12% • 21% 25% 7% 45%
9	9	165	21% 28% 35% 24% • 10%
10	A	76	12% 47% 36% 5%
10	B	76	13% 11% 47% 37% 5%
11	AA	1342	82% 80% 18% •
12	AB	181	61% 41% 31% 17% 11%
13	AC	329	66% 60% 6% • 33%
13	AD	329	90% 76% 15% 9%
14	AE	1407	72% 66% 24% • 5%
15	AF	91	84% 77% 13% 10%
16	AG	495	69% 31% 44% 21% •
17	C	75	9% 71% 16% • 12%
18	D	1542	• 70% 25% • •
19	E	87	14% 87% 10% • •
20	F	71	13% 87% 10% • •
21	G	241	20% 79% 13% • 7%
22	H	557	30% 25% 16% • • 54%
23	I	233	18% 80% 8% • 11%
24	J	206	17% 92% 7%
25	K	167	5% 76% 14% • • 7%
26	L	135	5% 67% 10% 23%
27	M	179	13% 71% 12% • • 16%
28	N	130	5% 90% 8% • •
29	O	130	18% 80% 17% • •
30	P	103	16% 67% 20% 8% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Q	129	8% 82% 9% 9%
32	R	124	88% 10%
33	S	101	17% 88% 9%
34	T	89	80% 17%
35	U	82	18% 87% 12%
36	V	84	87% 7% 5%
37	W	92	26% 79% 10% 10%
38	X	118	25% 75% 18% 5%
39	Y	142	22% 37% 40% 20%
40	Z	121	8% 7% 12% 6% 75%
41	a	2904	73% 23%
42	b	85	6% 84% 6% 11%
43	c	78	6% 87% 9%
44	d	120	81% 19%
45	e	63	16% 86% 11%
46	f	59	85% 12%
47	g	70	21% 81% 11% 6%
48	h	273	5% 85% 13%
49	i	57	5% 77% 19%
50	j	209	10% 88% 12%
51	k	55	15% 89% 5% 5%
52	l	201	13% 85% 14%
53	m	46	78% 17%
54	n	179	15% 75% 20%
55	o	65	9% 88% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
56	p	177	18% 90% 8%
57	q	38	24% 89% 8%
58	r	149	39% 88% 9%
59	s	142	15% 83% 15%
60	t	123	10% 80% 19%
61	u	144	10% 88% 12%
62	v	136	7% 91% 8%
63	w	127	5% 77% 17% 6%
64	x	117	16% 84% 15%
65	y	115	17% 89% 10%
66	z	118	8% 84% 14%

2 Entry composition (i)

There are 68 unique types of molecules in this entry. The entry contains 291173 atoms, of which 109913 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	0	103	1655	516	839	153	145	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	1	110	1779	532	922	166	156	3	0	0

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	2	94	1557	470	811	140	134	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
4	3	103	1632	498	844	148	142	0	0

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	4	94	1533	479	780	137	134	3	0	0

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	5	23	732	225	260	87	137	23	0	0

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
7	6	27	847	259	305	89	167	27	0	0

- Molecule 8 is a RNA chain called mRNA with 39 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
8	7	31	744	289	97	92	235	31	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	9	148	1117	705	196	209	7	0	0

- Molecule 10 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
10	A	76	2446	723	826	295	527	75	0	0
			Total	C	H	N	O	P		
10	B	76	2434	723	814	295	527	75	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AA	1340	10567	6631	1841	2052	43	0	0

- Molecule 12 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AB	161	1276	813	221	235	7	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AC	220	1690	1056	298	330	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AD	298	2073	1284	377	406	6	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	AE	1335	21000	6526	10612	1854	1958	50	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AF	82	650	396	122	131	1	0	0

- Molecule 16 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	AG	495	3852	2396	669	774	13	0	0

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	C	66	1103	344	559	102	97	1	0	0

- Molecule 18 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
18	D	1524	49126	14585	16423	6003	10591	1524	0	0

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	E	86	1388	414	719	138	114	3	0	0

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	F	70	1218	366	629	125	97	1	0	0

- Molecule 21 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	G	225	3545	1113	1785	316	323	8	0	0

- Molecule 22 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	H	259	3184	1073	1454	305	349	3	0	0

- Molecule 23 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	I	208	3346	1036	1710	307	290	3	0	0

- Molecule 24 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	J	205	3350	1026	1707	315	298	4	0	0

- Molecule 25 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	K	156	2348	717	1196	217	212	6	0	0

- Molecule 26 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	L	104	1694	536	846	153	152	7	0	0

- Molecule 27 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	M	151	2416	735	1235	227	215	4	0	0

- Molecule 28 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	N	129	2010	616	1031	173	184	6	0	0

- Molecule 29 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	O	127	2092	634	1070	206	179	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	P	99	1621	495	831	151	143	1	0	0

- Molecule 31 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	Q	117	1764	540	887	174	160	3	0	0

- Molecule 32 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	R	121	1940	580	1001	194	161	4	0	0

- Molecule 33 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	S	100	1649	499	844	164	139	3	0	0

- Molecule 34 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	T	88	1448	439	734	144	130	1	0	0

- Molecule 35 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	U	82	1315	406	666	128	114	1	0	0

- Molecule 36 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	V	80	1339	411	691	121	113	3	0	0

- Molecule 37 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	W	83	1351	424	688	126	111	2	0	0

- Molecule 38 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	X	116	1864	558	964	181	158	3	0	0

- Molecule 39 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Y	141	1032	651	179	196	6	0	0

- Molecule 40 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Z	30	227	144	33	47	3	0	0

- Molecule 41 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
41	a	2880	92918	27587	31077	11398	19976	2880	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	b	76	1181	360	599	117	104	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	c	77	1277	388	652	129	106	2	0	0

- Molecule 44 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
44	d	120	3870	1144	1301	468	837	120	0	0

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	e	62	1032	308	531	98	94	1	0	0

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	f	58	936	281	488	87	78	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	g	66	1042	323	520	99	94	6	0	0

- Molecule 48 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	h	271	4236	1288	2154	423	364	7	0	0

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	i	56	903	269	459	94	80	1	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	j	209	3182	979	1617	288	294	4	0	0

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
51	k	52	890	275	464	78	73	0	0

- Molecule 52 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
52	l	201	3171	974	1619	283	290	5	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	m	46	795	228	418	90	57	2	0	0

- Molecule 54 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	n	177	2853	899	1443	249	256	6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
55	o	64	1076	323	572	105	74	2	0	0

- Molecule 56 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
56	p	175	2671	826	1358	241	244	2	0	0

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
57	q	38	645	185	343	65	48	4	0	0

- Molecule 58 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
58	r	149	2259	699	1148	197	214	1	0	0

- Molecule 59 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
59	s	142	2291	714	1162	212	199	4	0	0

- Molecule 60 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
60	t	123	1969	593	1023	181	166	6	0	0

- Molecule 61 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
61	u	144	2182	654	1129	207	190	2	0	0

- Molecule 62 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
62	v	136	2231	686	1157	205	177	6	0	0

- Molecule 63 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
63	w	119	1945	588	994	195	163	5	0	0

- Molecule 64 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
64	x	116	1815	552	923	178	162	0	0

- Molecule 65 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
65	y	114	1879	574	962	179	163	1	0	0

- Molecule 66 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
66	z	117	1967	604	1020	192	151	0	0

- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
67	AE	1	1	1	0

- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

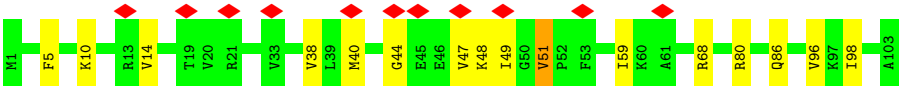
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
68	AE	2	2	2	0

3 Residue-property plots (i)

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

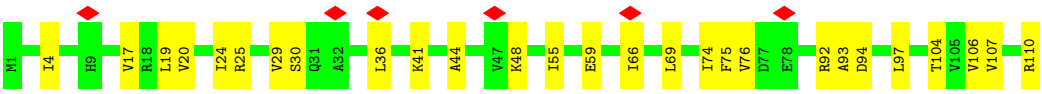
- Molecule 1: Ribosomal protein L21

Chain 0:



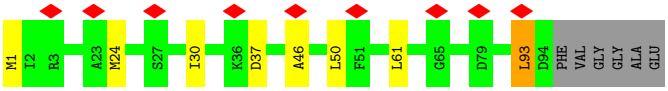
- Molecule 2: 50S ribosomal protein L22

Chain 1:



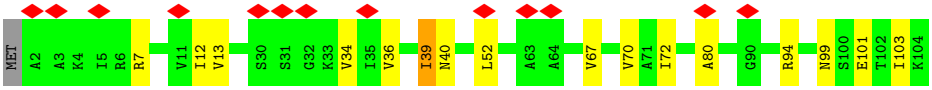
- Molecule 3: 50S ribosomal protein L23

Chain 2:



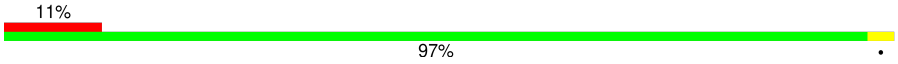
- Molecule 4: 50S ribosomal protein L24

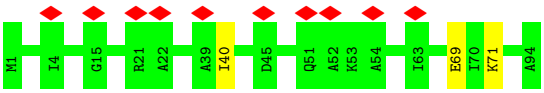
Chain 3:



- Molecule 5: 50S ribosomal protein L25

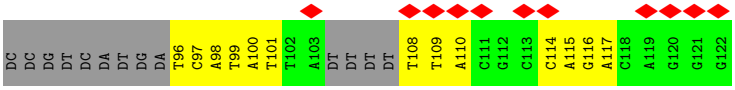
Chain 4:





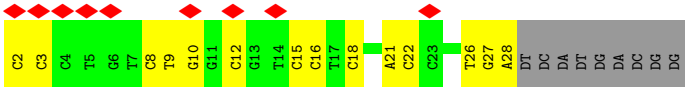
- Molecule 6: NT DNA

Chain 5: 31% 28% 36% 36%



- Molecule 7: T DNA

Chain 6: 25% 36% 39% 25%

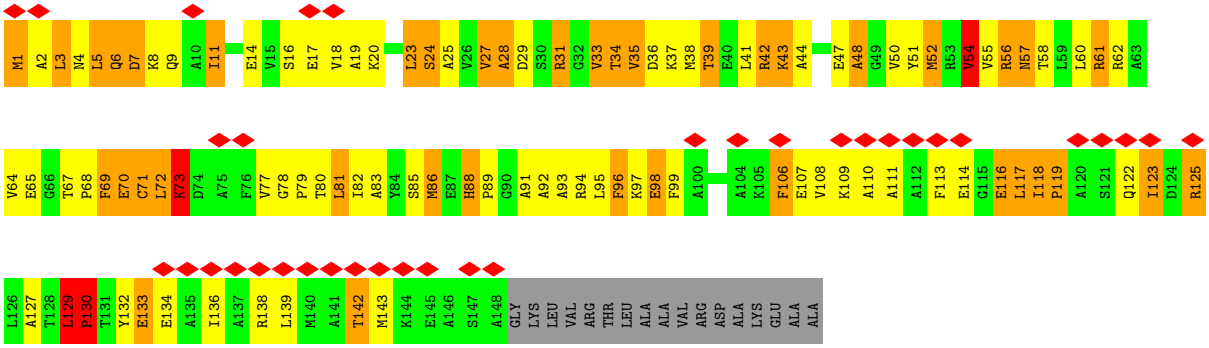


- Molecule 8: mRNA with 39 nt long spacer

Chain 7: 12% 21% 25% 7% 45%

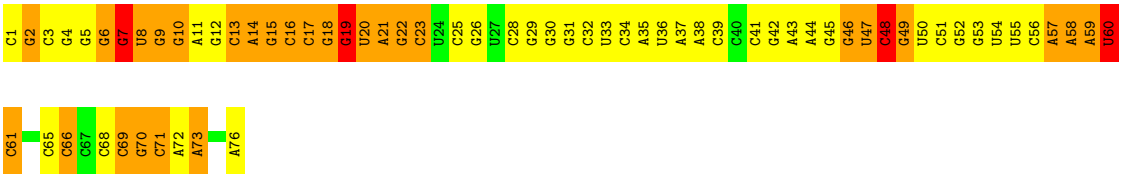
- Molecule 9: 50S ribosomal protein L10

Chain 9: 21% 28% 35% 24% 10%



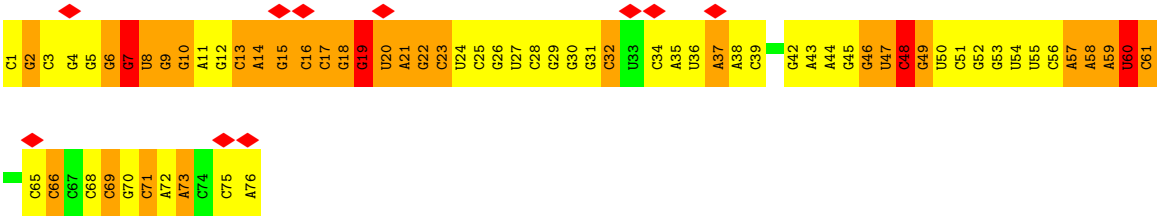
- Molecule 10: E-site and P-site tRNA (fMet)

Chain A: 12% 47% 36% 5%



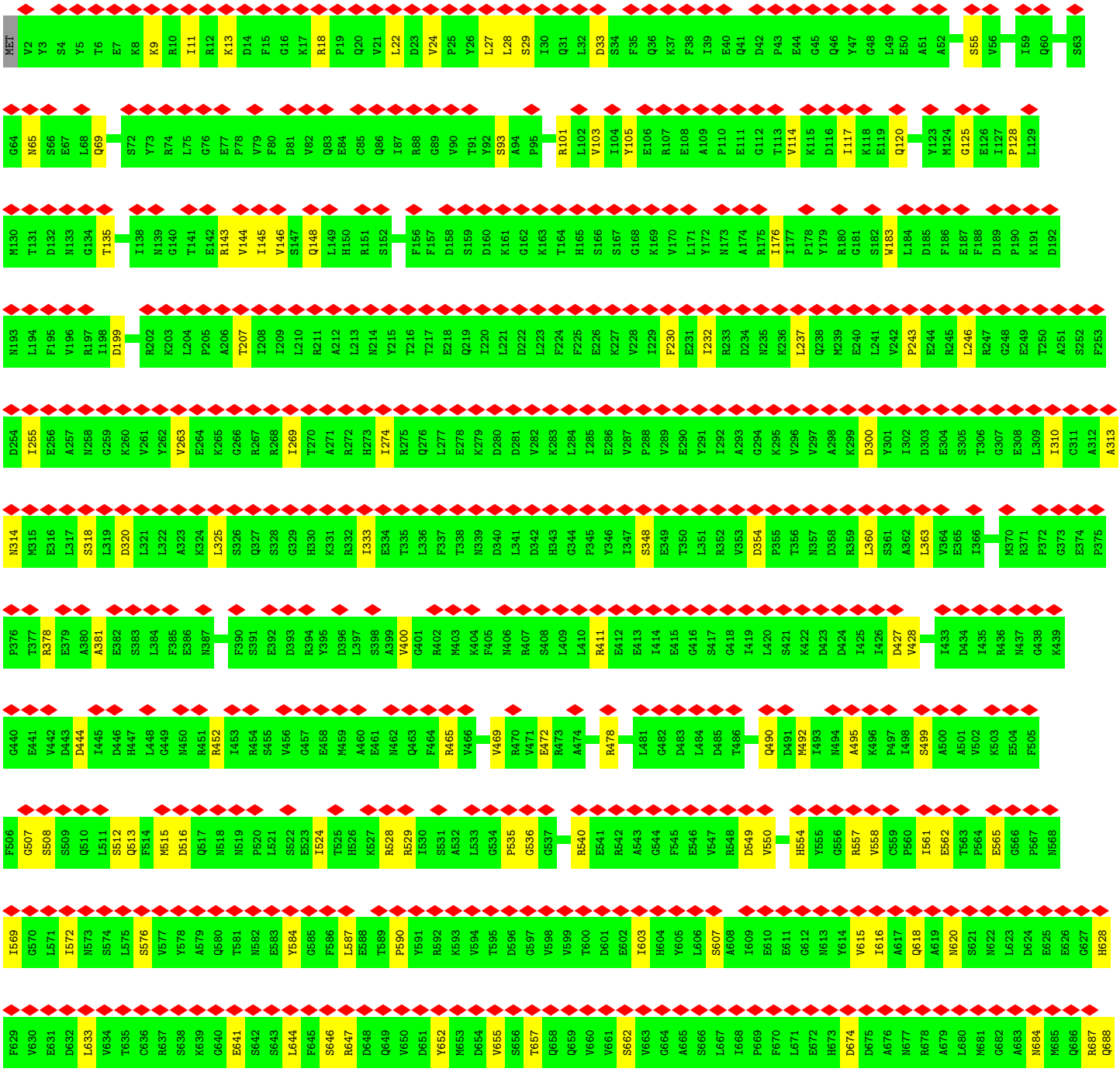
- Molecule 10: E-site and P-site tRNA (fMet)

Chain B: 13% 11% 47% 37% 5%



• Molecule 11: DNA-directed RNA polymerase subunit beta

Chain AA:



A689 V690 P691 T692 L693 R694 A695 D696 K697 P698 L699 V700 G701 T702 G703 M704 E705 R706 A707 V708 A709 V710 D711 S712 G713 V714 T715 A716 V717 A718 K719 R720 G721 G722 V723 V724 Q725 Y726 V727 D728 A729 S730 R731 I732 V733 I734 K735 V736 N737 E738 D739 E740 M741 Y742 P743 G744 E745 A746 G747 I748

D749 I750 Y751 N752 L753 T754 K755 Y756 T757 R758 Q761 N762 T763 C764 I765 N766 Q767 M768 P769 C770 V771 S772 L773 G774 E775 P776 V777 E778 R779 G780 D781 V782 L783 A784 D785 G786 P787 S788 T789 D790 L791 G792 E793 L794 A795 L796 G797 Q798 N799 M800 R801 V802 A803 F804 M805 P806 W807 N808 G809

Y810 N811 F812 E813 D814 S815 I816 L817 V818 S819 E820 R821 V822 V823 Q824 E825 D826 R827 F828 T829 T830 I831 H832 I833 Q834 E835 L836 A837 C838 V839 S840 R841 D842 T843 K844 L845 G846 P847 E848 E849 I850 T851 A852 D853 I854 P855 N856 V857 G858 E859 A860 A861 L862 S863 K864 L865 D866 E867 S868 G869

I870 V871 Y872 I873 G874 A875 E876 V877 T878 G879 G880 D881 I882 L883 V884 G885 K886 V887 T888 P889 K890 G891 E892 T893 Q894 L895 T896 P897 E898 E899 K900 L901 L902 R903 A904 I905 F906 G907 E908 K909 A910 S911 D912 V913 K914 D915 S916 S917 L918 R919 V920 P921 N922 G923 V924 S925 G926 T927 V928 I929

D930 V931 Q932 V933 F934 T935 R936 D937 G938 V939 E940 K941 D942 K943 R944 A945 L946 E947 I948 E949 E950 M951 Q952 L953 K954 Q955 A956 K957 K958 D959 L960 S961 E962 E963 L964 Q965 I966 L967 E968 A969 G970 L971 F972 S973 R974 I975 R976 A977 V978 L979 V980 A981 G982 G983 V984 E985 A986 E987 K988 L989

D990 K991 L992 P993 R994 D995 R996 W997 L998 E999 L1000 G1001 L1002 T1003 D1004 E1005 E1006 K1007 Q1008 N1009 Q1010 L1011 E1012 Q1013 L1014 A1015 E1016 Q1017 Y1018 D1019 E1020 L1021 K1022 H1023 E1024 F1025 E1026 K1027 K1028 L1029 E1030 A1031 K1032 R1033 R1034 K1035 I1036 T1037 Q1038 G1039 D1040 D1041 L1042 A1043 P1044 G1045 V1046 L1047 K1048 I1049

V1050 K1051 V1052 Y1053 L1054 A1055 V1056 K1057 R1058 R1059 I1060 Q1061 P1062 G1063 D1064 A1067 G1068 R1069 H1070 G1071 N1072 K1073 G1074 V1075 I1076 S1077 K1078 I1079 N1080 P1081 I1082 E1083 D1084 M1085 P1086 Y1087 D1088 E1089 N1090 G1091 T1092 P1093 V1094 D1095 I1096 V1097 L1098 N1099 P1100 L1101 G1102 V1103 P1104 S1105 R1106 M1107 N1108 I1109 G1110

Q1111 I1112 L1113 E1114 T1115 H1116 L1117 G1118 M1119 A1120 A1121 K1122 G1125 D1126 K1127 I1128 N1129 A1130 M1131 L1132 K1133 Q1134 Q1135 Q1136 E1137 V1138 A1139 K1140 L1141 R1142 E1143 F1144 T1145 Q1146 R1147 A1148 Y1149 D1150 L1151 G1152 A1153 D1154 V1155 R1156 Q1157 K1158 V1159 D1160 L1161 S1162 T1163 F1164 S1165 D1166 E1167 E1168 V1169 M1170 R1171

L1172 A1173 E1174 N1175 L1176 R1177 K1178 G1179 M1180 P1181 I1182 A1183 T1184 P1185 V1186 F1187 D1188 G1189 A1190 K1191 E1192 A1193 E1194 I1195 K1196 E1197 L1198 L1199 K1200 L1201 G1202 D1203 L1204 P1205 T1206 S1207 G1208 Q1209 I1210 R1211 L1212 Y1213 D1214 G1215 R1216 Q1217 T1217 G1218 E1219 Q1220 F1221 E1222 R1223 P1224 V1225 T1226 V1227 G1228 Y1229 M1230 Y1231

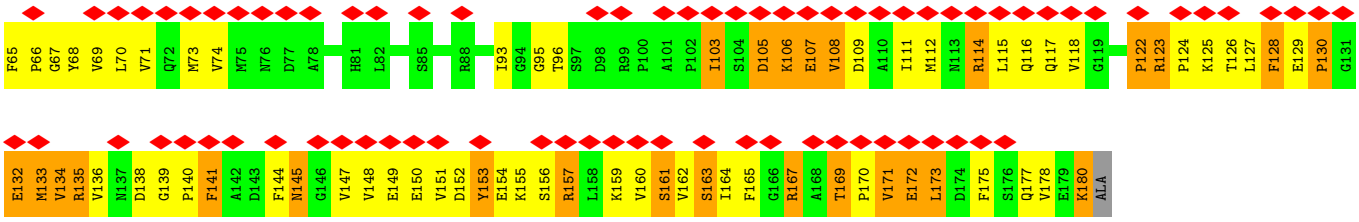
M1232 L1233 K1234 L1235 N1236 H1237 L1238 V1239 D1240 D1241 K1242 M1243 H1244 A1245 R1246 S1247 T1248 L1253 V1254 T1255 Q1256 G1260 G1261 K1262 A1263 Q1264 F1265 G1266 G1267 Q1268 G1271 E1272 M1273 E1274 V1275 L1278 E1279 A1280 Y1281 G1282 A1283 A1284 Y1285 T1286 L1287 M1290 V1298 N1299 T1302 K1303 M1304 Y1305 K1306

N1307 I1308 V1309 D1310 G1311 N1312 H1313 Q1314 M1315 E1316 P1317 F1323 K1328 E1329 S1332 L1333 G1334 I1335 N1336 I1337 E1338 L1339 E1340 D1341 GLU

- Molecule 12: Transcription termination/antitermination protein NusG

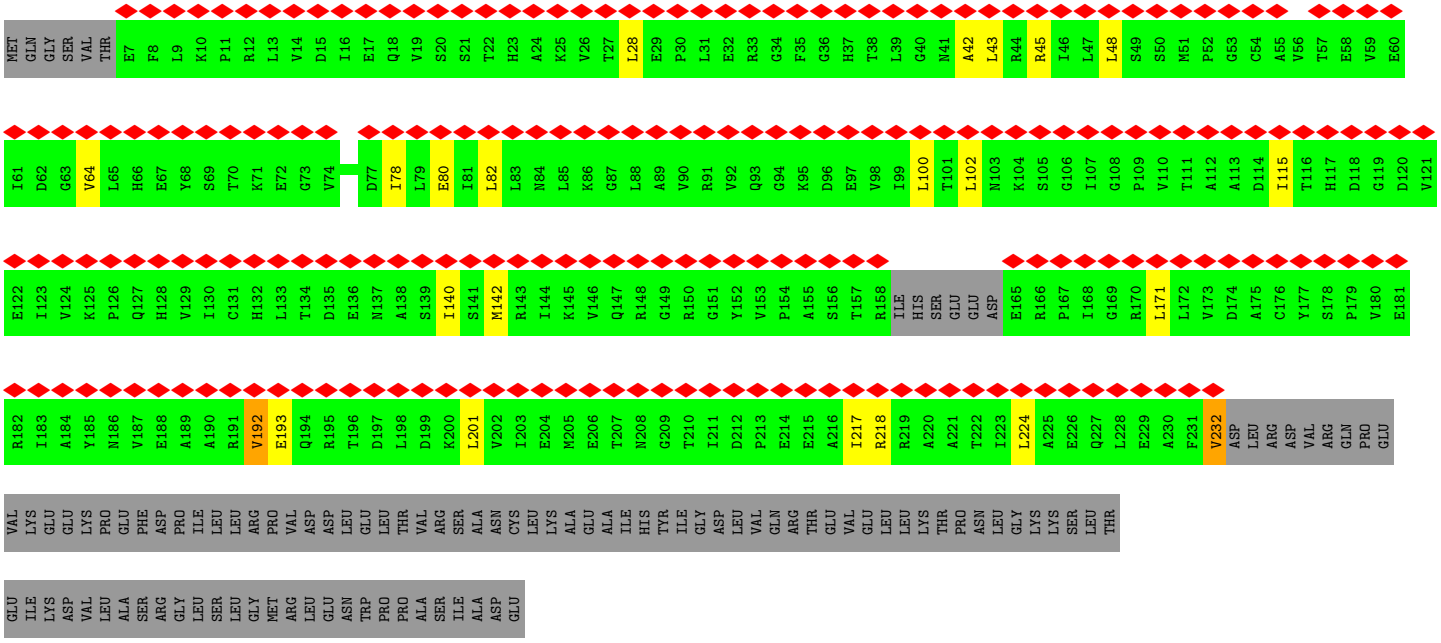
Chain AB:

MET SER GLU ALA PRO K6 K7 R8 W9 Y10 V11 S16 E19 G20 R21 V22 A23 T24 S25 L26 R27 E28 H29 I30 K31 L32 H33 N34 M35 E36 D37 L38 F39 G40 E41 V42 M43 V44 P45 T46 E47 E48 VAL VAL GLU ILE ARG GLY GLY GLN ARG ARG LYS SER GLU ARG K63 F64



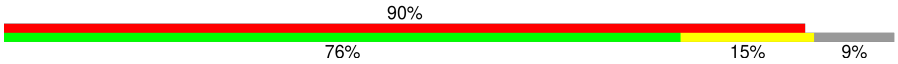
- Molecule 13: DNA-directed RNA polymerase subunit alpha

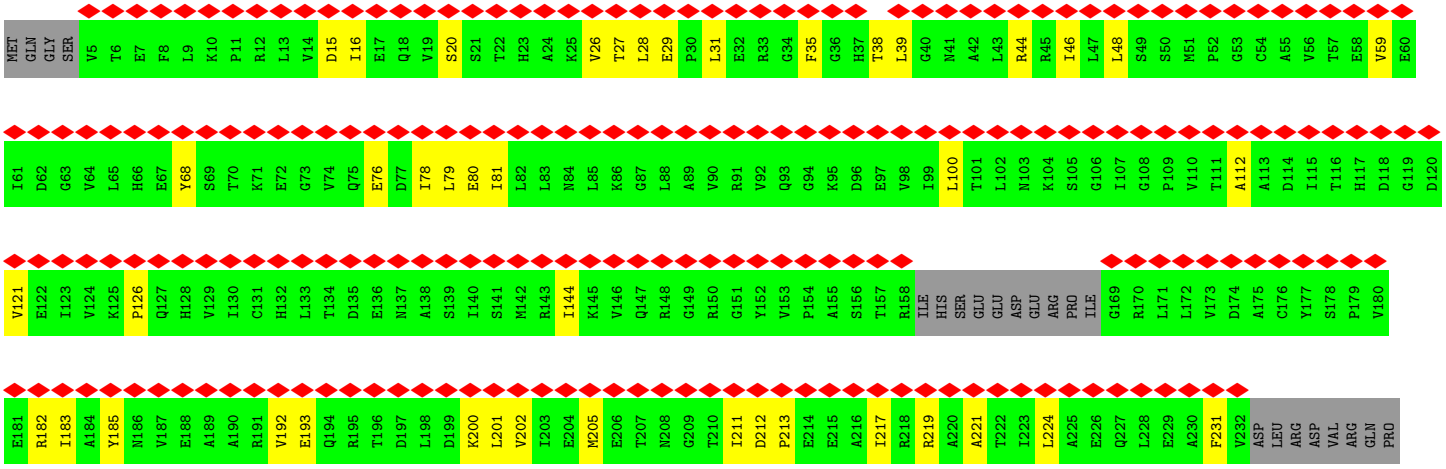
Chain AC:

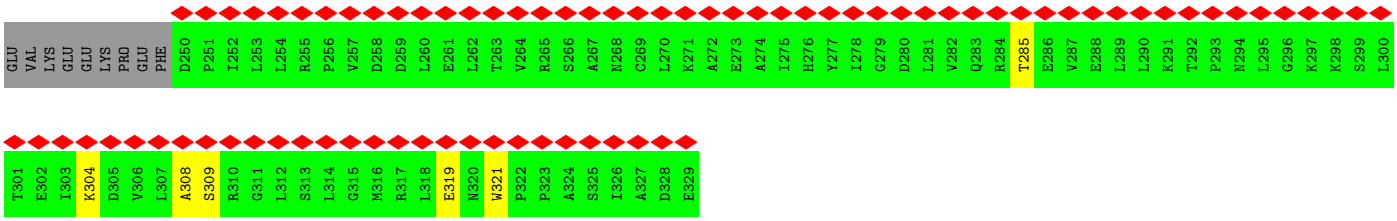


- Molecule 13: DNA-directed RNA polymerase subunit alpha

Chain AD:

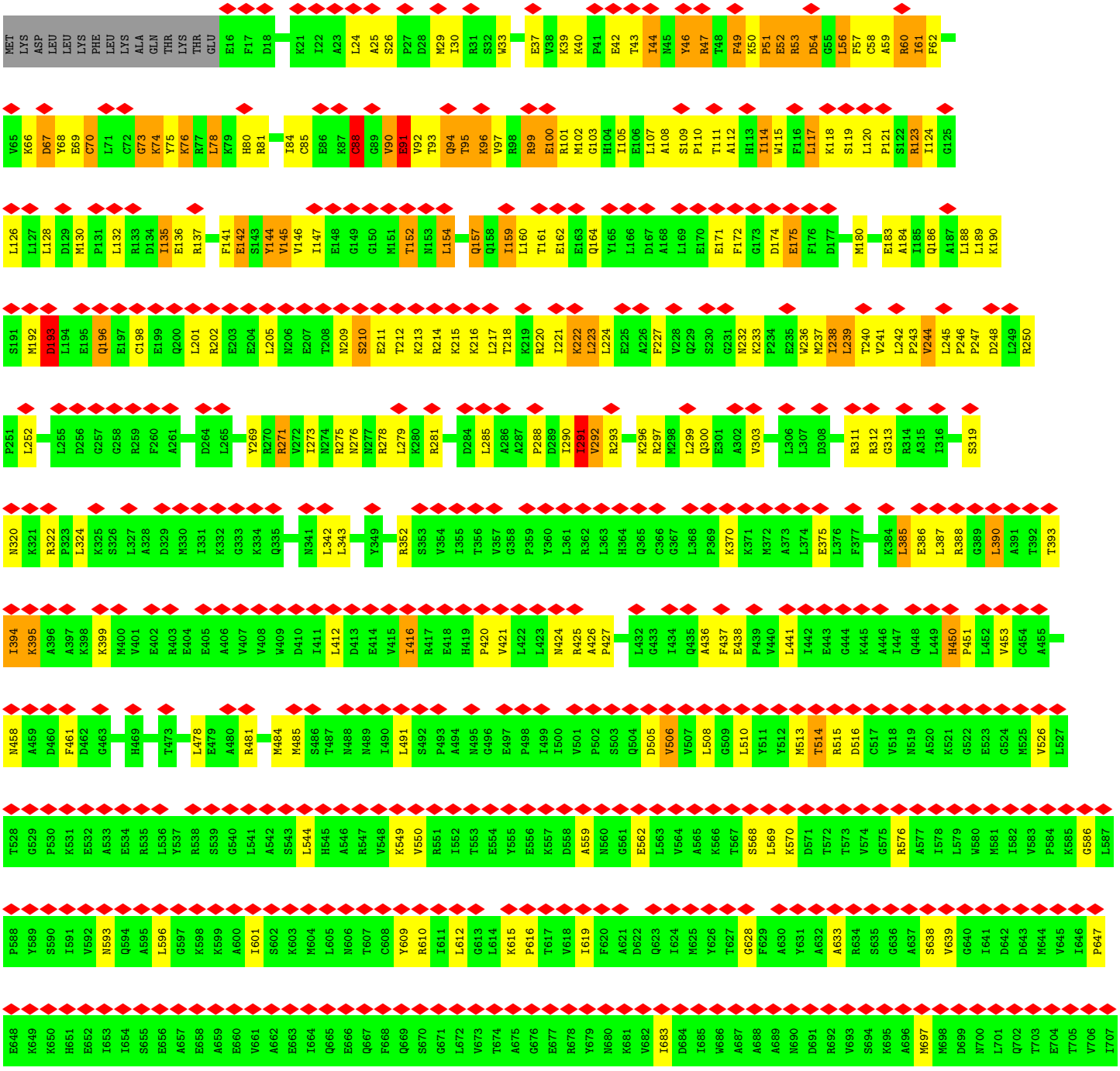






• Molecule 14: DNA-directed RNA polymerase subunit beta'

Chain AE:



N708 R709 D710 G711 Q712 E713 E714 K715 Q716 V717 S718 F719 N720 S721 I722 Y723 M724 M725 A726 D727 S728 G729 A730 R731 G732 S733 A734 A735 Q736 I737 R738 Q739 L740 A741 G742 M743 R744 G745 L746 M747 A748 K749 P750 D751 G752 S753 I754 I755 E756 T757 P758 I759 T760 A761 N762 F763 R764 E765 G766 L767

N768 V769 L770 Q771 Y772 F773 I774 S775 T776 H777 G778 A779 R780 K781 G782 L783 A784 D785 T786 A787 L788 K789 T790 T797 R798 R799 L800 Y801 D802 Y803 A804 Q805 D806 L807 V808 V809 D812 D813 C814 G815 T816 H817 E818 G819 I820 M821 M822 T823 P824 V825 I826 E827 G828 G829 D830 V831 K832 E833

P834 L835 R836 D837 R838 V839 L840 G841 R842 V843 T844 A845 E846 D847 V848 L849 K850 P851 G852 T853 A854 D855 I856 L857 V858 P859 R860 N861 T862 L863 L864 H865 E866 Q867 W868 C869 D870 L871 L872 E873 E874 N875 S876 V877 D878 A879 V880 K881 V882 R883 S884 V885 V886 S887 C888 D889 T890 D891 F892 G893

V894 C895 A896 H897 C898 Y899 G900 R901 D902 L903 A904 R905 G906 H907 I908 I909 N910 K911 G912 E913 A914 I915 G916 V917 I918 A919 A920 Q921 S922 I923 G924 E925 P926 G927 T928 Q929 L930 T931 M932 R933 THR PHE HIS ILE GLY GLY ALA ALA SER ARG ALA ALA ALA GLU S948 S949 I950 Q951 V952 K953

N954 K955 G956 S957 I958 K959 L960 S961 N962 V963 K964 S965 V966 V967 N968 S969 S970 G971 K972 L973 V974 I975 T976 S977 R978 N979 T980 E981 L982 K983 L984 I985 D986 E987 F988 G989 R990 T991 K992 E993 S994 Y995 K996 V997 P998 Y999 G1000 A1001 V1002 L1003 A1004 K1005 G1006 D1007 G1008 E1009 Q1010 V1011 A1012 G1013

G1014 E1015 T1016 V1017 A1018 N1019 W1020 D1021 P1022 H1023 T1024 M1025 P1026 V1027 I1028 T1029 E1030 V1031 S1032 G1033 F1034 V1035 R1036 F1037 T1038 D1039 M1040 I1041 D1042 G1043 Q1044 I1045 I1046 T1047 R1048 Q1049 T1050 D1051 E1052 L1053 T1054 G1055 L1056 S1057 S1058 L1059 V1060 V1061 L1062 D1063 S1064 A1065 E1066 R1067 T1068 A1069 G1070 G1071 K1072 D1073

L1074 R1075 P1076 A1077 L1078 K1079 I1080 V1081 D1082 A1083 Q1084 G1085 N1086 D1087 V1088 L1089 I1090 P1091 G1092 T1093 D1094 M1095 P1096 A1097 Q1098 Y1099 F1100 L1101 P1102 G1103 K1104 A1105 I1106 V1107 Q1108 L1109 E1110 D1111 G1112 V1113 Q1114 I1115 S1116 S1117 G1118 D1119 T1120 L1121 A1122 R1123 I1124 P1125 Q1126 GLU SER GLY GLY GLY THR LYS ASP

ILE THR G1136 G1137 L1138 P1139 R1140 V1141 A1142 D1143 L1144 F1145 E1146 A1147 R1148 R1149 P1150 K1151 E1152 P1153 A1154 I1155 L1156 A1157 E1158 I1159 S1160 G1161 I1162 V1163 S1164 F1165 G1166 K1167 E1168 T1169 K1170 G1171 K1172 R1173 R1174 L1175 V1176 I1177 T1178 P1179 V1180 D1181 G1182 S1183 D1184 P1185 Y1186 E1187 E1188 M1189 I1190 P1191 K1192 W1193

R1194 Q1195 L1196 N1197 V1198 F1199 E1200 G1201 E1202 R1203 V1204 E1205 R1206 G1207 D1208 V1209 I1210 S1211 D1212 G1213 P1214 E1215 A1216 P1217 H1218 D1219 I1220 L1221 R1222 L1223 R1224 G1225 V1226 H1227 A1228 V1229 T1230 R1231 Y1232 I1233 V1234 N1235 E1236 V1237 Q1238 D1239 V1240 Y1241 R1242 L1243 Q1244 G1245 I1248 N1249 D1250 K1251 H1252 I1253 E1254

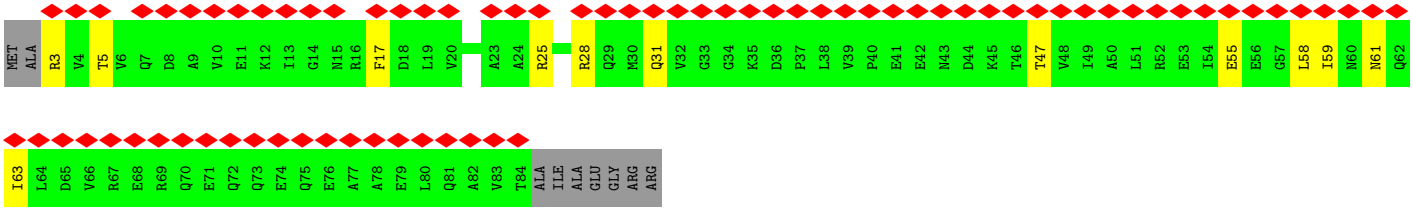
V1255 I1256 V1257 R1258 Q1259 M1260 L1261 R1262 K1263 A1264 T1265 I1266 V1267 N1268 A1269 G1270 S1271 S1272 D1273 F1274 L1275 E1276 G1277 E1278 Q1279 V1280 E1281 R1284 A1288 N1289 R1290 E1291 L1292 E1293 A1294 N1295 G1296 K1297 V1298 T1301 Y1302 S1303 R1304 D1305 L1306 L1307 G1308 I1309 T1310 K1311 A1312 S1313 L1314 A1315 T1316 E1317 S1318

F1319 I1320 S1321 S1324 F1325 Q1326 T1329 R1330 V1331 L1332 T1333 A1336 V1337 A1338 G1339 K1340 E1343 L1344 R1345 G1346 L1347 K1348 E1349 N1350 V1351 I1352 V1353 G1354 R1355 L1356 I1357 P1358 A1359 G1360 T1361 G1362 Y1363 A1364 D1368 R1369 M1370 R1371 R1372 R1373 ALA ALA GLY GLU ALA PRO ALA ALA PRO GLN VAL

THR ALA GLU ASP ALA SER ALA SER LEU ALA GLU LEU LEU ASN ALA GLY LEU GLY GLY SER ASP ASN GLU

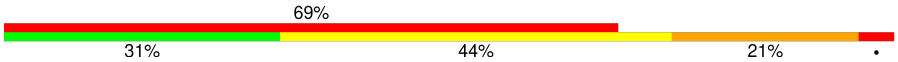
- Molecule 15: DNA-directed RNA polymerase subunit omega

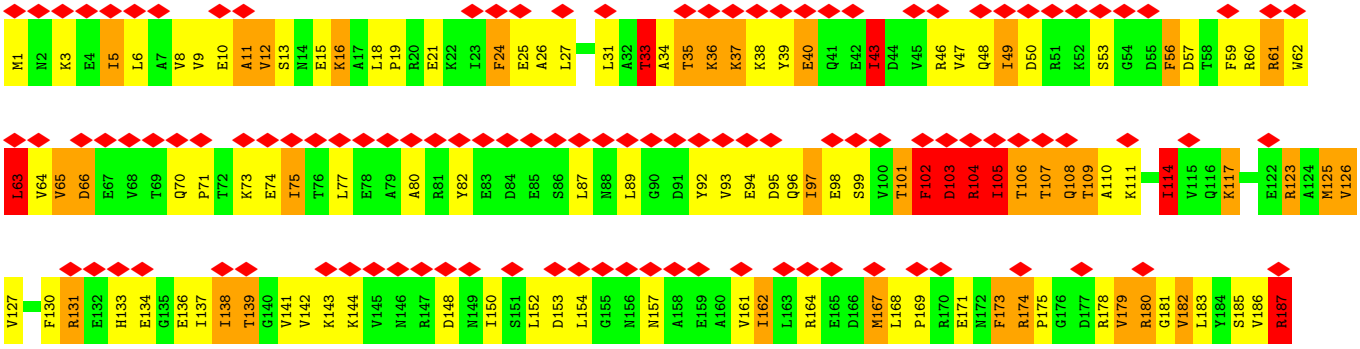
Chain AF: 84% 77% 13% 10%

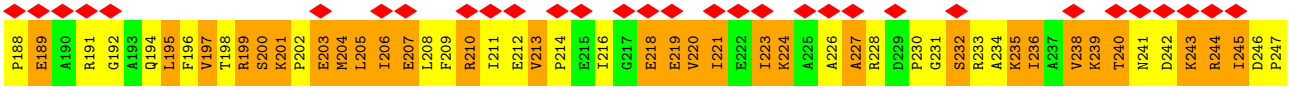


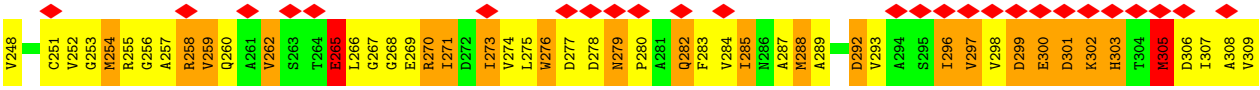
• Molecule 16: Transcription termination/antitermination protein NusA

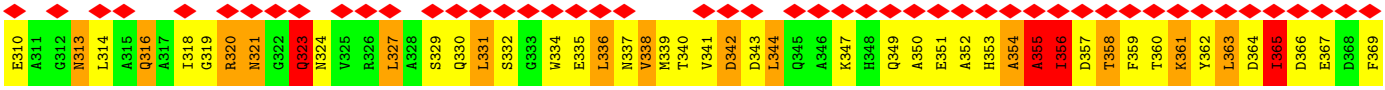
Chain AG:

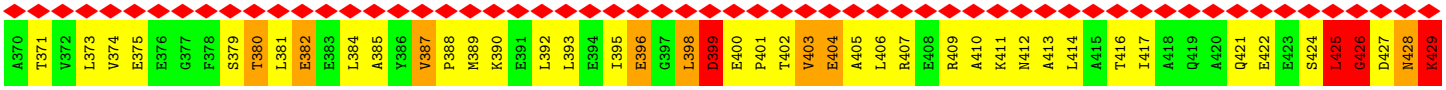


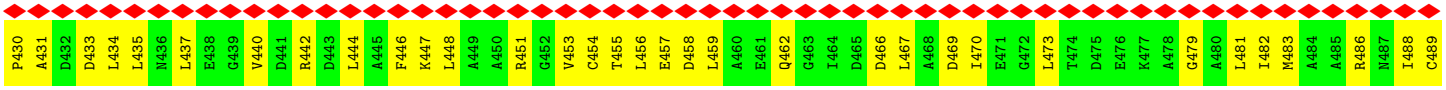


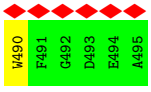






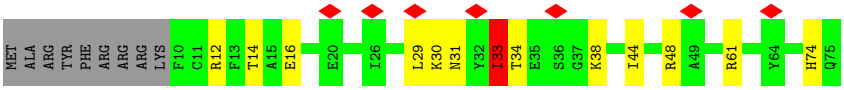






• Molecule 17: 30S ribosomal protein S18

Chain C:



• Molecule 18: 16S rRNA

Chain D: 70% 25%

A1 U4 U5 G6 A7 A8 G9 U13 U17 C18 A19 U20 G21 G22 U29 A32 G35 C36 U37 G38 G39 C40 G41 C47 C48 U49 A50 A51 C52 A53 C54 A60 G69 U70 A71 A72 C73 A74 G75 G76 G82 C83 U84 C87 U88 U89 C90 U91

G94 C95 U96 G107 G108 A109 C110 A120 U121 G122 G128 A131 G141 G144 G145 G148 A149 A152 A160 G164 U170 U173 A181 A182 C183 A196 A197 G198 G204 U208 U209 C210 G211 G212 G213 C214 C215 U216 C217 U218 U219 G220 C221

G226 U245 A246 G247 G251 U252 A253 G258 A262 G266 C267 C271 A279 G289 U294 G299 G305 A306 A321 G324 A325 G326 A327 C328 A329 G332 G337 A338 G347 C352 A353 G354 C355 G360 U367 A371 G372 A373 A374 U375

G376 A382 A383 G384 C385 A389 C392 A393 A397 U398 G404 U405 G406 A412 G413 A414 U421 C422 G423 G424 G428 U429 A430 A431 U439 C440 G446 A451 G457 U458 A459 A460 U463 U464 U467 A468 C469 A478 U479 U480 G481 G484 U485 U486

A495 A496 A502 C503 C504 G505 A509 A510 C511 G515 U G517 C518 C519 G526 G C528 G529 G530 U531 A532 A533 G542 A547 G548 C549 G550 U551 U552 A559 U562 A563 G568 A572 A573 C576 G577 C578 A579 C580 G581 A596 G604 U605 U610

A622 C623 G628 G633 U641 A642 A649 G650 U653 C658 A665 G666 A673 G674 U684 G685 U686 A687 G700 G722 U723 G724 G731 G734 C735 C736 A747 G748 G755 G760 A767 A768 G769 A777 A780 G791 A792 U793 A794

U798 G799 A815 A816 C817 C826 U827 U828 G829 G832 C841 U842 U843 G844 A845 G849 A860 G861 A864 A865 C868 G869 A872 A873 G874 U884 G887 G890 G902 A906 U911 C912 A913 A914 A915 U916 G926 G927 C934 A935 G945

A946 G947 C948 G954 U960 U961 C962 G963 A964 U965 G C A968 A969 G972 G973 A974 A975 G976 A977 A978 C979 U982 U991 U992 G993 A996 C999 A1004 U1008 U1009 U1017 G1018 A1021 G1024 U1025 G1026 C1027 C1028 U1029 U1030 C1031 G1032 C1037 G1043 A1044

C1045 A1046 C1059 U1060 G1061 G1064 U1065 U1085 U1086 G1094 U1095 G1099 C1100 A1101 A1102 C1103 G1124 U1125 U1126 G1133 G1134 U1135 C1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 A1145 A1146 A1151 A1152 C1158 U1159 A1167 U1168 A1169 A1170 A1171 G1174 G1175 A1176 G1177 G1184

U1189 G1190 A1196 A1197 G1206 G C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 C1218 A1219 A1225 C1226 A1227 C1228 U1235 A1236 C1237 A1238 A1239 U1240 G1255 A1256 A1257 G1258 C1259 G1260 A1275 G1276 C1277 G1278 G1279 A1280 A1285 U1286 A1287 A1299 G1300 U1301 C1302 G1305 U1308 G1309 G1310

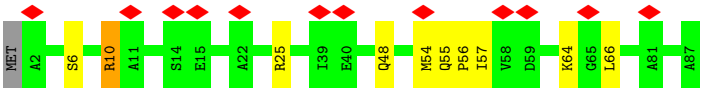
A1311 G1312 C1317 C1320 G1323 A1324 A1329 U1330 A1333 G1334 U1335 G1338 A1339 A1340 A1346 G1347 G1353 G1356 A1357 U1358 A1363 C1366 C1367 A1368 C1369 G1370 G1371 C1378 G1379 U1380 U1381 U1391 C1395 A1396 C1397 A1398 G1401 C C1403 C1404 G1405 U1406 C A1408 C1409

A1410 G1417 A1418 G1419 A1429 G1432 A1441 A1446 A1447 C1448 C1452 G1453 G1473 U1474 G1475 G1482 G1487 U1490 G1491 A1492 A1493 G1494 U1495 C1496 G1497 U A1499 A1500 C1501 A1502 A1503 G1504 G1505 U1506 A1513 G1514 G1515 G1516 G1517 A A C1520 G1526 G1529 G1530 A1534

C C U C C U U A

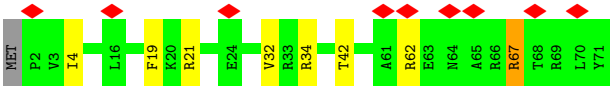
• Molecule 19: 30S ribosomal protein S20

Chain E:



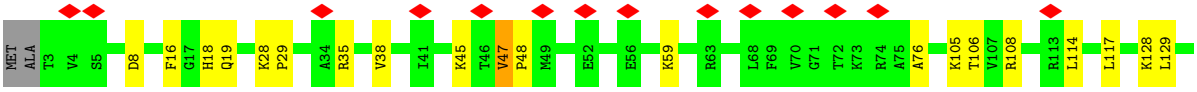
• Molecule 20: 30S ribosomal protein S21

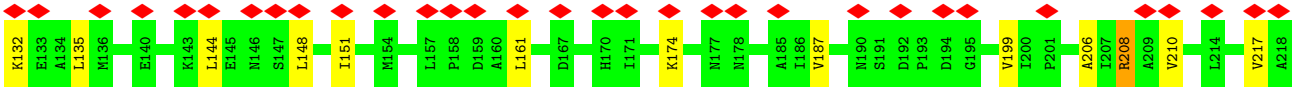
Chain F:

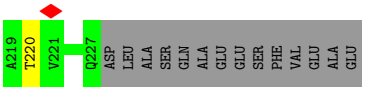


• Molecule 21: 30S ribosomal protein S2

Chain G:

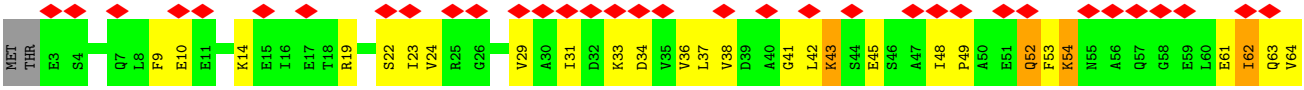


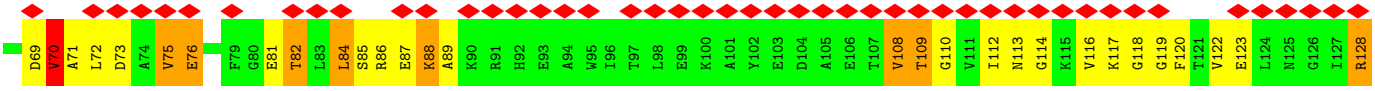


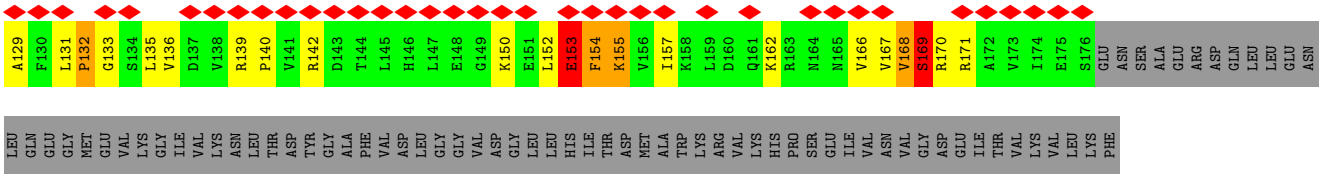


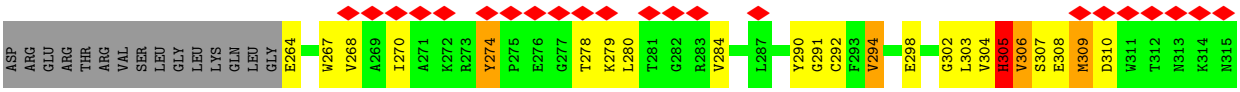
• Molecule 22: 30S ribosomal protein S1

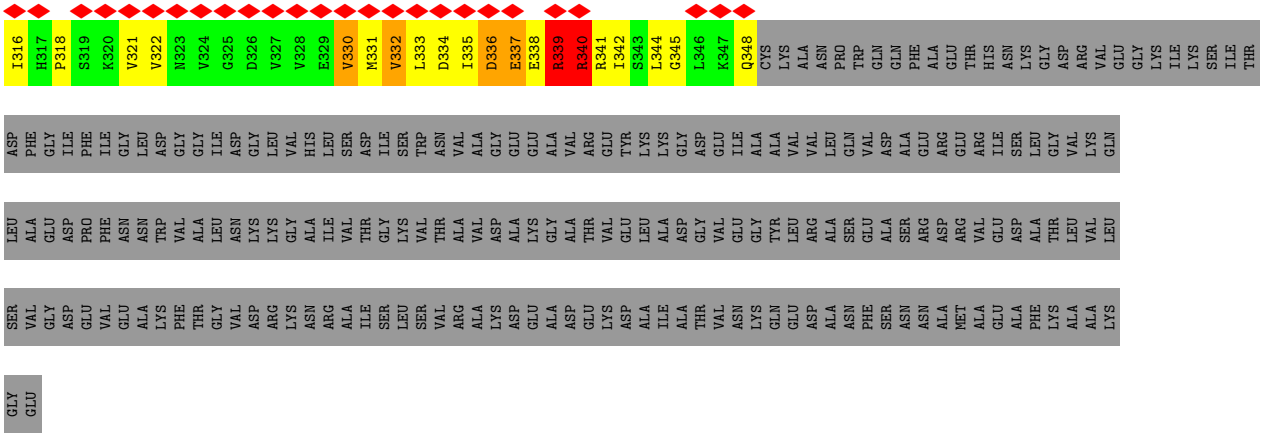
Chain H:





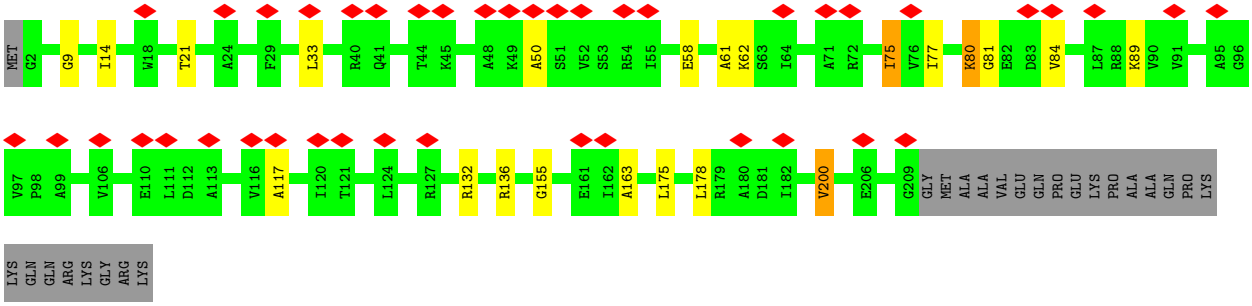






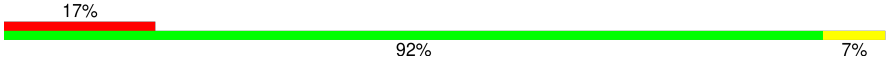
- Molecule 23: 30S ribosomal protein S3

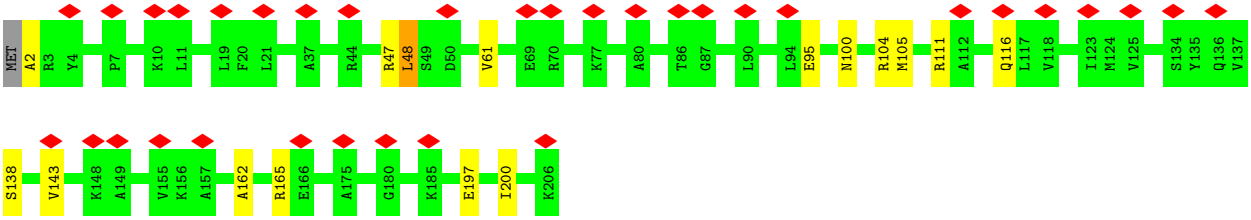
Chain I:



- Molecule 24: 30S ribosomal protein S4

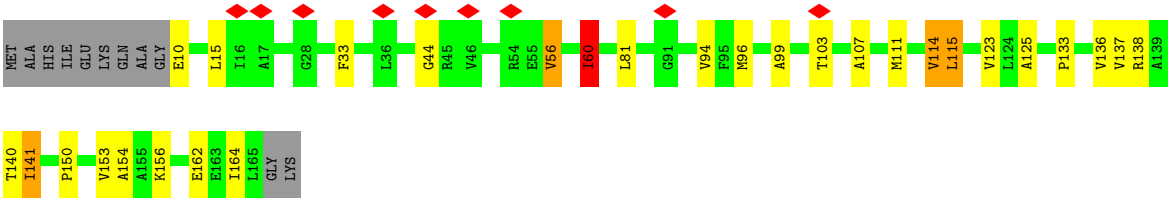
Chain J:





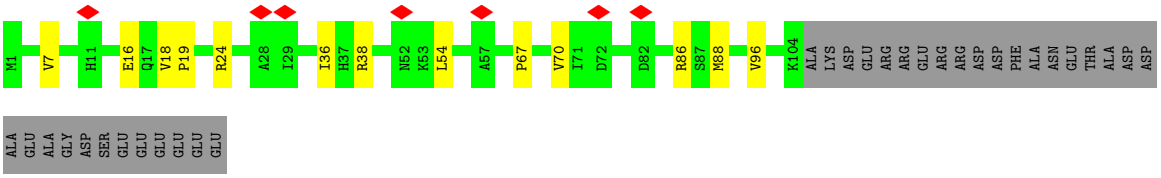
- Molecule 25: 30S ribosomal protein S5

Chain K:



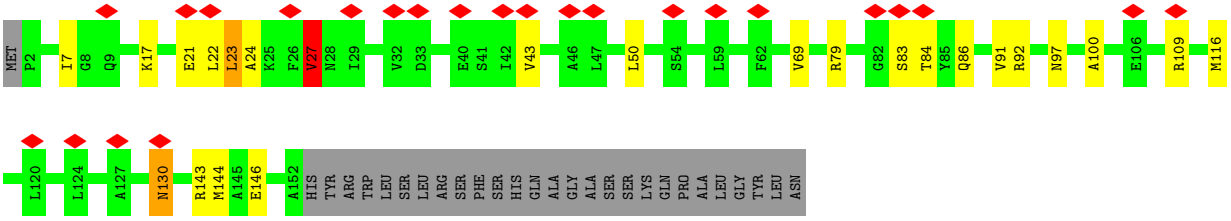
- Molecule 26: 30S ribosomal protein S6

Chain L:



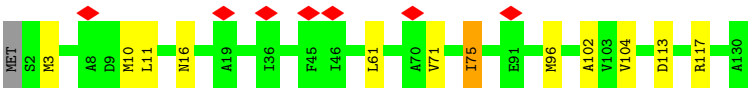
- Molecule 27: 30S ribosomal protein S7

Chain M:



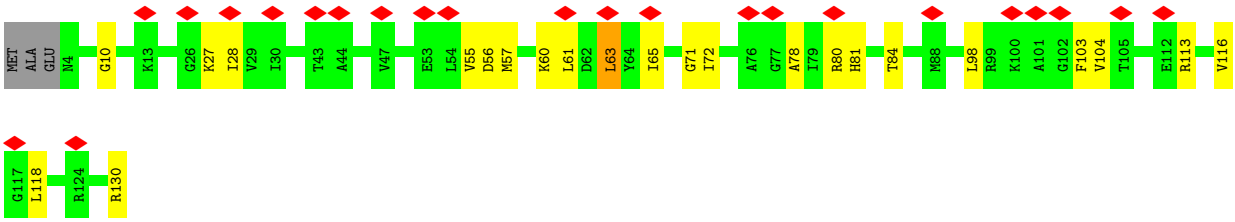
- Molecule 28: 30S ribosomal protein S8

Chain N:



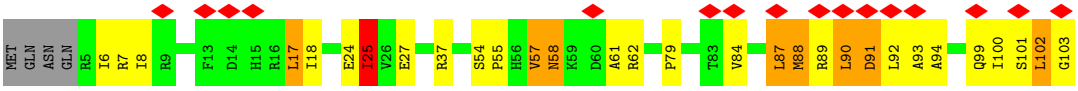
- Molecule 29: 30S ribosomal protein S9

Chain O:



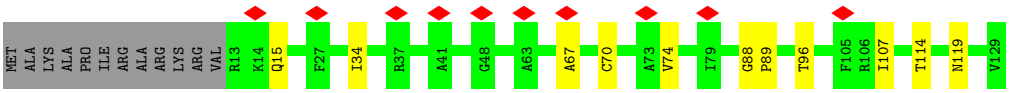
- Molecule 30: 30S ribosomal protein S10

Chain P:

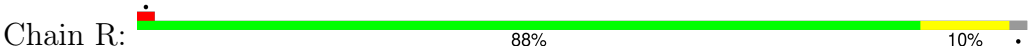


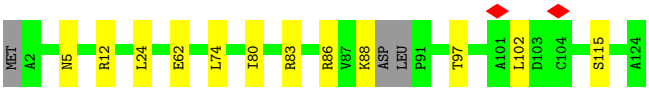
- Molecule 31: 30S ribosomal protein S11

Chain Q:

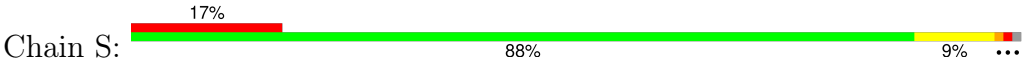


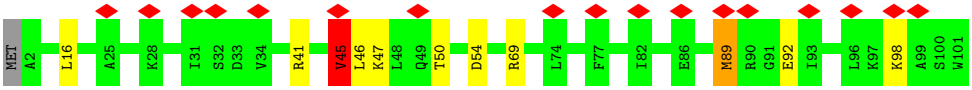
• Molecule 32: 30S ribosomal protein S12



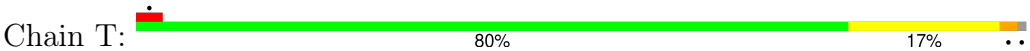


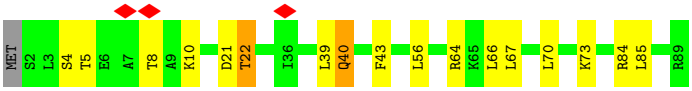
• Molecule 33: 30S ribosomal protein S14



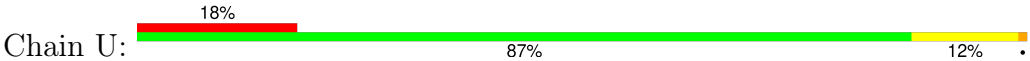


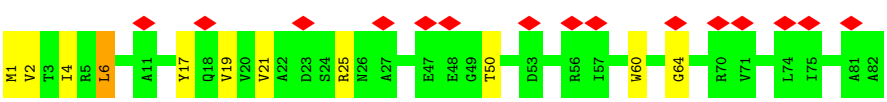
• Molecule 34: Small ribosomal subunit protein uS15



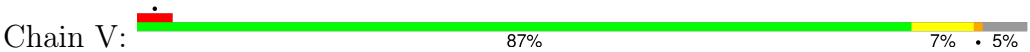


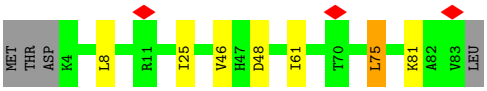
• Molecule 35: 30S ribosomal protein S16



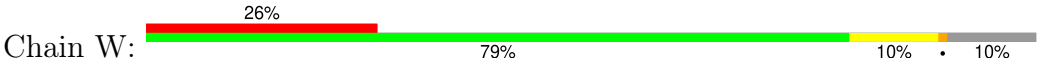


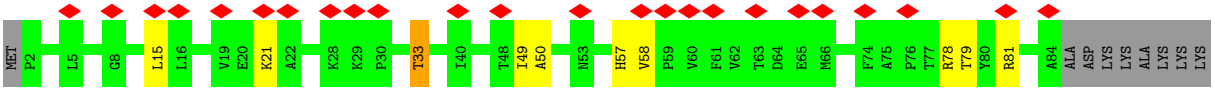
• Molecule 36: 30S ribosomal protein S17





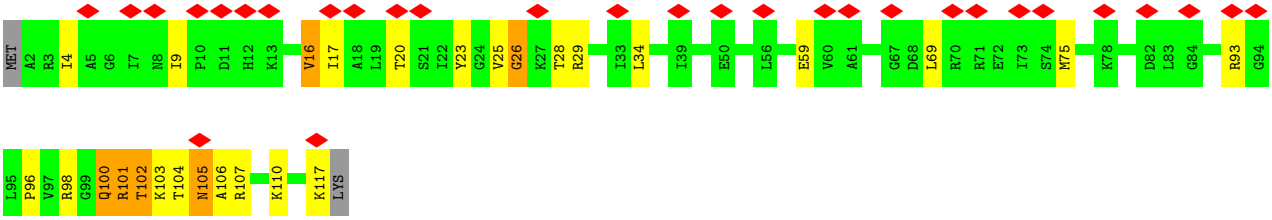
• Molecule 37: 30S ribosomal protein S19





• Molecule 38: 30S ribosomal protein S13

Chain X:

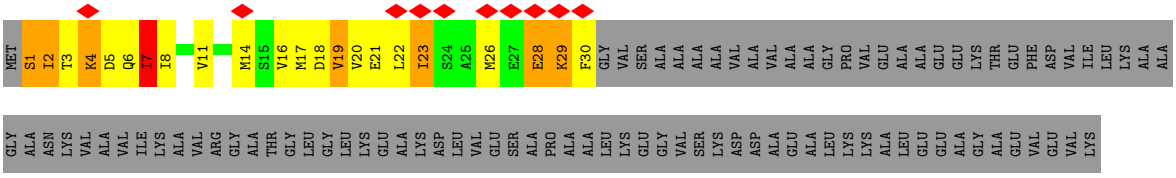


- Molecule 39: 50S ribosomal protein L11

Chain Y:

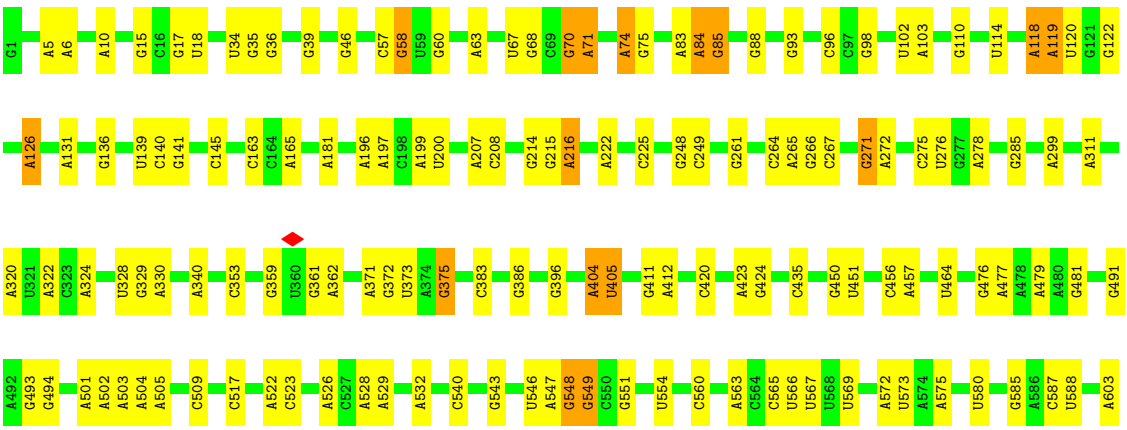
- Molecule 40: 50S ribosomal protein L7/L12

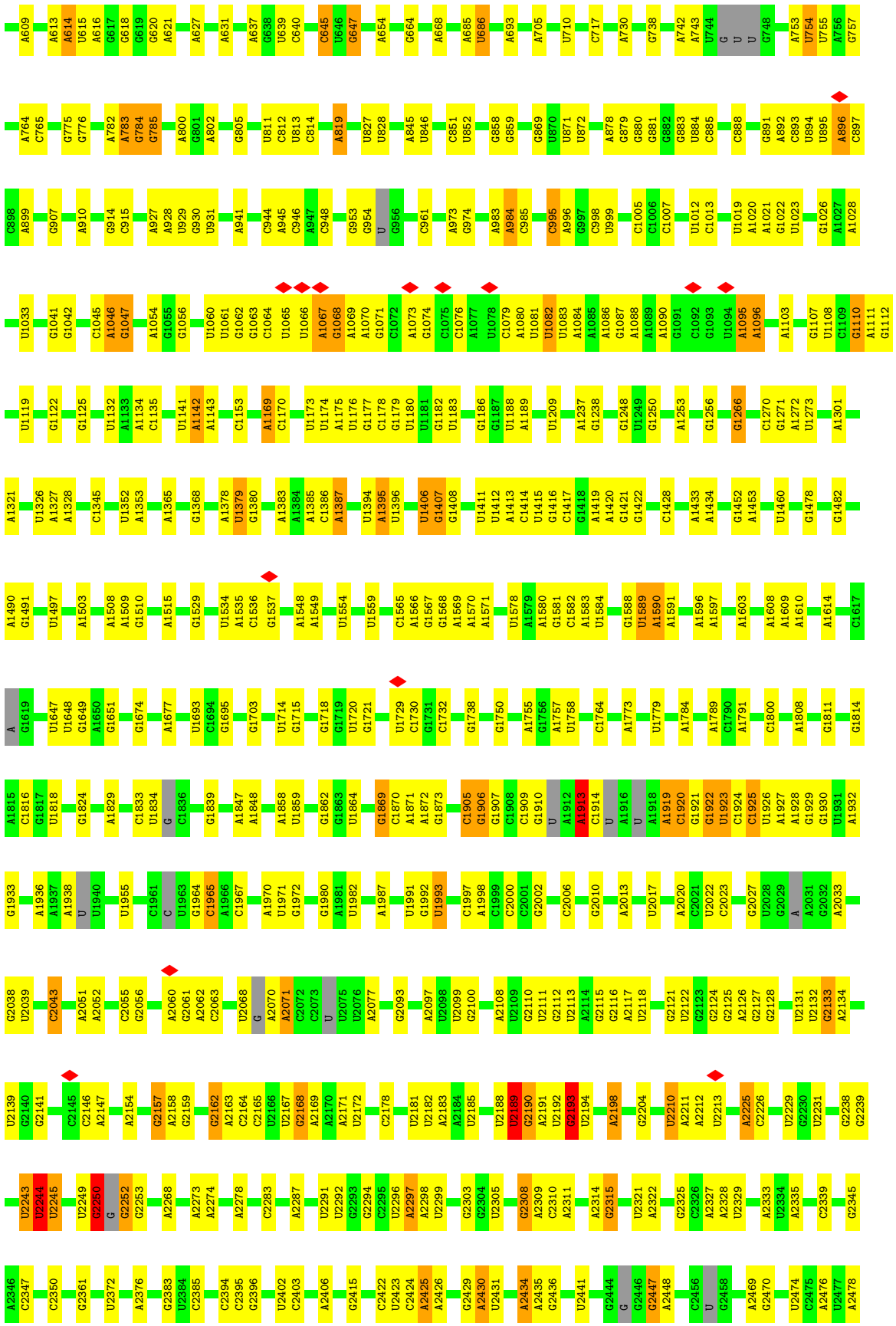
Chain Z:

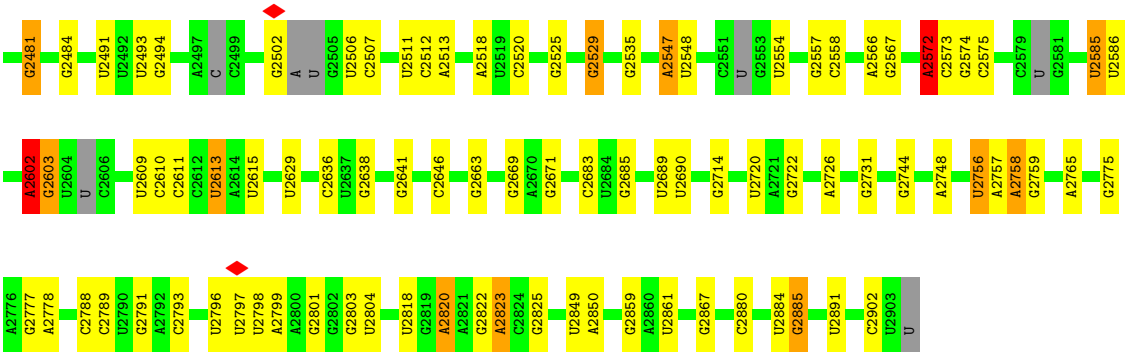


- Molecule 41: 23S rRNA

Chain a:

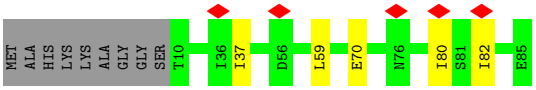



A609 A613 A614 U615 A616 G617 G618 G619 G620 A621 A627 A631 A637 G638 U639 C640 C645 U646 G647 A654 G664 A668 A685 U686 A693 A705 U710 C717 A730 G738 A742 A743 U744 G U U G748 A753 U754 U755 A756 G757
A764 C765 G775 G776 A782 A783 G784 G785 A800 G801 A802 G805 U811 C812 U813 C814 A819 U827 U828 A845 U846 C851 U852 G858 G859 G869 U870 U871 U872 A878 G879 G880 G881 G882 G883 U884 C885 C888 G891 A892 C893 U894 U895 A896 C897
C898 A899 G907 A910 G914 C915 A927 A928 U929 G930 U931 A941 C944 A945 C946 A947 C948 G953 G954 U G956 C961 A973 G974 A983 A984 C985 C995 A996 G997 C998 U999 C1005 C1006 C1007 U1012 C1013 U1019 A1020 A1021 G1022 U1023 G1026 A1027 A1028
U1033 G1041 G1042 C1045 A1046 G1047 A1054 G1055 G1056 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 A1103 G1107 U1108 C1109 G1110 A1111 G1112
U1119 G1122 G1125 U1132 A1133 A1134 C1135 U1141 A1142 A1143 C1153 A1169 C1170 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 G1186 G1187 U1188 A1189 U1209 A1237 G1238 G1248 U1249 G1250 A1253 G1256 G1266 C1270 G1271 A1272 U1273 A1301
A1321 U1326 A1327 A1328 C1345 U1352 A1353 A1365 G1368 A1378 U1379 G1380 A1383 A1384 A1385 C1386 A1387 U1394 A1395 U1396 U1406 G1407 G1408 U1411 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 G1421 G1422 C1428 A1433 A1434 G1452 A1453 U1460 G1478 G1482
A1490 G1491 U1497 A1503 A1508 A1509 G1510 A1515 G1529 U1534 A1535 C1536 G1537 A1548 A1549 U1554 U1559 C1565 A1566 G1567 G1568 A1569 A1570 A1571 U1578 A1579 A1580 G1581 C1582 A1583 U1584 G1588 U1589 A1590 A1591 A1596 A1597 A1603 A1608 A1609 A1610 A1614 C1617
A G1619 U1647 U1648 G1649 A1650 G1651 G1674 A1677 U1693 C1694 G1695 G1703 U1714 G1715 G1718 G1719 U1720 G1721 U1729 C1730 G1731 C1732 G1738 G1750 A1755 G1756 A1757 U1758 C1764 A1773 U1779 A1784 A1789 C1790 A1791 C1800 A1808 G1811 G1814
A1815 C1816 G1817 U1818 G1824 A1829 C1833 U1834 G C1836 G1839 A1847 A1848 A1858 U1859 G1862 G1863 U1864 G1869 C1870 A1871 A1872 G1873 C1905 G1906 G1907 C1908 C1909 G1910 U A1912 A1913 C1914 U A1916 U A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 U1926 A1927 A1928 G1929 G1930 U1931 A1932
G1933 A1936 A1937 A1938 U U1940 U1955 C1961 C U1963 G1964 G1965 A1966 C1967 A1970 U1971 G1972 G1980 A1981 U1982 A1987 U1991 G1992 U1993 C1997 A1998 C1999 C2000 C2001 G2002 C2006 G2010 A2013 U2017 A2020 C2021 U2022 C2023 G2027 U2028 G2029 A A2031 G2032 A2033
G2038 U2039 C2043 A2051 A2052 C2055 G2056 A2060 G2061 A2062 C2063 U2068 G A2070 A2071 C2072 C2073 U U2075 U2076 A2077 G2093 A2097 U2098 U2099 G2100 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 U2131 U2132 G2133 A2134
U2139 G2140 G2141 C2145 C2146 A2147 A2154 G2157 A2158 G2159 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 C2178 U2181 U2182 A2183 A2184 U2185 U2188 U2189 G2190 A2191 U2192 G2193 U2194 A2198 G2204 U2210 A2211 A2212 U2213 A2225 C2226 U2229 G2230 U2231 G2238 G2239
U2243 U2244 U2245 U2249 G2250 G G2252 G2253 A2268 A2273 A2274 A2278 C2283 A2287 U2291 U2292 G2293 G2294 C2295 U2296 A2297 A2298 U2299 G2303 G2304 U2305 G2308 A2309 C2310 A2311 A2314 G2315 U2321 A2322 G2325 C2326 A2327 A2328 U2329 A2333 U2334 A2335 C2339 G2345
A2346 C2347 C2350 G2361 U2372 A2376 G2383 U2384 C2385 C2394 C2395 G2396 U2402 C2403 A2406 G2415 C2422 U2423 C2424 A2425 A2426 G2429 A2430 U2431 A2434 A2435 G2436 U2441 G2444 G G2446 G2447 A2448 C2456 U G2458 A2469 G2470 U2474 C2475 A2476 U2477 A2478



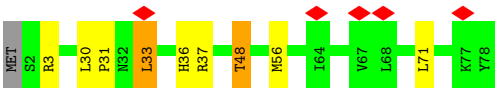
- Molecule 42: 50S ribosomal protein L27

Chain b:



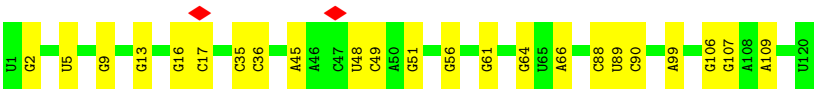
- Molecule 43: 50S ribosomal protein L28

Chain c:



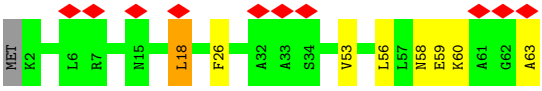
- Molecule 44: 5S rRNA

Chain d:



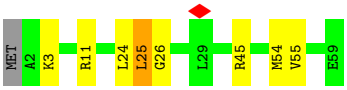
- Molecule 45: 50S ribosomal protein L29

Chain e:



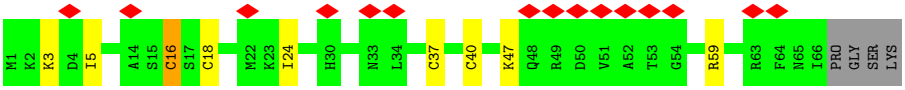
- Molecule 46: 50S ribosomal protein L30

Chain f:



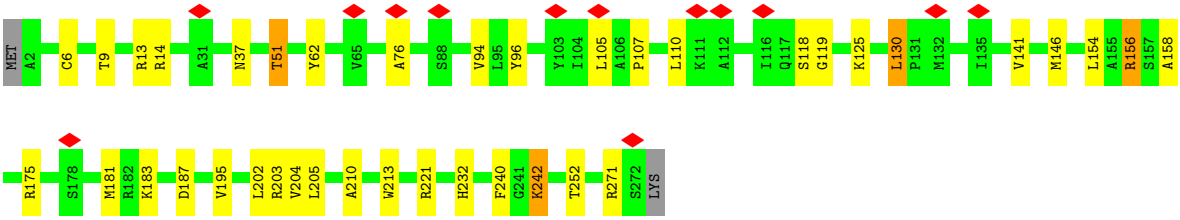
- Molecule 47: 50S ribosomal protein L31

Chain g: 21% 81% 11% • 6%



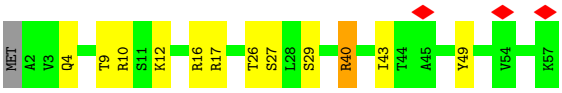
• Molecule 48: 50S ribosomal protein L2

Chain h: 5% 85% 13% ••



• Molecule 49: 50S ribosomal protein L32

Chain i: 5% 77% 19% • •

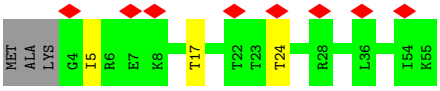


• Molecule 50: 50S ribosomal protein L3

Chain j: 10% 88% 12%

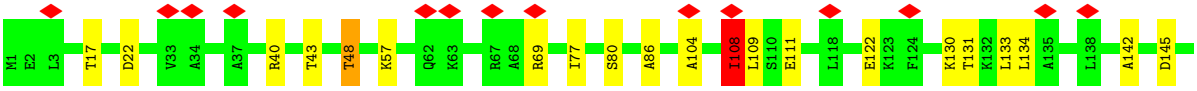
• Molecule 51: 50S ribosomal protein L33

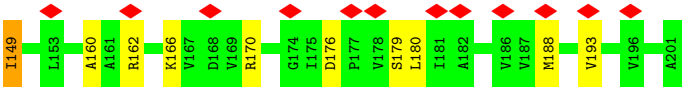
Chain k: 15% 89% 5% 5%



• Molecule 52: 50S ribosomal protein L4

Chain l: 13% 85% 14% •



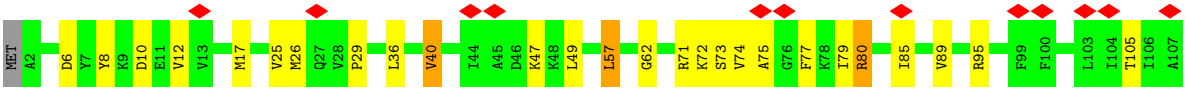


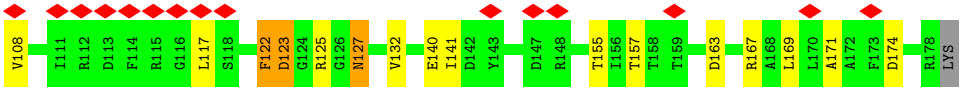
• Molecule 53: 50S ribosomal protein L34

Chain m:

• Molecule 54: 50S ribosomal protein L5

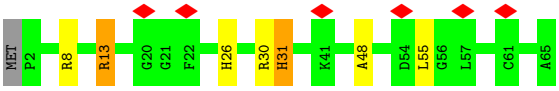
Chain n:





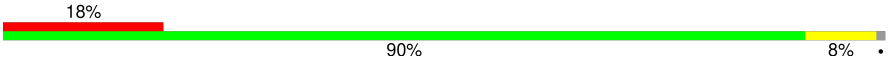
• Molecule 55: 50S ribosomal protein L35

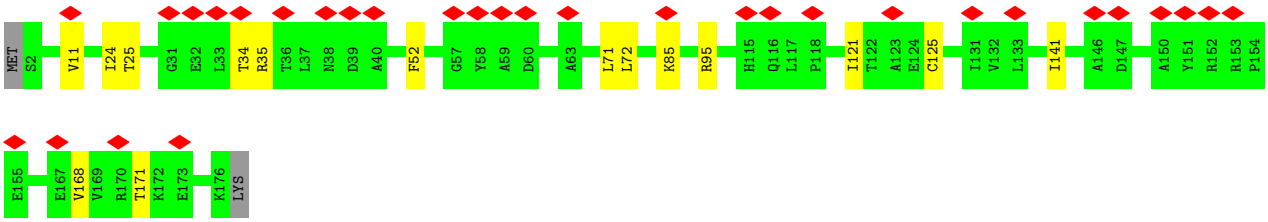
Chain o:



• Molecule 56: 50S ribosomal protein L6

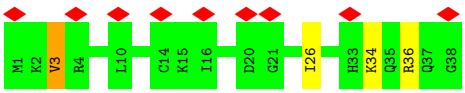
Chain p:





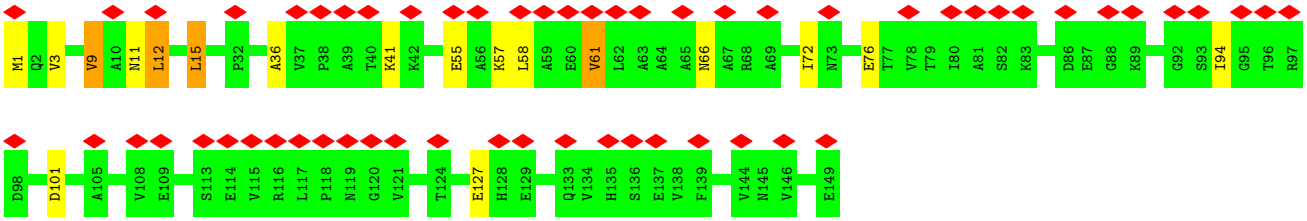
• Molecule 57: 50S ribosomal protein L36

Chain q:



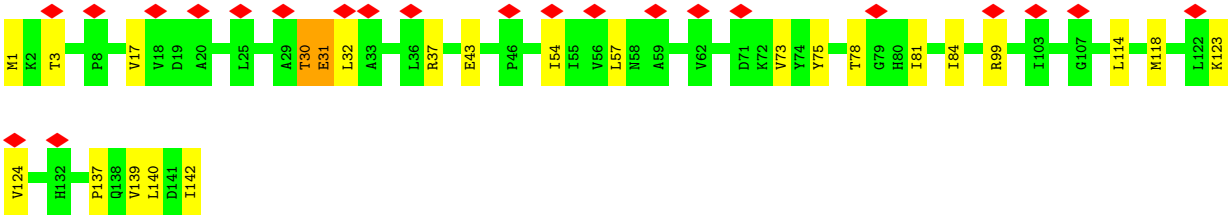
• Molecule 58: 50S ribosomal protein L9

Chain r:



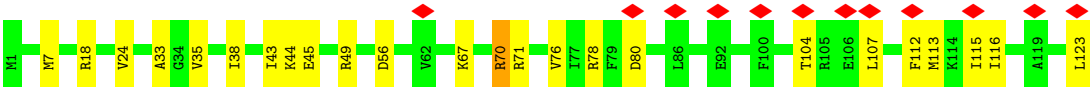
- Molecule 59: 50S ribosomal protein L13

Chain s:



- Molecule 60: 50S ribosomal protein L14

Chain t:

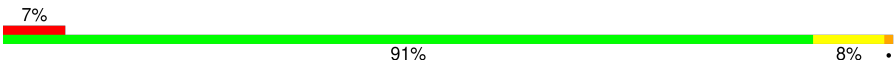


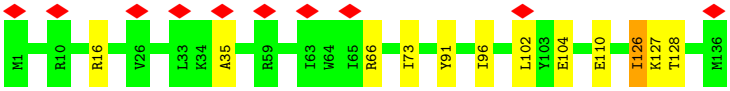
- Molecule 61: 50S ribosomal protein L15

Chain u:

- Molecule 62: 50S ribosomal protein L16

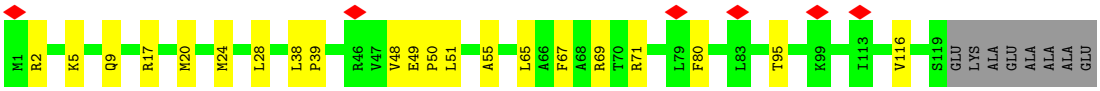
Chain v:





- Molecule 63: 50S ribosomal protein L17

Chain w:

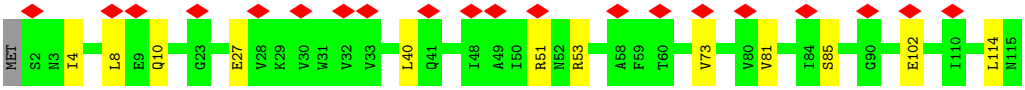


- Molecule 64: 50S ribosomal protein L18

Chain x:

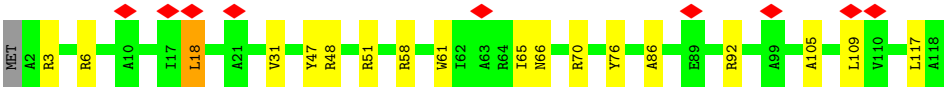
- Molecule 65: 50S ribosomal protein L19

Chain y:



- Molecule 66: 50S ribosomal protein L20

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.087	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.00000001	Depositor
Map size (Å)	533.2, 533.2, 533.2	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.50	0/829	0.74	0/1107
2	1	0.67	0/864	1.08	0/1156
3	2	0.54	0/752	0.89	0/1005
4	3	0.47	0/796	0.77	0/1062
5	4	0.52	0/766	0.88	0/1025
6	5	0.64	1/528 (0.2%)	0.55	0/810
7	6	0.56	1/603 (0.2%)	0.56	0/926
8	7	0.62	3/717 (0.4%)	0.90	4/1110 (0.4%)
9	9	1.15	3/1131 (0.3%)	1.30	3/1524 (0.2%)
10	A	0.36	0/1810	0.72	2/2821 (0.1%)
10	B	0.44	0/1810	0.87	9/2821 (0.3%)
11	AA	0.39	0/10736	0.63	0/14487
12	AB	0.55	0/1304	0.78	1/1759 (0.1%)
13	AC	0.38	0/1710	0.61	0/2317
13	AD	0.30	0/2091	0.59	0/2847
14	AE	0.56	10/10545 (0.1%)	0.79	27/14236 (0.2%)
15	AF	0.30	0/652	0.61	0/879
16	AG	0.97	5/3897 (0.1%)	1.40	49/5273 (0.9%)
17	C	0.66	0/553	1.14	1/743 (0.1%)
18	D	0.40	9/36610 (0.0%)	0.75	38/57091 (0.1%)
19	E	0.76	0/675	1.32	0/895
20	F	0.72	0/597	1.20	0/792
21	G	0.65	0/1791	1.08	1/2413 (0.0%)
22	H	0.76	4/1746 (0.2%)	1.58	34/2382 (1.4%)
23	I	0.59	0/1663	0.99	0/2241
24	J	0.63	0/1665	1.08	0/2227
25	K	0.64	1/1165 (0.1%)	1.06	2/1568 (0.1%)
26	L	0.58	0/867	0.94	0/1171
27	M	0.68	0/1195	1.19	3/1602 (0.2%)
28	N	0.56	0/989	0.91	0/1326
29	O	0.59	0/1034	1.02	1/1375 (0.1%)
30	P	0.64	0/800	1.13	4/1082 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	Q	0.55	0/893	0.91	0/1205
32	R	0.50	0/952	0.81	0/1274
33	S	0.64	0/817	1.11	1/1088 (0.1%)
34	T	0.69	0/722	1.21	0/964
35	U	0.58	0/659	0.99	0/884
36	V	0.46	0/657	0.73	0/881
37	W	0.51	0/680	0.83	0/915
38	X	0.67	0/909	1.21	3/1215 (0.2%)
39	Y	1.04	0/1046	1.09	1/1410 (0.1%)
40	Z	1.02	0/227	1.12	0/304
41	a	0.41	3/69247 (0.0%)	0.75	55/107985 (0.1%)
42	b	0.51	0/589	0.76	0/779
43	c	0.63	0/635	0.97	0/848
44	d	0.37	0/2872	0.69	0/4478
45	e	0.69	0/502	1.19	0/667
46	f	0.62	0/452	1.02	0/605
47	g	0.56	0/531	0.99	1/709 (0.1%)
48	h	0.54	0/2121	0.85	0/2852
49	i	0.53	0/450	0.94	0/599
50	j	0.60	0/1586	0.87	0/2134
51	k	0.47	0/433	0.80	0/576
52	l	0.61	0/1571	1.03	1/2113 (0.0%)
53	m	0.69	0/380	1.22	0/498
54	n	0.63	0/1434	1.18	10/1926 (0.5%)
55	o	0.64	0/513	1.11	1/676 (0.1%)
56	p	0.58	0/1333	0.89	0/1805
57	q	0.51	0/303	0.88	0/397
58	r	0.63	0/1122	0.98	1/1515 (0.1%)
59	s	0.68	0/1152	1.02	0/1551
60	t	0.57	0/955	0.88	0/1279
61	u	0.55	0/1062	0.95	1/1413 (0.1%)
62	v	0.60	0/1093	0.97	0/1460
63	w	0.68	0/964	1.13	0/1289
64	x	0.61	0/902	1.09	0/1209
65	y	0.53	0/929	0.79	0/1242
66	z	0.80	0/960	1.25	0/1278
All	All	0.50	40/194544 (0.0%)	0.84	254/286096 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	A	0	2
10	B	0	2
12	AB	0	1
13	AC	0	1
13	AD	0	3
14	AE	0	5
16	AG	0	6
22	H	0	3
38	X	0	1
All	All	0	24

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	130	PRO	N-CA	18.14	1.70	1.47
16	AG	429	LYS	C-N	13.82	1.51	1.33
14	AE	93	THR	CA-C	12.11	1.69	1.52
22	H	169	SER	N-CA	11.81	1.61	1.46
14	AE	291	ILE	CA-C	11.52	1.67	1.52
18	D	1516	G	O3'-P	-10.71	1.45	1.61
14	AE	70	CYS	CA-CB	-8.86	1.41	1.53
18	D	1339	A	O3'-P	8.48	1.73	1.61
8	7	55	G	C1'-N9	-7.50	1.36	1.48
8	7	2	U	C1'-N1	7.12	1.59	1.48
16	AG	246	ASP	C-N	7.00	1.50	1.33
22	H	88	LYS	N-CA	6.98	1.55	1.46
6	5	109	DT	O3'-P	6.81	1.71	1.61
18	D	145	G	O3'-P	6.74	1.71	1.61
18	D	196	A	O3'-P	6.58	1.71	1.61
22	H	168	VAL	C-N	6.39	1.42	1.33
18	D	1275	A	O3'-P	6.36	1.70	1.61
16	AG	355	ALA	N-CA	6.26	1.54	1.46
41	a	2434	A	O3'-P	6.02	1.70	1.61
16	AG	355	ALA	CA-C	5.96	1.60	1.52
18	D	1515	G	O3'-P	-5.92	1.52	1.61
18	D	1395	C	O3'-P	5.72	1.69	1.61
22	H	88	LYS	CA-C	5.67	1.60	1.52
14	AE	90	VAL	CA-C	5.63	1.60	1.52
18	D	1490	U	O3'-P	5.56	1.69	1.61
7	6	10	DG	C1'-N9	-5.40	1.35	1.46
8	7	18	U	C1'-N1	5.29	1.56	1.48
25	K	56	VAL	CA-CB	5.29	1.57	1.54
14	AE	424	ASN	CG-ND2	-5.28	1.22	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	1492	A	O3'-P	5.27	1.69	1.61
41	a	1905	C	O3'-P	5.25	1.69	1.61
14	AE	1350	ASN	CG-ND2	-5.24	1.22	1.33
41	a	2167	U	O3'-P	5.19	1.69	1.61
14	AE	777	HIS	CD2-NE2	-5.18	1.32	1.37
14	AE	777	HIS	ND1-CE1	5.18	1.37	1.32
14	AE	291	ILE	N-CA	5.14	1.52	1.46
9	9	129	LEU	C-N	5.12	1.45	1.33
9	9	116	GLU	N-CA	5.11	1.49	1.46
16	AG	99	SER	N-CA	5.11	1.49	1.46
14	AE	1268	ASN	CG-ND2	-5.08	1.22	1.33

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	AE	291	ILE	CA-C-N	20.29	158.49	121.97
14	AE	291	ILE	C-N-CA	20.29	158.49	121.97
16	AG	104	ARG	CA-C-N	17.90	154.19	121.97
16	AG	104	ARG	C-N-CA	17.90	154.19	121.97
18	D	1516	G	O3'-P-O5'	17.53	130.29	104.00
22	H	88	LYS	CA-C-N	17.03	143.71	120.38
22	H	88	LYS	C-N-CA	17.03	143.71	120.38
10	B	29	G	C3'-C2'-O2'	15.98	134.67	110.70
9	9	129	LEU	CA-C-N	15.92	139.75	119.84
9	9	129	LEU	C-N-CA	15.92	139.75	119.84
18	D	1516	G	P-O3'-C3'	-15.58	96.83	120.20
16	AG	246	ASP	CA-C-N	14.45	137.90	119.84
16	AG	246	ASP	C-N-CA	14.45	137.90	119.84
16	AG	354	ALA	O-C-N	-13.68	107.31	122.09
22	H	332	VAL	N-CA-C	13.67	124.56	110.62
22	H	169	SER	N-CA-C	12.78	138.01	110.80
22	H	330	VAL	N-CA-C	12.13	126.86	109.51
22	H	305	HIS	N-CA-C	11.91	131.02	111.37
16	AG	429	LYS	CA-C-N	11.51	132.24	119.92
16	AG	429	LYS	C-N-CA	11.51	132.24	119.92
14	AE	291	ILE	CB-CA-C	10.67	128.78	111.29
16	AG	24	PHE	CA-CB-CG	-10.58	103.22	113.80
16	AG	105	ILE	CA-C-N	10.23	136.97	120.60
16	AG	105	ILE	C-N-CA	10.23	136.97	120.60
14	AE	90	VAL	N-CA-C	9.89	122.19	107.75
41	a	2244	U	C1'-C2'-O2'	-9.79	93.71	108.40
54	n	73	SER	N-CA-CB	-9.61	94.52	110.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	D	1206	G	C4'-C3'-O3'	9.52	127.28	113.00
30	P	54	SER	CA-C-N	9.40	129.09	118.85
30	P	54	SER	C-N-CA	9.40	129.09	118.85
41	a	2250	G	C4'-C3'-O3'	-9.19	95.61	109.40
16	AG	103	ASP	CA-CB-CG	9.04	121.64	112.60
18	D	1401	G	C4'-C3'-O3'	8.75	126.12	113.00
18	D	428	G	C4'-C3'-O3'	8.73	122.50	109.40
9	9	130	PRO	CA-N-CD	-8.66	99.88	112.00
8	7	1	A	O3'-P-O5'	-8.59	91.12	104.00
22	H	339	ARG	CA-C-N	8.57	137.90	121.54
22	H	339	ARG	C-N-CA	8.57	137.90	121.54
33	S	45	VAL	N-CA-CB	8.43	120.41	110.55
41	a	2296	U	C4'-C3'-O3'	8.42	122.03	109.40
41	a	404	A	C2'-C3'-O3'	8.41	122.12	109.50
18	D	1515	G	O3'-P-O5'	-8.40	91.40	104.00
8	7	4	U	C2'-C3'-O3'	8.34	122.01	109.50
30	P	57	VAL	N-CA-C	8.27	120.01	107.77
16	AG	35	THR	CA-CB-OG1	-8.24	97.24	109.60
16	AG	292	ASP	O-C-N	-8.23	107.47	122.44
16	AG	109	THR	CB-CA-C	8.19	124.77	110.85
41	a	2252	G	N9-C1'-C2'	-8.17	99.75	112.00
18	D	197	A	C2'-C3'-O3'	8.13	121.70	109.50
16	AG	108	GLN	N-CA-CB	8.07	123.56	110.40
18	D	1401	G	N9-C1'-C2'	-7.94	100.09	112.00
41	a	2425	A	C2'-C3'-O3'	7.83	121.24	109.50
22	H	155	LYS	CA-C-N	-7.80	110.90	121.66
22	H	155	LYS	C-N-CA	-7.80	110.90	121.66
18	D	1493	A	C2'-C3'-O3'	7.73	125.29	113.70
41	a	2071	A	C4'-C3'-O3'	-7.71	101.43	113.00
54	n	75	ALA	CA-C-N	7.66	129.71	120.14
54	n	75	ALA	C-N-CA	7.66	129.71	120.14
22	H	52	GLN	N-CA-C	-7.63	104.11	113.50
14	AE	903	LEU	CA-C-N	7.63	136.11	121.54
14	AE	903	LEU	C-N-CA	7.63	136.11	121.54
22	H	84	LEU	N-CA-C	7.63	120.99	110.24
22	H	168	VAL	CA-C-N	7.62	136.09	121.54
22	H	168	VAL	C-N-CA	7.62	136.09	121.54
18	D	1339	A	P-O3'-C3'	7.58	131.58	120.20
38	X	102	THR	CB-CA-C	7.58	123.42	110.84
18	D	1499	A	N9-C1'-C2'	-7.55	100.67	112.00
25	K	60	ILE	N-CA-CB	7.54	119.38	110.55
18	D	528	C	N1-C1'-C2'	-7.52	100.72	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	AG	33	THR	CA-C-N	7.50	135.86	121.54
16	AG	33	THR	C-N-CA	7.50	135.86	121.54
16	AG	102	PHE	CA-C-N	7.49	135.84	121.54
16	AG	102	PHE	C-N-CA	7.49	135.84	121.54
25	K	56	VAL	O-C-N	7.45	125.19	120.42
54	n	73	SER	CB-CA-C	7.44	122.91	110.79
10	B	28	C	P-O3'-C3'	7.41	131.32	120.20
22	H	336	ASP	CB-CA-C	-7.40	98.73	110.79
21	G	47	VAL	O-C-N	7.34	125.12	120.42
16	AG	108	GLN	N-CA-C	-7.32	103.81	112.89
41	a	783	A	C4'-C3'-O3'	7.31	123.96	113.00
41	a	2602	A	C4'-C3'-O3'	7.26	120.29	109.40
18	D	1497	G	C1'-C2'-O2'	-7.26	97.52	108.40
16	AG	426	GLY	O-C-N	-7.22	113.31	122.70
54	n	108	VAL	O-C-N	7.22	125.19	120.07
10	B	29	G	N9-C1'-C2'	-7.17	101.24	112.00
41	a	896	A	C4'-C3'-O3'	7.13	120.09	109.40
41	a	2162	G	C4'-C3'-O3'	7.09	120.04	109.40
18	D	196	A	P-O3'-C3'	7.08	130.82	120.20
41	a	2225	A	C4'-C3'-O3'	7.03	119.94	109.40
41	a	1379	U	C2'-C3'-O3'	7.02	124.23	113.70
41	a	2244	U	C4'-C3'-O3'	6.96	123.44	113.00
27	M	27	VAL	N-CA-CB	6.92	118.65	110.55
22	H	140	PRO	N-CA-CB	6.91	110.51	103.25
12	AB	122	PRO	N-CA-CB	6.90	110.50	103.25
41	a	2252	G	C4'-C3'-O3'	6.84	123.26	113.00
22	H	340	ARG	CA-C-N	-6.82	112.53	123.23
22	H	340	ARG	C-N-CA	-6.82	112.53	123.23
16	AG	102	PHE	N-CA-C	6.81	125.30	110.80
54	n	71	ARG	CA-C-N	6.79	134.04	122.37
54	n	71	ARG	C-N-CA	6.79	134.04	122.37
16	AG	104	ARG	O-C-N	6.71	131.52	122.59
22	H	170	ARG	N-CA-C	6.66	119.63	110.24
41	a	2243	U	C4'-C3'-O3'	6.64	122.97	113.00
18	D	517	G	C5'-C4'-C3'	6.64	125.16	115.20
18	D	526	C	C4'-C3'-O3'	6.62	122.94	113.00
22	H	87	GLU	N-CA-C	-6.60	104.09	111.28
58	r	61	VAL	N-CA-CB	6.57	118.24	110.55
22	H	303	LEU	N-CA-C	6.55	121.11	112.13
54	n	127	ASN	CB-CA-C	6.55	121.70	110.77
29	O	72	ILE	N-CA-C	-6.54	105.33	111.48
41	a	2189	U	C1'-C2'-O2'	-6.54	102.00	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	a	2167	U	P-O3'-C3'	6.53	129.99	120.20
22	H	112	ILE	N-CA-C	6.52	117.09	106.72
16	AG	106	THR	OG1-CB-CG2	-6.51	96.28	109.30
22	H	132	PRO	N-CA-CB	6.51	110.21	103.38
41	a	894	U	C2'-C3'-O3'	6.51	119.26	109.50
22	H	155	LYS	N-CA-C	-6.49	98.33	108.90
14	AE	450	HIS	CB-CG-CD2	-6.48	122.78	131.20
18	D	526	C	N1-C1'-C2'	-6.48	102.28	112.00
55	o	13	ARG	N-CA-C	6.47	121.00	113.18
18	D	1340	A	C1'-C2'-O2'	6.46	118.09	108.40
54	n	127	ASN	CA-CB-CG	-6.43	106.17	112.60
16	AG	355	ALA	CB-CA-C	6.38	123.11	110.42
18	D	69	G	C4'-C3'-O3'	-6.36	103.46	113.00
41	a	754	U	N1-C1'-C2'	6.36	121.54	112.00
16	AG	103	ASP	CA-C-N	6.35	133.67	121.54
16	AG	103	ASP	C-N-CA	6.35	133.67	121.54
14	AE	61	ILE	CA-C-N	-6.33	114.04	121.64
14	AE	61	ILE	C-N-CA	-6.33	114.04	121.64
41	a	2434	A	P-O3'-C3'	6.32	129.68	120.20
18	D	1208	C	N1-C1'-C2'	-6.32	102.53	112.00
8	7	47	U	C4'-C3'-O3'	6.30	118.86	109.40
14	AE	777	HIS	CB-CG-CD2	-6.30	123.02	131.20
16	AG	109	THR	N-CA-C	-6.29	104.50	111.36
22	H	153	GLU	N-CA-C	-6.25	97.48	110.80
41	a	2425	A	C4'-C3'-O3'	6.24	118.76	109.40
17	C	33	ILE	CA-C-O	-6.21	114.97	121.93
10	B	28	C	O3'-P-O5'	-6.20	94.70	104.00
16	AG	403	VAL	N-CA-C	-6.18	104.26	111.00
22	H	113	ASN	N-CA-C	6.15	118.07	111.36
14	AE	70	CYS	CB-CA-C	6.14	120.36	110.29
18	D	1206	G	N9-C1'-C2'	-6.12	102.83	112.00
16	AG	108	GLN	CB-CA-C	-6.11	97.23	109.99
16	AG	404	GLU	N-CA-C	-6.09	104.95	112.38
18	D	1408	A	C4'-C3'-O3'	6.06	122.09	113.00
41	a	271	G	C4'-C3'-O3'	6.05	118.47	109.40
16	AG	71	PRO	N-CA-C	6.04	122.57	113.81
18	D	1516	G	OP1-P-O3'	-6.04	89.88	108.00
16	AG	33	THR	CA-CB-CG2	6.00	120.69	110.50
41	a	2210	U	C4'-C3'-O3'	5.99	118.39	109.40
14	AE	90	VAL	CA-C-O	-5.98	114.17	120.39
27	M	92	ARG	CA-C-N	5.98	125.46	119.24
27	M	92	ARG	C-N-CA	5.98	125.46	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	D	550	G	C3'-C2'-O2'	5.97	119.65	110.70
41	a	1913	A	C2'-C3'-O3'	5.96	118.44	109.50
41	a	2820	A	C4'-C3'-O3'	-5.95	104.08	113.00
41	a	2308	G	C2'-C3'-O3'	-5.89	104.86	113.70
52	l	108	ILE	N-CA-CB	5.89	118.55	110.54
22	H	109	THR	N-CA-C	-5.87	99.08	109.06
38	X	26	GLY	N-CA-C	-5.86	104.28	112.13
22	H	150	LYS	N-CA-C	5.86	118.26	110.53
22	H	75	VAL	N-CA-C	5.84	116.53	108.12
14	AE	291	ILE	N-CA-CB	-5.84	101.60	111.23
41	a	2756	U	C4'-C3'-O3'	5.83	118.15	109.40
54	n	72	LYS	N-CA-C	-5.81	99.18	109.06
18	D	1275	A	P-O3'-C3'	5.81	128.91	120.20
16	AG	66	ASP	N-CA-C	-5.79	103.95	111.71
10	A	48	C	N1-C1'-C2'	5.78	120.67	112.00
41	a	1905	C	P-O3'-C3'	5.77	128.85	120.20
14	AE	91	GLU	N-CA-C	5.76	123.08	110.80
41	a	70	G	C4'-C3'-O3'	5.76	118.03	109.40
10	B	29	G	O5'-C5'-C4'	-5.75	102.87	111.50
18	D	1490	U	P-O3'-C3'	5.75	128.83	120.20
18	D	1406	U	N1-C1'-C2'	-5.74	103.39	112.00
18	D	976	G	C4'-C3'-O3'	-5.74	104.40	113.00
18	D	1492	A	P-O3'-C3'	5.73	128.79	120.20
41	a	2168	G	C4'-C3'-O3'	-5.72	104.41	113.00
10	B	48	C	N1-C1'-C2'	5.70	120.55	112.00
16	AG	220	VAL	N-CA-C	-5.68	108.32	113.71
18	D	1340	A	C5'-C4'-C3'	5.66	124.48	116.00
41	a	1757	A	C4'-C3'-O3'	-5.65	104.52	113.00
14	AE	450	HIS	CB-CG-ND1	5.62	131.13	122.70
41	a	2017	U	C2'-C3'-O3'	-5.62	105.28	113.70
22	H	114	GLY	N-CA-C	5.61	121.23	111.14
41	a	2731	G	C4'-C3'-O3'	-5.60	104.60	113.00
16	AG	101	THR	CA-CB-OG1	5.59	117.99	109.60
18	D	780	A	C4'-C3'-O3'	-5.57	104.65	113.00
16	AG	74	GLU	CB-CA-C	-5.53	101.62	110.14
41	a	1568	G	C4'-C3'-O3'	-5.53	104.70	113.00
14	AE	93	THR	CB-CA-C	5.48	121.33	110.42
41	a	2447	G	C2'-C3'-O3'	-5.48	101.28	109.50
14	AE	93	THR	CA-C-N	5.47	133.15	121.45
14	AE	93	THR	C-N-CA	5.47	133.15	121.45
16	AG	354	ALA	CA-C-N	-5.43	111.16	121.54
16	AG	354	ALA	C-N-CA	-5.43	111.16	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	D	1499	A	C4'-C3'-O3'	5.42	121.14	113.00
41	a	2572	A	C4'-C3'-O3'	-5.42	101.27	109.40
16	AG	355	ALA	N-CA-CB	5.41	119.63	110.49
14	AE	777	HIS	CB-CG-ND1	5.39	130.78	122.70
41	a	2481	G	C4'-C3'-O3'	-5.38	104.92	113.00
14	AE	69	GLU	CA-C-N	-5.36	113.94	121.72
14	AE	69	GLU	C-N-CA	-5.36	113.94	121.72
18	D	864	A	N9-C1'-C2'	5.36	120.04	112.00
41	a	375	G	C2'-C3'-O3'	5.36	121.74	113.70
18	D	1145	A	C4'-C3'-O3'	-5.36	104.97	113.00
14	AE	90	VAL	O-C-N	-5.35	117.53	123.20
18	D	517	G	C4'-C3'-O3'	-5.34	101.38	109.40
41	a	2068	U	C4'-C3'-O3'	-5.34	104.98	113.00
16	AG	105	ILE	N-CA-CB	-5.34	102.42	111.23
41	a	2020	A	C4'-C3'-O3'	-5.33	105.00	113.00
18	D	145	G	P-O3'-C3'	5.33	128.20	120.20
41	a	944	C	C4'-C3'-O3'	-5.33	105.00	113.00
14	AE	70	CYS	N-CA-C	-5.33	101.09	109.25
8	7	10	U	C2'-C3'-O3'	5.33	117.49	109.50
10	B	35	A	P-O3'-C3'	5.32	128.18	120.20
41	a	1270	C	C2'-C3'-O3'	-5.32	105.72	113.70
14	AE	73	GLY	N-CA-C	5.30	125.75	113.18
18	D	1395	C	P-O3'-C3'	5.28	128.12	120.20
47	g	5	ILE	N-CA-C	5.28	117.65	111.05
41	a	2231	U	C1'-C2'-O2'	5.27	116.31	108.40
41	a	2529	G	C4'-C3'-O3'	-5.27	105.09	113.00
39	Y	5	GLN	O-C-N	5.27	124.73	120.83
10	B	60	U	C2'-C3'-O3'	5.25	117.37	109.50
14	AE	88	CYS	N-CA-C	5.24	120.32	113.88
41	a	479	A	C4'-C3'-O3'	5.22	117.22	109.40
10	A	60	U	C2'-C3'-O3'	5.21	117.32	109.50
14	AE	61	ILE	CA-C-O	-5.19	115.55	120.95
38	X	102	THR	CA-C-O	-5.19	114.95	121.02
41	a	1834	U	C4'-C3'-O3'	-5.19	105.22	113.00
61	u	101	ILE	N-CA-C	5.18	116.47	112.12
22	H	128	ARG	CA-C-N	-5.17	114.12	122.81
22	H	128	ARG	C-N-CA	-5.17	114.12	122.81
16	AG	107	THR	CA-C-N	-5.17	112.09	121.14
16	AG	107	THR	C-N-CA	-5.17	112.09	121.14
41	a	2245	U	N1-C1'-C2'	-5.15	104.27	112.00
41	a	126	A	C4'-C3'-O3'	-5.14	105.29	113.00
41	a	423	A	C2'-C3'-O3'	-5.13	106.00	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	D	1335	U	C4'-C3'-O3'	-5.13	105.30	113.00
30	P	25	ILE	N-CA-CB	5.12	117.51	110.54
16	AG	114	ILE	N-CA-C	-5.12	105.51	110.42
41	a	528	A	C4'-C3'-O3'	-5.11	105.33	113.00
14	AE	1184	ASP	N-CA-C	5.09	121.06	109.81
22	H	154	PHE	N-CA-C	-5.07	100.44	109.06
16	AG	105	ILE	O-C-N	5.06	128.90	122.57
16	AG	65	VAL	CA-C-N	5.06	131.62	121.81
16	AG	65	VAL	C-N-CA	5.06	131.62	121.81
16	AG	107	THR	CA-C-O	-5.05	113.17	119.18
41	a	614	A	C2'-C3'-O3'	5.03	117.04	109.50
41	a	328	U	C4'-C3'-O3'	-5.03	105.46	113.00
41	a	2193	G	C2'-C3'-O3'	5.02	121.23	113.70
16	AG	356	ILE	N-CA-C	-5.02	107.83	111.90
22	H	108	VAL	N-CA-C	-5.01	98.92	109.34
41	a	2335	A	C4'-C3'-O3'	-5.01	105.48	113.00
10	B	19	G	N9-C1'-C2'	5.00	119.51	112.00

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	19	G	Sidechain
10	A	7	G	Sidechain
12	AB	44	VAL	Mainchain
13	AC	192	VAL	Peptide
13	AD	20	SER	Peptide
13	AD	319	GLU	Peptide
13	AD	321	TRP	Peptide
14	AE	1184	ASP	Peptide
14	AE	1326	GLN	Peptide
14	AE	313	GLY	Peptide
14	AE	416	ILE	Peptide
14	AE	804	ALA	Peptide
16	AG	102	PHE	Peptide
16	AG	104	ARG	Peptide,Mainchain
16	AG	11	ALA	Peptide
16	AG	292	ASP	Mainchain
16	AG	426	GLY	Mainchain
10	B	19	G	Sidechain
10	B	7	G	Sidechain
22	H	274	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
22	H	81	GLU	Peptide
22	H	82	THR	Peptide
38	X	100	GLN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	816	839	839	8	0
2	1	857	922	922	14	0
3	2	746	811	811	5	0
4	3	788	844	844	11	0
5	4	753	780	780	0	0
6	5	472	260	260	26	0
7	6	542	305	306	24	0
8	7	647	97	321	106	0
9	9	1117	0	1153	168	0
10	A	1620	826	826	173	0
10	B	1620	814	827	141	0
11	AA	10567	0	10584	316	0
12	AB	1276	0	1244	270	0
13	AC	1690	0	1714	15	0
13	AD	2073	0	1889	46	0
14	AE	10388	10612	10610	383	0
15	AF	650	0	658	12	0
16	AG	3852	0	3826	815	0
17	C	544	559	560	24	0
18	D	32703	16423	16459	239	0
19	E	669	719	719	4	0
20	F	589	629	629	8	0
21	G	1760	1785	1785	46	0
22	H	1730	1454	1454	212	0
23	I	1636	1710	1710	43	0
24	J	1643	1707	1707	16	0
25	K	1152	1196	1196	21	0
26	L	848	846	846	3	0
27	M	1181	1235	1235	34	0
28	N	979	1031	1031	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	O	1022	1070	1070	12	0
30	P	790	831	831	106	0
31	Q	877	887	887	4	0
32	R	939	1001	1001	6	0
33	S	805	844	844	6	0
34	T	714	734	734	7	0
35	U	649	666	666	4	0
36	V	648	691	691	4	0
37	W	663	688	688	3	0
38	X	900	964	964	58	0
39	Y	1032	0	1088	90	0
40	Z	227	0	237	19	0
41	a	61841	31077	31123	301	0
42	b	582	599	599	3	0
43	c	625	652	652	4	0
44	d	2569	1301	1301	3	0
45	e	501	531	531	5	0
46	f	448	488	488	5	0
47	g	522	520	520	11	0
48	h	2082	2154	2154	19	0
49	i	444	459	458	6	0
50	j	1565	1617	1616	16	0
51	k	426	464	464	0	0
52	l	1552	1619	1619	14	0
53	m	377	418	418	10	0
54	n	1410	1443	1444	29	0
55	o	504	572	572	3	0
56	p	1313	1358	1358	7	0
57	q	302	343	343	1	0
58	r	1111	1148	1148	6	0
59	s	1129	1162	1162	14	0
60	t	946	1023	1023	12	0
61	u	1053	1129	1129	8	0
62	v	1074	1157	1157	5	0
63	w	951	994	994	8	0
64	x	892	923	923	8	0
65	y	917	962	962	4	0
66	z	947	1020	1019	13	0
67	AE	1	0	0	0	0
68	AE	2	0	0	0	0
All	All	181260	109913	132623	3352	0

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

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

All (3352) 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)
16:AG:425:LEU:CD2	16:AG:429:LYS:HE2	1.21	1.61
16:AG:287:ALA:CA	16:AG:331:LEU:HD12	1.18	1.59
17:C:12:ARG:HG3	22:H:264:GLU:CB	1.30	1.59
22:H:131:LEU:CB	22:H:167:VAL:CA	1.78	1.58
16:AG:168:LEU:CD2	16:AG:231:GLY:HA3	1.34	1.53
11:AA:901:LEU:CD1	16:AG:8:VAL:HG13	1.31	1.52
16:AG:363:LEU:CD2	16:AG:410:ALA:H	1.24	1.51
16:AG:393:LEU:CB	16:AG:398:LEU:CD2	1.83	1.50
16:AG:287:ALA:CB	16:AG:331:LEU:HD12	1.41	1.50
16:AG:287:ALA:HA	16:AG:331:LEU:CD1	1.38	1.50
16:AG:425:LEU:CA	16:AG:429:LYS:HE3	1.40	1.50
22:H:131:LEU:CB	22:H:167:VAL:HA	1.03	1.47
12:AB:139:GLY:HA3	30:P:102:LEU:CD1	1.46	1.46
9:9:130:PRO:N	9:9:130:PRO:CA	1.70	1.45
16:AG:425:LEU:HD23	16:AG:429:LYS:CE	1.45	1.44
12:AB:173:LEU:HD11	30:P:102:LEU:CD2	1.49	1.43
9:9:31:ARG:NE	41:a:1054:A:H5'	1.31	1.43
16:AG:363:LEU:CD2	16:AG:410:ALA:N	1.82	1.42
16:AG:168:LEU:CD2	16:AG:231:GLY:CA	1.98	1.39
16:AG:393:LEU:CD2	16:AG:398:LEU:CD2	1.99	1.39
16:AG:168:LEU:HD22	16:AG:231:GLY:CA	1.49	1.38
8:7:14:U:H5'	23:I:132:ARG:NH1	1.40	1.36
16:AG:187:ARG:HB3	16:AG:188:PRO:CD	1.45	1.36
11:AA:901:LEU:HD11	16:AG:8:VAL:CG1	1.55	1.36
16:AG:437:LEU:HD21	16:AG:456:LEU:CD1	1.54	1.36
22:H:71:ALA:C	22:H:72:LEU:HD12	1.49	1.36
16:AG:385:ALA:CB	16:AG:411:LYS:HE3	1.56	1.35
9:9:57:ASN:OD1	9:9:62:ARG:CG	1.75	1.34
16:AG:393:LEU:CA	16:AG:398:LEU:CD2	2.05	1.34
18:D:1358:U:O4	18:D:1363:A:N1	1.60	1.33
22:H:118:GLY:O	22:H:133:GLY:CA	1.74	1.33
16:AG:393:LEU:CA	16:AG:398:LEU:HD22	1.59	1.32
41:a:1839:G:H1'	41:a:1927:A:C8	1.62	1.32
16:AG:434:LEU:HD22	16:AG:459:LEU:CD1	1.58	1.32
16:AG:387:VAL:HG12	16:AG:388:PRO:CD	1.57	1.32
16:AG:393:LEU:HB3	16:AG:398:LEU:CD2	1.51	1.32
13:AD:285:THR:CB	16:AG:82:TYR:CE1	2.14	1.31
16:AG:434:LEU:CD2	16:AG:456:LEU:HA	1.58	1.31

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:849:GLU:HG2	16:AG:104:ARG:NH1	1.45	1.31
16:AG:393:LEU:CD2	16:AG:398:LEU:HD21	1.57	1.30
16:AG:448:LEU:HD21	16:AG:473:LEU:CD1	1.61	1.30
16:AG:353:HIS:O	16:AG:356:ILE:HG23	1.13	1.28
22:H:118:GLY:O	22:H:133:GLY:HA3	1.27	1.28
41:a:1021:A:N1	41:a:1141:U:O4	1.63	1.28
11:AA:854:ILE:N	16:AG:105:ILE:HG23	1.44	1.28
18:D:1308:U:H2'	38:X:98:ARG:NH2	1.48	1.28
16:AG:393:LEU:CG	16:AG:398:LEU:HD21	1.63	1.27
8:7:21:U:OP2	23:I:80:LYS:HA	1.28	1.27
16:AG:434:LEU:HA	16:AG:456:LEU:CD2	1.64	1.27
9:9:31:ARG:CZ	41:a:1054:A:H5'	1.63	1.27
12:AB:65:PHE:CE2	12:AB:111:ILE:HD11	1.70	1.27
18:D:1227:A:OP2	38:X:110:LYS:HE3	1.35	1.26
16:AG:363:LEU:HD23	16:AG:410:ALA:N	1.38	1.25
11:AA:858:GLY:H	11:AA:861:ALA:CB	1.49	1.25
16:AG:425:LEU:HA	16:AG:429:LYS:CE	1.64	1.25
17:C:12:ARG:CG	22:H:264:GLU:CB	2.15	1.25
18:D:1308:U:H3'	38:X:98:ARG:CZ	1.43	1.24
16:AG:355:ALA:CB	16:AG:382:GLU:CD	2.10	1.24
16:AG:353:HIS:C	16:AG:356:ILE:HG23	1.62	1.24
16:AG:387:VAL:CG1	16:AG:388:PRO:HD2	1.67	1.24
10:A:32:C:O4'	27:M:144:MET:HE1	1.09	1.23
10:A:18:G:N7	10:A:57:A:N6	1.87	1.23
18:D:948:C:OP2	38:X:105:ASN:OD1	1.53	1.23
16:AG:355:ALA:HA	16:AG:382:GLU:OE2	1.37	1.22
6:5:100:DA:OP1	12:AB:16:SER:O	1.56	1.22
12:AB:165:PHE:N	30:P:88:MET:HG3	1.52	1.22
16:AG:355:ALA:HB2	16:AG:382:GLU:OE1	1.40	1.22
16:AG:363:LEU:HD23	16:AG:409:ARG:C	1.63	1.22
16:AG:393:LEU:HA	16:AG:398:LEU:CD2	1.69	1.22
16:AG:123:ARG:HH12	16:AG:191:ARG:CA	1.36	1.22
16:AG:433:ASP:O	16:AG:456:LEU:HD11	1.35	1.22
9:9:88:HIS:HB3	9:9:89:PRO:CD	1.70	1.22
11:AA:853:ASP:C	16:AG:105:ILE:HG23	1.64	1.22
18:D:563:A:N1	18:D:884:U:O4	1.73	1.22
6:5:100:DA:OP1	12:AB:16:SER:OG	1.58	1.21
16:AG:362:TYR:O	16:AG:413:ALA:HB2	1.35	1.21
18:D:1308:U:C2'	38:X:98:ARG:NH2	2.03	1.21
10:B:18:G:N7	10:B:57:A:N6	1.87	1.21
12:AB:19:GLU:O	12:AB:44:VAL:HG11	1.37	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:267:TRP:CZ2	22:H:340:ARG:HG2	1.75	1.21
16:AG:287:ALA:CA	16:AG:331:LEU:CD1	2.02	1.20
16:AG:393:LEU:HD22	16:AG:398:LEU:CD2	1.71	1.20
16:AG:425:LEU:CG	16:AG:429:LYS:HE2	1.69	1.20
12:AB:139:GLY:CA	30:P:102:LEU:HD13	1.70	1.20
12:AB:167:ARG:NE	23:I:61:ALA:O	1.73	1.20
16:AG:123:ARG:NH1	16:AG:191:ARG:C	1.98	1.19
12:AB:23:ALA:HB2	12:AB:44:VAL:CG2	1.70	1.19
12:AB:140:PRO:CD	30:P:102:LEU:HB2	1.70	1.19
16:AG:442:ARG:O	16:AG:446:PHE:CD2	1.95	1.18
16:AG:287:ALA:CB	16:AG:331:LEU:CD1	2.16	1.18
12:AB:19:GLU:HG2	12:AB:44:VAL:HG13	1.20	1.18
16:AG:353:HIS:O	16:AG:357:ASP:N	1.77	1.18
8:7:21:U:OP2	23:I:80:LYS:CA	1.91	1.18
11:AA:849:GLU:CG	16:AG:104:ARG:HH11	1.55	1.18
16:AG:393:LEU:HD22	16:AG:398:LEU:CD1	1.73	1.17
16:AG:437:LEU:CD2	16:AG:456:LEU:HD13	1.74	1.17
12:AB:65:PHE:CD2	12:AB:111:ILE:HD11	1.78	1.17
16:AG:355:ALA:HA	16:AG:382:GLU:CD	1.71	1.16
9:9:31:ARG:NE	41:a:1054:A:C5'	2.07	1.16
16:AG:381:LEU:HA	16:AG:384:LEU:HD12	1.21	1.16
11:AA:913:VAL:HG21	16:AG:108:GLN:NE2	1.56	1.15
10:B:70:G:H2'	10:B:71:C:H5"	1.22	1.15
11:AA:859:GLU:O	11:AA:863:SER:HB3	1.46	1.14
16:AG:123:ARG:NH1	16:AG:191:ARG:O	1.80	1.14
10:A:70:G:H2'	10:A:71:C:H5"	1.23	1.13
11:AA:848:GLU:HG2	11:AA:888:THR:HG22	1.14	1.13
12:AB:173:LEU:CD1	30:P:102:LEU:CD2	2.26	1.13
22:H:135:LEU:CB	22:H:167:VAL:CB	2.27	1.13
22:H:267:TRP:CE2	22:H:340:ARG:HG2	1.84	1.13
10:A:32:C:O4'	27:M:144:MET:CE	1.97	1.12
12:AB:155:LYS:HB2	18:D:1277:C:OP2	1.48	1.12
17:C:44:ILE:HD13	22:H:339:ARG:CG	1.78	1.12
13:AD:285:THR:CB	16:AG:82:TYR:CD1	2.32	1.12
16:AG:393:LEU:CD2	16:AG:398:LEU:CD1	2.27	1.12
16:AG:422:GLU:HA	16:AG:426:GLY:CA	1.79	1.12
22:H:119:GLY:HA2	22:H:133:GLY:HA2	1.14	1.12
16:AG:355:ALA:HB1	16:AG:382:GLU:CG	1.77	1.12
17:C:44:ILE:HD13	22:H:339:ARG:HG2	1.18	1.12
16:AG:393:LEU:HD22	16:AG:398:LEU:HD11	1.28	1.11
9:9:142:THR:HG21	40:Z:7:ILE:HG12	1.21	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:1329:A:OP1	38:X:28:THR:HB	1.47	1.11
12:AB:173:LEU:CD1	30:P:102:LEU:HD23	1.79	1.11
16:AG:393:LEU:CB	16:AG:398:LEU:HD21	1.58	1.11
8:7:47:U:O2	11:AA:1253:LEU:HD12	1.48	1.11
16:AG:285:ILE:CG1	16:AG:293:VAL:HG11	1.80	1.11
16:AG:434:LEU:HA	16:AG:456:LEU:HD21	1.25	1.11
16:AG:254:MET:CG	16:AG:257:ALA:HB2	1.80	1.11
21:G:19:GLN:CD	22:H:76:GLU:HB3	1.67	1.11
16:AG:285:ILE:HG23	16:AG:293:VAL:HG12	1.25	1.10
16:AG:425:LEU:HA	16:AG:429:LYS:HG3	1.33	1.10
9:9:50:VAL:HG22	39:Y:119:ALA:CB	1.82	1.10
11:AA:853:ASP:OD1	16:AG:105:ILE:HG21	1.47	1.10
16:AG:353:HIS:O	16:AG:356:ILE:CG2	1.99	1.10
16:AG:424:SER:O	16:AG:429:LYS:HG2	1.47	1.10
11:AA:858:GLY:H	11:AA:861:ALA:HB3	1.12	1.10
16:AG:187:ARG:HB3	16:AG:188:PRO:HD2	1.21	1.10
16:AG:425:LEU:HA	16:AG:429:LYS:CG	1.80	1.10
16:AG:279:ASN:OD1	16:AG:280:PRO:HD3	1.50	1.10
30:P:87:LEU:HD23	30:P:100:ILE:HD13	1.32	1.10
16:AG:123:ARG:HH12	16:AG:191:ARG:C	1.57	1.10
16:AG:393:LEU:HB3	16:AG:398:LEU:HD23	1.26	1.10
16:AG:434:LEU:CD2	16:AG:459:LEU:HD12	1.81	1.10
9:9:57:ASN:OD1	9:9:62:ARG:HG3	1.44	1.09
12:AB:23:ALA:HB2	12:AB:44:VAL:HG21	1.25	1.09
12:AB:165:PHE:HA	30:P:88:MET:O	1.53	1.09
18:D:1308:U:C3'	38:X:98:ARG:NH2	2.16	1.09
18:D:1308:U:C3'	38:X:98:ARG:CZ	2.30	1.09
12:AB:23:ALA:HB2	12:AB:44:VAL:CB	1.81	1.08
12:AB:66:PRO:HG2	14:AE:281:ARG:NH2	1.66	1.08
22:H:267:TRP:CH2	22:H:340:ARG:HG2	1.87	1.08
24:J:162:ALA:HA	24:J:165:ARG:CZ	1.83	1.08
16:AG:181:GLY:HA2	16:AG:204:MET:SD	1.93	1.08
18:D:1308:U:C2'	38:X:98:ARG:HH21	1.63	1.08
11:AA:887:VAL:HG21	11:AA:913:VAL:HG22	1.33	1.08
16:AG:425:LEU:CD2	16:AG:429:LYS:CE	2.13	1.08
41:a:1839:G:C8	41:a:1927:A:H1'	1.87	1.08
16:AG:393:LEU:HD22	16:AG:398:LEU:HD21	1.25	1.07
21:G:19:GLN:CD	22:H:76:GLU:CB	2.19	1.07
12:AB:165:PHE:CZ	30:P:91:ASP:HA	1.88	1.07
16:AG:451:ARG:HH12	16:AG:467:LEU:C	1.62	1.07
9:9:88:HIS:CB	9:9:89:PRO:HD3	1.83	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AC:232:VAL:C	13:AD:221:ALA:HB3	1.80	1.07
16:AG:385:ALA:CB	16:AG:411:LYS:CE	2.33	1.07
16:AG:434:LEU:HD23	16:AG:456:LEU:HD23	1.10	1.07
8:7:3:G:H5"	18:D:1500:A:N6	1.70	1.07
12:AB:155:LYS:NZ	18:D:1278:G:OP2	1.88	1.07
22:H:71:ALA:O	22:H:72:LEU:HD12	1.53	1.07
9:9:129:LEU:N	9:9:130:PRO:HD3	1.66	1.06
16:AG:434:LEU:CD2	16:AG:456:LEU:CA	2.33	1.06
11:AA:857:VAL:HG12	11:AA:861:ALA:CB	1.84	1.06
16:AG:434:LEU:HD23	16:AG:456:LEU:HA	1.34	1.06
16:AG:451:ARG:NH1	16:AG:467:LEU:HA	1.68	1.06
16:AG:363:LEU:HD21	16:AG:410:ALA:H	0.94	1.06
21:G:19:GLN:CG	22:H:75:VAL:HG22	1.84	1.06
8:7:14:U:C5'	23:I:132:ARG:HH12	1.68	1.06
11:AA:900:LYS:HZ2	16:AG:11:ALA:CB	1.69	1.06
16:AG:365:ILE:HD13	16:AG:406:LEU:CD2	1.85	1.06
16:AG:430:PRO:HG2	16:AG:435:LEU:HD21	1.29	1.06
16:AG:434:LEU:HD21	16:AG:456:LEU:HA	1.26	1.06
12:AB:140:PRO:HD3	30:P:102:LEU:HB2	1.32	1.06
21:G:19:GLN:HG3	22:H:75:VAL:HG22	1.38	1.06
16:AG:387:VAL:HG12	16:AG:388:PRO:HD2	1.06	1.05
16:AG:187:ARG:HB3	16:AG:188:PRO:HD3	1.32	1.05
12:AB:11:VAL:HG23	12:AB:103:ILE:HD11	1.39	1.05
16:AG:302:LYS:H	16:AG:302:LYS:HE3	1.16	1.04
16:AG:365:ILE:HD13	16:AG:406:LEU:HD22	1.37	1.04
12:AB:138:ASP:HB3	12:AB:177:GLN:HA	1.37	1.04
10:B:18:G:N2	10:B:55:U:O2	1.90	1.04
11:AA:854:ILE:HG12	11:AA:855:PRO:HD2	1.39	1.04
12:AB:140:PRO:HD2	30:P:102:LEU:HD13	1.32	1.04
16:AG:285:ILE:HG13	16:AG:293:VAL:CG1	1.86	1.04
16:AG:385:ALA:HB1	16:AG:411:LYS:HE3	1.35	1.04
22:H:162:LYS:CB	22:H:298:GLU:CD	2.30	1.04
12:AB:165:PHE:CE1	30:P:91:ASP:HA	1.93	1.04
16:AG:285:ILE:HG23	16:AG:293:VAL:CG1	1.87	1.04
16:AG:363:LEU:HG	16:AG:410:ALA:HB2	1.37	1.04
16:AG:393:LEU:CB	16:AG:398:LEU:HD23	1.80	1.04
14:AE:24:LEU:HG	14:AE:232:ASN:HD21	1.17	1.03
18:D:1227:A:OP2	38:X:110:LYS:CE	2.06	1.03
22:H:19:ARG:O	22:H:72:LEU:HB2	1.57	1.03
9:9:129:LEU:H	9:9:130:PRO:HD3	0.90	1.03
11:AA:1313:HIS:CD2	15:AF:31:GLN:HE22	1.75	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:155:LYS:NZ	18:D:1277:C:H3'	1.71	1.03
10:B:56:C:H2'	10:B:57:A:H5"	1.39	1.03
10:B:70:G:C2'	10:B:71:C:H5"	1.89	1.03
10:A:18:G:N2	10:A:55:U:O2	1.90	1.03
11:AA:854:ILE:HG12	11:AA:855:PRO:CD	1.89	1.03
16:AG:422:GLU:HA	16:AG:426:GLY:HA3	1.33	1.03
16:AG:448:LEU:CD2	16:AG:473:LEU:CD1	2.36	1.03
12:AB:154:GLU:O	18:D:1276:G:OP2	1.75	1.03
16:AG:168:LEU:HD21	16:AG:231:GLY:CA	1.83	1.03
10:B:56:C:O4'	54:n:80:ARG:NH2	1.91	1.03
18:D:1329:A:OP1	38:X:28:THR:CB	2.07	1.03
8:7:11:U:O2'	25:K:33:PHE:CE1	2.11	1.02
8:7:21:U:OP2	23:I:80:LYS:HG2	1.59	1.02
10:A:56:C:H2'	10:A:57:A:H5"	1.39	1.02
11:AA:909:LYS:HD3	11:AA:909:LYS:H	1.16	1.02
12:AB:128:PHE:CE1	12:AB:175:PHE:HB3	1.93	1.02
16:AG:187:ARG:CB	16:AG:188:PRO:CD	2.37	1.02
16:AG:425:LEU:CG	16:AG:429:LYS:CE	2.34	1.02
16:AG:437:LEU:CD2	16:AG:456:LEU:CD1	2.34	1.02
22:H:290:TYR:O	22:H:305:HIS:O	1.77	1.02
30:P:17:LEU:HD21	30:P:93:ALA:CB	1.90	1.02
9:9:93:ALA:O	9:9:129:LEU:HD12	1.60	1.02
10:A:70:G:C2'	10:A:71:C:H5"	1.89	1.02
16:AG:425:LEU:CA	16:AG:429:LYS:CE	2.30	1.02
16:AG:425:LEU:C	16:AG:429:LYS:HE3	1.84	1.02
16:AG:422:GLU:HA	16:AG:426:GLY:N	1.74	1.01
16:AG:361:LYS:CE	16:AG:417:ILE:HG12	1.90	1.01
11:AA:857:VAL:HG12	11:AA:861:ALA:HB1	1.03	1.01
16:AG:361:LYS:HE2	16:AG:417:ILE:HG12	1.39	1.01
16:AG:363:LEU:HD23	16:AG:409:ARG:CA	1.89	1.01
12:AB:128:PHE:CZ	12:AB:175:PHE:HB3	1.94	1.01
16:AG:434:LEU:HD21	16:AG:456:LEU:CA	1.89	1.01
12:AB:155:LYS:HZ1	18:D:1277:C:C3'	1.74	1.01
16:AG:168:LEU:HD22	16:AG:231:GLY:HA2	1.40	1.01
16:AG:363:LEU:CD2	16:AG:409:ARG:HB2	1.91	1.01
16:AG:393:LEU:CG	16:AG:398:LEU:CD2	2.30	1.01
18:D:13:U:N3	18:D:915:A:C6	2.29	1.01
14:AE:111:THR:HG23	14:AE:300:GLN:CD	1.86	1.00
16:AG:365:ILE:CG2	16:AG:409:ARG:NH1	2.23	1.00
41:a:2297:A:N1	41:a:2321:U:C4	2.29	1.00
12:AB:140:PRO:HD2	30:P:102:LEU:CD1	1.91	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:38:VAL:CG2	22:H:75:VAL:HG21	1.90	1.00
11:AA:549:ASP:OD2	14:AE:750:PRO:HB3	1.60	1.00
13:AD:308:ALA:CB	16:AG:96:GLN:CB	2.34	1.00
16:AG:434:LEU:CD2	16:AG:456:LEU:HD23	1.92	1.00
16:AG:287:ALA:HA	16:AG:331:LEU:HD11	1.41	0.99
16:AG:355:ALA:HB1	16:AG:382:GLU:HG3	1.41	0.99
10:B:56:C:H5'	54:n:80:ARG:CZ	1.90	0.99
16:AG:393:LEU:HD23	16:AG:398:LEU:HD22	1.43	0.99
16:AG:123:ARG:NH1	16:AG:191:ARG:CA	2.11	0.99
16:AG:131:ARG:O	16:AG:134:GLU:HG3	1.61	0.99
21:G:38:VAL:HG22	22:H:75:VAL:HG21	1.44	0.99
16:AG:287:ALA:HB2	16:AG:331:LEU:CD1	1.91	0.99
22:H:131:LEU:CB	22:H:167:VAL:CB	2.40	0.99
16:AG:434:LEU:HD23	16:AG:456:LEU:CD2	1.91	0.99
18:D:13:U:O4	18:D:20:U:O4	1.79	0.99
10:A:32:C:C4'	27:M:144:MET:HE1	1.93	0.99
16:AG:362:TYR:O	16:AG:413:ALA:CB	2.10	0.99
16:AG:393:LEU:CD2	16:AG:398:LEU:HD11	1.90	0.99
18:D:1308:U:H2'	38:X:98:ARG:HH21	1.06	0.99
12:AB:165:PHE:H	30:P:88:MET:HA	1.27	0.99
8:7:21:U:OP2	23:I:80:LYS:CG	2.09	0.98
11:AA:849:GLU:HB2	11:AA:887:VAL:CG1	1.93	0.98
16:AG:442:ARG:O	16:AG:446:PHE:HD2	1.34	0.98
13:AD:308:ALA:CB	16:AG:96:GLN:HB3	1.92	0.98
16:AG:168:LEU:HD21	16:AG:230:PRO:C	1.89	0.98
16:AG:228:ARG:HA	16:AG:327:LEU:HD11	1.46	0.98
16:AG:336:LEU:HD12	16:AG:336:LEU:H	1.26	0.98
9:9:88:HIS:CB	9:9:89:PRO:CD	2.41	0.98
11:AA:1268:GLN:NE2	14:AE:352:ARG:HD2	1.78	0.98
22:H:118:GLY:O	22:H:133:GLY:HA2	1.63	0.98
9:9:31:ARG:CD	41:a:1054:A:H5'	1.94	0.98
12:AB:140:PRO:CD	30:P:102:LEU:CB	2.41	0.98
16:AG:393:LEU:HD22	16:AG:398:LEU:CG	1.93	0.98
9:9:129:LEU:H	9:9:130:PRO:CD	1.77	0.97
11:AA:895:LEU:HD23	11:AA:895:LEU:H	1.29	0.97
16:AG:168:LEU:HD21	16:AG:231:GLY:N	1.76	0.97
11:AA:913:VAL:CG2	16:AG:108:GLN:NE2	2.10	0.97
8:7:14:U:C5'	23:I:132:ARG:NH1	2.26	0.97
10:A:32:C:O2'	27:M:86:GLN:CG	2.12	0.97
22:H:119:GLY:CA	22:H:133:GLY:HA2	1.95	0.97
41:a:1839:G:C1'	41:a:1927:A:C8	2.47	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:853:ASP:C	16:AG:105:ILE:CG2	2.38	0.97
12:AB:19:GLU:O	12:AB:44:VAL:CG1	2.13	0.97
16:AG:393:LEU:CA	16:AG:398:LEU:HD23	1.87	0.97
16:AG:214:PRO:O	16:AG:218:GLU:OE2	1.83	0.96
8:7:2:U:P	18:D:1505:G:H8	1.87	0.96
16:AG:424:SER:O	16:AG:429:LYS:CG	2.13	0.96
16:AG:433:ASP:O	16:AG:456:LEU:CD1	2.13	0.96
9:9:142:THR:HG21	40:Z:7:ILE:CG1	1.96	0.96
16:AG:279:ASN:CG	16:AG:280:PRO:CD	2.38	0.96
41:a:1839:G:O4'	41:a:1927:A:O4'	1.82	0.96
16:AG:380:THR:O	16:AG:384:LEU:CD1	2.13	0.96
13:AC:232:VAL:C	13:AD:221:ALA:CB	2.37	0.96
16:AG:387:VAL:HG12	16:AG:388:PRO:HD3	1.47	0.96
16:AG:258:ARG:HH11	16:AG:258:ARG:HG2	1.31	0.95
9:9:57:ASN:OD1	9:9:62:ARG:HG2	1.64	0.95
11:AA:887:VAL:CG2	11:AA:913:VAL:HG22	1.97	0.95
7:6:15:DC:N4	7:6:16:DC:N4	2.15	0.95
12:AB:64:PHE:HB2	14:AE:285:LEU:HD21	1.46	0.95
12:AB:139:GLY:CA	30:P:102:LEU:CD1	2.36	0.95
16:AG:393:LEU:HA	16:AG:398:LEU:HD22	0.95	0.95
11:AA:900:LYS:NZ	16:AG:11:ALA:HB1	1.82	0.95
41:a:67:U:N3	41:a:74:A:C6	2.35	0.95
8:7:14:U:H5'	23:I:132:ARG:HH12	1.01	0.94
16:AG:451:ARG:NH1	16:AG:467:LEU:CA	2.30	0.94
30:P:17:LEU:HD21	30:P:93:ALA:HB1	1.49	0.94
6:5:100:DA:P	12:AB:16:SER:HG	1.89	0.94
12:AB:140:PRO:CD	30:P:102:LEU:HD13	1.96	0.94
16:AG:363:LEU:HG	16:AG:410:ALA:CB	1.97	0.94
18:D:13:U:N3	18:D:915:A:N6	2.16	0.94
16:AG:171:GLU:OE2	16:AG:267:GLY:HA3	1.68	0.94
18:D:1308:U:H3'	38:X:98:ARG:NH2	1.76	0.94
12:AB:141:PHE:CE2	12:AB:171:VAL:HG11	2.02	0.94
16:AG:440:VAL:CG2	16:AG:481:LEU:HD22	1.97	0.94
14:AE:68:TYR:O	14:AE:75:TYR:CE2	2.20	0.94
16:AG:254:MET:HG2	16:AG:257:ALA:CB	1.97	0.94
12:AB:165:PHE:N	30:P:88:MET:HA	1.82	0.93
16:AG:365:ILE:CD1	16:AG:406:LEU:HD22	1.97	0.93
22:H:71:ALA:C	22:H:72:LEU:CD1	2.42	0.93
11:AA:857:VAL:CG1	11:AA:861:ALA:HB1	1.97	0.93
11:AA:901:LEU:CG	16:AG:8:VAL:HG13	1.98	0.93
16:AG:363:LEU:CG	16:AG:410:ALA:HB2	1.99	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:13:U:C4	18:D:915:A:N6	2.36	0.93
41:a:1839:G:O4'	41:a:1927:A:C1'	2.16	0.93
10:A:72:A:H2'	10:A:73:A:H5"	1.48	0.93
16:AG:254:MET:CG	16:AG:257:ALA:CB	2.47	0.93
8:7:4:U:O2'	18:D:1403:C:O2	1.87	0.93
16:AG:279:ASN:CG	16:AG:280:PRO:HD3	1.93	0.93
10:A:32:C:O2'	27:M:86:GLN:HG3	1.68	0.93
10:A:68:C:H2'	10:A:69:C:H5"	1.51	0.93
11:AA:901:LEU:CD1	16:AG:8:VAL:CG1	2.28	0.93
16:AG:183:LEU:HG	16:AG:197:VAL:HG13	1.51	0.93
10:B:72:A:H2'	10:B:73:A:H5"	1.49	0.93
12:AB:65:PHE:CE2	12:AB:111:ILE:CD1	2.51	0.93
16:AG:448:LEU:HD21	16:AG:473:LEU:HD11	1.48	0.93
9:9:88:HIS:HB3	9:9:89:PRO:HD3	0.93	0.92
11:AA:900:LYS:NZ	16:AG:11:ALA:CB	2.31	0.92
12:AB:165:PHE:H	30:P:88:MET:HG3	1.32	0.92
16:AG:448:LEU:HD21	16:AG:473:LEU:HD13	1.48	0.92
22:H:119:GLY:HA3	22:H:131:LEU:O	1.68	0.92
30:P:87:LEU:CD2	30:P:100:ILE:HD13	1.99	0.92
11:AA:853:ASP:OD2	16:AG:103:ASP:HB2	1.69	0.92
16:AG:393:LEU:HD23	16:AG:398:LEU:CD2	1.93	0.92
16:AG:123:ARG:CZ	16:AG:191:ARG:O	2.17	0.92
22:H:135:LEU:HA	22:H:157:ILE:CB	1.98	0.92
13:AD:285:THR:CB	16:AG:82:TYR:HE1	1.72	0.92
11:AA:858:GLY:N	11:AA:861:ALA:CB	2.33	0.92
9:9:50:VAL:HG22	39:Y:119:ALA:HB1	1.50	0.92
10:B:75:C:OP1	41:a:2602:A:C8	2.22	0.92
11:AA:858:GLY:H	11:AA:861:ALA:HB2	1.34	0.92
12:AB:140:PRO:HD2	30:P:102:LEU:CG	2.00	0.92
16:AG:240:THR:OG1	16:AG:247:PRO:HG3	1.68	0.91
16:AG:355:ALA:HB2	16:AG:382:GLU:CD	1.83	0.91
16:AG:434:LEU:HD22	16:AG:459:LEU:HD12	0.93	0.91
11:AA:1313:HIS:HD2	15:AF:31:GLN:HE22	0.98	0.91
16:AG:453:VAL:HG13	16:AG:458:ASP:CB	2.00	0.91
18:D:13:U:C4	18:D:20:U:O4	2.24	0.91
16:AG:451:ARG:NH1	16:AG:466:ASP:O	2.02	0.91
16:AG:425:LEU:HA	16:AG:429:LYS:CD	2.01	0.91
9:9:93:ALA:O	9:9:129:LEU:CD1	2.19	0.91
10:A:56:C:H1'	41:a:2112:G:C6	2.06	0.91
16:AG:200:SER:O	16:AG:230:PRO:HG2	1.71	0.91
16:AG:363:LEU:HD22	16:AG:409:ARG:HB2	1.53	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:363:LEU:HD23	16:AG:409:ARG:CB	2.00	0.91
39:Y:104:GLN:HG2	39:Y:108:ILE:HD11	1.53	0.91
11:AA:900:LYS:HZ2	16:AG:11:ALA:HB3	1.32	0.90
16:AG:385:ALA:HB3	16:AG:411:LYS:CE	2.00	0.90
16:AG:434:LEU:HD21	16:AG:455:THR:O	1.69	0.90
10:B:68:C:H2'	10:B:69:C:H5"	1.51	0.90
14:AE:24:LEU:HB2	14:AE:232:ASN:OD1	1.71	0.90
41:a:2013:A:N6	41:a:2613:U:H3	1.68	0.90
8:7:2:U:P	18:D:1505:G:C8	2.64	0.90
9:9:129:LEU:N	9:9:130:PRO:CD	2.34	0.90
14:AE:136:GLU:OE1	14:AE:312:ARG:NH1	2.04	0.90
16:AG:240:THR:OG1	16:AG:247:PRO:CG	2.20	0.90
11:AA:641:GLU:OE2	14:AE:749:LYS:NZ	2.03	0.90
8:7:21:U:OP1	23:I:81:GLY:N	2.03	0.90
12:AB:167:ARG:HG2	12:AB:167:ARG:HH21	1.35	0.90
16:AG:123:ARG:HH12	16:AG:191:ARG:HA	1.32	0.90
16:AG:365:ILE:HG21	16:AG:409:ARG:NH1	1.87	0.90
16:AG:453:VAL:HG23	16:AG:462:GLN:NE2	1.87	0.90
22:H:119:GLY:HA2	22:H:133:GLY:CA	2.01	0.90
11:AA:855:PRO:CB	16:AG:109:THR:HG21	2.02	0.90
10:B:18:G:N2	10:B:58:A:N7	2.19	0.90
22:H:279:LYS:HA	22:H:331:MET:HB3	1.54	0.90
41:a:1406:U:O2'	41:a:1407:G:C5'	2.19	0.90
41:a:2314:A:H1'	54:n:155:THR:HG21	1.54	0.89
12:AB:65:PHE:HD1	14:AE:285:LEU:HD23	1.38	0.89
16:AG:174:ARG:HB3	16:AG:175:PRO:HD2	1.51	0.89
16:AG:422:GLU:CA	16:AG:426:GLY:HA3	2.02	0.89
10:A:18:G:N2	10:A:58:A:N7	2.19	0.89
12:AB:167:ARG:CZ	23:I:61:ALA:O	2.20	0.89
22:H:162:LYS:N	22:H:298:GLU:OE2	2.06	0.89
14:AE:202:ARG:HG2	14:AE:202:ARG:HH11	1.35	0.89
16:AG:434:LEU:HD23	16:AG:456:LEU:CA	2.00	0.89
6:5:114:DC:H5"	14:AE:1148:ARG:NH2	1.87	0.89
16:AG:425:LEU:CA	16:AG:429:LYS:HG3	2.02	0.89
39:Y:21:PRO:HB2	39:Y:22:PRO:HD3	1.54	0.88
11:AA:857:VAL:HG11	11:AA:862:LEU:HD12	1.53	0.88
16:AG:393:LEU:CD2	16:AG:398:LEU:HD22	1.90	0.88
9:9:50:VAL:CG2	39:Y:119:ALA:HB3	2.04	0.88
12:AB:155:LYS:HZ1	18:D:1277:C:H3'	1.28	0.88
21:G:18:HIS:HA	22:H:43:LYS:HD2	1.55	0.88
22:H:131:LEU:CB	22:H:167:VAL:N	2.37	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:434:LEU:HD21	16:AG:455:THR:C	1.97	0.88
8:7:3:G:C5'	18:D:1500:A:H62	1.85	0.88
11:AA:913:VAL:HG21	16:AG:108:GLN:HE21	1.36	0.88
12:AB:167:ARG:NH1	23:I:62:LYS:O	2.07	0.88
12:AB:11:VAL:HG23	12:AB:103:ILE:CD1	2.03	0.88
16:AG:168:LEU:HD22	16:AG:231:GLY:HA3	1.00	0.88
30:P:87:LEU:HD23	30:P:100:ILE:CD1	2.02	0.88
12:AB:95:GLY:O	14:AE:162:GLU:CD	2.16	0.88
16:AG:187:ARG:CB	16:AG:188:PRO:HD2	2.03	0.88
16:AG:363:LEU:HG	16:AG:410:ALA:CA	2.04	0.88
16:AG:434:LEU:HA	16:AG:456:LEU:HD23	1.53	0.88
16:AG:302:LYS:HE3	16:AG:302:LYS:N	1.87	0.88
10:A:33:U:H5"	27:M:84:THR:HG21	1.55	0.88
11:AA:857:VAL:HG11	11:AA:862:LEU:CD1	2.04	0.88
12:AB:19:GLU:HG2	12:AB:44:VAL:CG1	2.04	0.88
12:AB:140:PRO:HD2	30:P:102:LEU:CB	2.03	0.87
12:AB:128:PHE:HZ	12:AB:175:PHE:C	1.82	0.87
12:AB:140:PRO:CB	30:P:6:ILE:HD11	2.04	0.87
14:AE:68:TYR:C	14:AE:75:TYR:HE2	1.80	0.87
12:AB:11:VAL:CG2	12:AB:103:ILE:HD11	2.03	0.87
12:AB:23:ALA:CB	12:AB:44:VAL:HG21	2.04	0.87
16:AG:168:LEU:HD23	16:AG:231:GLY:HA3	1.56	0.87
16:AG:422:GLU:HA	16:AG:426:GLY:H	1.34	0.87
11:AA:858:GLY:O	11:AA:861:ALA:N	2.07	0.87
12:AB:155:LYS:NZ	18:D:1278:G:P	2.48	0.87
16:AG:486:ARG:O	16:AG:490:TRP:HD1	1.57	0.87
9:9:142:THR:CG2	40:Z:7:ILE:HG12	2.03	0.87
22:H:348:GLN:N	22:H:348:GLN:OE1	2.08	0.87
12:AB:173:LEU:HD11	30:P:102:LEU:HD23	0.88	0.87
16:AG:141:VAL:HG22	16:AG:178:ARG:HG2	1.57	0.87
16:AG:362:TYR:C	16:AG:413:ALA:CB	2.48	0.87
24:J:162:ALA:HB2	24:J:165:ARG:NH2	1.90	0.87
11:AA:1313:HIS:HD2	15:AF:31:GLN:NE2	1.71	0.86
16:AG:302:LYS:O	16:AG:302:LYS:NZ	2.08	0.86
17:C:31:ASN:OD1	22:H:268:VAL:HG22	1.74	0.86
30:P:17:LEU:CD2	30:P:93:ALA:HB3	2.03	0.86
12:AB:155:LYS:HZ2	18:D:1278:G:P	1.98	0.86
14:AE:425:ARG:NH1	14:AE:458:ASN:O	2.08	0.86
41:a:783:A:N3	41:a:783:A:H2'	1.89	0.86
16:AG:362:TYR:C	16:AG:413:ALA:HB2	1.99	0.86
4:3:34:VAL:HG13	4:3:67:VAL:HG22	1.58	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:171:GLU:CD	16:AG:267:GLY:HA3	1.99	0.86
16:AG:385:ALA:HB1	16:AG:411:LYS:CE	2.04	0.86
16:AG:453:VAL:HG13	16:AG:458:ASP:HB2	1.55	0.86
12:AB:44:VAL:HG22	12:AB:69:VAL:HG13	1.56	0.86
16:AG:287:ALA:HA	16:AG:331:LEU:HD12	0.87	0.86
16:AG:434:LEU:HD12	16:AG:454:CYS:O	1.76	0.86
9:9:31:ARG:CD	41:a:1054:A:H4'	2.06	0.86
9:9:52:MET:C	9:9:52:MET:HE3	2.00	0.86
18:D:197:A:C6	18:D:221:C:H4'	2.11	0.86
16:AG:393:LEU:HB3	16:AG:398:LEU:HD21	1.25	0.86
11:AA:855:PRO:HB3	16:AG:109:THR:CG2	2.06	0.85
24:J:61:VAL:HG21	24:J:200:ILE:HD11	1.57	0.85
12:AB:167:ARG:HH11	23:I:62:LYS:C	1.84	0.85
22:H:267:TRP:CD2	22:H:340:ARG:HG2	2.12	0.85
47:g:16:CYS:CB	47:g:37:CYS:HB3	2.05	0.85
10:A:16:C:O2	41:a:2181:U:H5'	1.76	0.85
16:AG:254:MET:CB	16:AG:257:ALA:HB2	2.07	0.85
16:AG:430:PRO:HG2	16:AG:435:LEU:CD2	2.05	0.85
22:H:162:LYS:CA	22:H:298:GLU:OE2	2.17	0.85
10:A:18:G:N7	10:A:57:A:C6	2.44	0.85
14:AE:68:TYR:O	14:AE:75:TYR:HE2	1.58	0.85
16:AG:248:VAL:HG13	16:AG:273:ILE:HB	1.56	0.85
16:AG:355:ALA:CA	16:AG:382:GLU:CD	2.49	0.85
14:AE:24:LEU:HG	14:AE:232:ASN:ND2	1.90	0.85
16:AG:385:ALA:HB3	16:AG:411:LYS:HE3	1.57	0.85
16:AG:448:LEU:CD2	16:AG:473:LEU:HD11	2.05	0.85
12:AB:103:ILE:HD12	12:AB:107:GLU:CD	2.00	0.85
14:AE:68:TYR:HB3	14:AE:75:TYR:OH	1.77	0.85
39:Y:81:LYS:O	39:Y:81:LYS:HE3	1.75	0.85
9:9:125:ARG:NH1	9:9:125:ARG:HA	1.92	0.85
12:AB:141:PHE:CZ	12:AB:171:VAL:HG11	2.12	0.85
39:Y:60:VAL:HG13	39:Y:66:PHE:HB3	1.58	0.85
12:AB:167:ARG:HE	23:I:61:ALA:C	1.85	0.84
22:H:135:LEU:CB	22:H:167:VAL:C	2.50	0.84
16:AG:243:LYS:HB3	16:AG:245:ILE:HD11	1.60	0.84
10:B:18:G:N7	10:B:57:A:C6	2.44	0.84
41:a:67:U:N3	41:a:74:A:N6	2.25	0.84
14:AE:26:SER:HB2	14:AE:236:TRP:CZ2	2.12	0.84
16:AG:387:VAL:CG1	16:AG:388:PRO:CD	2.41	0.84
22:H:131:LEU:CB	22:H:166:VAL:O	2.26	0.84
25:K:111:MET:HE2	25:K:125:ALA:HB1	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:136:VAL:HG22	12:AB:178:VAL:HG12	1.57	0.84
16:AG:61:ARG:HD3	16:AG:63:LEU:HD21	1.57	0.84
41:a:2303:G:C2	41:a:2314:A:C2	2.66	0.84
12:AB:173:LEU:HD11	30:P:102:LEU:HD21	1.57	0.84
22:H:267:TRP:CH2	22:H:340:ARG:CG	2.61	0.84
11:AA:909:LYS:HD3	11:AA:909:LYS:N	1.87	0.84
16:AG:203:GLU:HA	16:AG:206:ILE:HG12	1.60	0.84
16:AG:287:ALA:HB2	16:AG:331:LEU:HD13	1.58	0.84
16:AG:387:VAL:CB	16:AG:388:PRO:HD2	2.06	0.84
10:A:72:A:C2'	10:A:73:A:H5"	2.08	0.84
12:AB:96:THR:HB	14:AE:162:GLU:HG3	1.60	0.84
22:H:332:VAL:HG11	22:H:335:ILE:HG13	1.57	0.84
21:G:16:PHE:HB3	22:H:43:LYS:HA	1.60	0.84
12:AB:165:PHE:H	30:P:88:MET:CA	1.91	0.83
16:AG:433:ASP:C	16:AG:456:LEU:HG	2.03	0.83
22:H:267:TRP:CZ3	22:H:340:ARG:HG2	2.12	0.83
9:9:31:ARG:CD	41:a:1054:A:C4'	2.57	0.83
17:C:12:ARG:HH22	22:H:268:VAL:CG2	1.91	0.83
8:7:3:G:H5"	18:D:1500:A:H62	1.40	0.83
16:AG:285:ILE:CG2	16:AG:293:VAL:HG12	2.06	0.83
18:D:1227:A:H5'	38:X:110:LYS:NZ	1.93	0.83
8:7:21:U:OP2	23:I:80:LYS:CB	2.26	0.83
12:AB:133:MET:H	12:AB:133:MET:HE2	1.43	0.83
39:Y:102:ARG:HB3	39:Y:141:ASP:HA	1.61	0.83
16:AG:354:ALA:HA	16:AG:357:ASP:HB3	1.60	0.83
9:9:57:ASN:OD1	9:9:62:ARG:CD	2.27	0.83
11:AA:848:GLU:HG2	11:AA:888:THR:CG2	2.03	0.83
16:AG:127:VAL:CG2	16:AG:192:GLY:HA2	2.09	0.83
13:AD:308:ALA:HB2	16:AG:96:GLN:CB	1.77	0.83
16:AG:210:ARG:HG3	16:AG:216:ILE:HB	1.59	0.83
7:6:21:DA:N1	8:7:51:G:N2	2.26	0.83
12:AB:23:ALA:HB2	12:AB:44:VAL:HB	1.58	0.83
16:AG:425:LEU:HA	16:AG:429:LYS:HE3	0.95	0.83
9:9:31:ARG:HH11	9:9:31:ARG:HG3	1.41	0.83
12:AB:139:GLY:HA3	30:P:102:LEU:HD13	0.83	0.83
10:B:56:C:H5'	54:n:80:ARG:NE	1.93	0.83
41:a:1021:A:N6	41:a:1141:U:H3	1.77	0.83
16:AG:252:VAL:HA	16:AG:259:VAL:HG23	1.61	0.82
8:7:2:U:OP2	18:D:1505:G:C8	2.32	0.82
11:AA:858:GLY:N	11:AA:861:ALA:HB3	1.94	0.82
14:AE:141:PHE:HE2	14:AE:296:LYS:HB2	1.44	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:285:ILE:CB	16:AG:293:VAL:HG11	2.09	0.82
16:AG:353:HIS:CA	16:AG:356:ILE:HG23	2.09	0.82
10:A:68:C:C2'	10:A:69:C:H5"	2.08	0.82
16:AG:213:VAL:HG11	16:AG:251:CYS:HA	1.59	0.82
11:AA:849:GLU:HB2	11:AA:887:VAL:HG12	1.59	0.82
12:AB:173:LEU:CD1	30:P:102:LEU:HD21	2.08	0.82
16:AG:285:ILE:HG13	16:AG:293:VAL:HG11	1.45	0.82
39:Y:20:SER:HB3	39:Y:21:PRO:HD3	1.59	0.82
11:AA:854:ILE:HG13	11:AA:887:VAL:HB	1.58	0.82
16:AG:279:ASN:CG	16:AG:280:PRO:HD2	2.03	0.82
10:B:68:C:C2'	10:B:69:C:H5"	2.08	0.82
8:7:2:U:OP1	18:D:1505:G:C8	2.32	0.82
16:AG:425:LEU:HG	16:AG:429:LYS:CE	2.08	0.82
22:H:267:TRP:CZ3	22:H:340:ARG:CG	2.63	0.82
22:H:305:HIS:CD2	22:H:306:VAL:H	1.98	0.82
9:9:31:ARG:HD2	41:a:1054:A:H4'	1.62	0.82
9:9:50:VAL:HG22	39:Y:119:ALA:HB3	1.60	0.82
16:AG:380:THR:O	16:AG:384:LEU:HD11	1.80	0.82
30:P:17:LEU:CD2	30:P:93:ALA:CB	2.58	0.82
41:a:1019:U:H3	41:a:1142:A:N6	1.77	0.82
14:AE:141:PHE:CE2	14:AE:296:LYS:HB2	2.15	0.82
16:AG:285:ILE:CG2	16:AG:293:VAL:CG1	2.57	0.82
16:AG:365:ILE:CG2	16:AG:409:ARG:HH12	1.91	0.82
9:9:62:ARG:HG2	9:9:62:ARG:HH21	1.44	0.81
10:A:56:C:C2'	10:A:57:A:H5"	2.10	0.81
12:AB:11:VAL:CG2	12:AB:103:ILE:CD1	2.58	0.81
16:AG:451:ARG:HH12	16:AG:467:LEU:CA	1.92	0.81
22:H:155:LYS:CB	22:H:169:SER:CB	2.58	0.81
41:a:1406:U:O2'	41:a:1407:G:H5"	1.79	0.81
12:AB:140:PRO:CB	30:P:84:VAL:HG21	2.10	0.81
14:AE:1169:THR:OG1	14:AE:1192:LYS:NZ	2.13	0.81
16:AG:365:ILE:CD1	16:AG:406:LEU:CD2	2.57	0.81
16:AG:362:TYR:HA	16:AG:413:ALA:CB	2.09	0.81
10:B:72:A:C2'	10:B:73:A:H5"	2.09	0.81
22:H:122:VAL:O	22:H:129:ALA:N	2.13	0.81
9:9:3:LEU:HD13	9:9:5:LEU:HG	1.61	0.81
16:AG:133:HIS:ND1	16:AG:136:GLU:OE1	2.13	0.81
18:D:37:U:N3	18:D:397:A:N6	2.28	0.81
41:a:1839:G:C1'	41:a:1927:A:N9	2.43	0.81
7:6:18:DC:H42	8:7:53:G:H1	1.26	0.81
10:B:54:U:H3	10:B:58:A:N6	1.78	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:56:C:C2'	10:B:57:A:H5"	2.11	0.81
21:G:19:GLN:OE1	22:H:75:VAL:O	1.85	0.81
8:7:2:U:OP1	18:D:1505:G:H8	1.62	0.81
11:AA:855:PRO:HB2	16:AG:109:THR:HG21	1.62	0.81
16:AG:362:TYR:HA	16:AG:413:ALA:HB1	1.62	0.81
13:AD:308:ALA:HB1	16:AG:96:GLN:HB3	1.61	0.81
14:AE:111:THR:HG23	14:AE:300:GLN:OE1	1.81	0.81
16:AG:451:ARG:HH11	16:AG:467:LEU:HA	1.42	0.81
39:Y:27:LEU:HD12	39:Y:27:LEU:O	1.81	0.81
16:AG:12:VAL:HB	16:AG:16:LYS:HG3	1.61	0.81
16:AG:425:LEU:HG	16:AG:429:LYS:CD	2.10	0.81
16:AG:451:ARG:NE	16:AG:470:ILE:HG13	1.95	0.81
11:AA:808:ASN:H	14:AE:633:ALA:HB2	1.44	0.81
16:AG:361:LYS:CD	16:AG:417:ILE:HG12	2.10	0.81
9:9:31:ARG:CZ	41:a:1054:A:C5'	2.49	0.81
11:AA:848:GLU:CG	11:AA:888:THR:HG22	2.06	0.81
10:B:7:G:H4'	10:B:8:U:OP1	1.81	0.81
17:C:12:ARG:CB	22:H:264:GLU:CB	2.59	0.81
13:AD:308:ALA:HB2	16:AG:96:GLN:HB3	1.54	0.80
16:AG:425:LEU:HD23	16:AG:429:LYS:HE2	0.81	0.80
16:AG:434:LEU:CG	16:AG:455:THR:C	2.54	0.80
22:H:123:GLU:HA	22:H:128:ARG:HA	1.63	0.80
16:AG:353:HIS:C	16:AG:356:ILE:CG2	2.50	0.80
16:AG:379:SER:OG	16:AG:384:LEU:HD21	1.81	0.80
18:D:972:C:O2'	30:P:57:VAL:CG2	2.29	0.80
7:6:21:DA:N1	8:7:51:G:C2	2.49	0.80
10:A:54:U:H3	10:A:58:A:N6	1.78	0.80
11:AA:858:GLY:N	11:AA:861:ALA:HB2	1.96	0.80
16:AG:365:ILE:HG21	16:AG:409:ARG:HH12	1.42	0.80
47:g:18:CYS:HB3	47:g:40:CYS:CB	2.12	0.80
24:J:162:ALA:CA	24:J:165:ARG:NH2	2.44	0.80
39:Y:72:THR:OG1	39:Y:73:PRO:HD2	1.81	0.80
41:a:2297:A:N1	41:a:2321:U:O4	2.14	0.80
54:n:125:ARG:O	54:n:127:ASN:ND2	2.14	0.80
12:AB:23:ALA:CB	12:AB:44:VAL:HB	2.10	0.80
12:AB:165:PHE:H	30:P:88:MET:CG	1.95	0.80
10:B:22:G:H2'	10:B:23:C:C6	2.16	0.80
18:D:1329:A:P	38:X:28:THR:HB	2.22	0.80
18:D:1397:C:OP1	18:D:1397:C:H2'	1.81	0.80
41:a:1019:U:H3	41:a:1142:A:H61	1.28	0.80
9:9:28:ALA:H	9:9:110:ALA:HA	1.44	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:128:PHE:CZ	12:AB:175:PHE:CB	2.64	0.80
16:AG:226:ALA:HA	16:AG:236:ILE:HG13	1.61	0.80
10:B:76:A:H1'	41:a:2494:G:P	2.20	0.80
41:a:2298:A:C4	41:a:2321:U:C5	2.70	0.80
16:AG:437:LEU:HD21	16:AG:456:LEU:HD13	0.81	0.80
10:A:18:G:N2	10:A:58:A:C5	2.50	0.80
12:AB:148:VAL:HB	12:AB:160:VAL:HG22	1.64	0.80
9:9:39:THR:HA	9:9:42:ARG:HD2	1.64	0.80
9:9:43:LYS:HD2	9:9:43:LYS:C	2.05	0.80
16:AG:133:HIS:HD1	16:AG:136:GLU:CD	1.90	0.80
16:AG:381:LEU:HA	16:AG:384:LEU:CD1	2.09	0.80
16:AG:451:ARG:NH1	16:AG:467:LEU:C	2.40	0.80
8:7:21:U:H5'	23:I:80:LYS:HE2	1.64	0.79
14:AE:37:GLU:O	14:AE:61:ILE:HD11	1.82	0.79
16:AG:451:ARG:NH2	16:AG:470:ILE:HG13	1.97	0.79
10:A:7:G:H4'	10:A:8:U:OP1	1.81	0.79
11:AA:618:GLN:HG3	14:AE:770:LEU:HD13	1.64	0.79
16:AG:363:LEU:CG	16:AG:410:ALA:N	2.45	0.79
16:AG:425:LEU:CA	16:AG:429:LYS:CG	2.60	0.79
16:AG:430:PRO:CG	16:AG:435:LEU:HD21	2.10	0.79
30:P:17:LEU:HD21	30:P:93:ALA:HB3	1.62	0.79
16:AG:440:VAL:CG2	16:AG:481:LEU:CD2	2.60	0.79
9:9:31:ARG:CD	41:a:1054:A:C5'	2.58	0.79
10:A:58:A:O2'	10:A:59:A:H3'	1.81	0.79
11:AA:855:PRO:CB	16:AG:109:THR:CG2	2.59	0.79
16:AG:447:LYS:O	16:AG:470:ILE:CD1	2.31	0.79
24:J:162:ALA:CB	24:J:165:ARG:NH2	2.44	0.79
41:a:585:G:N7	66:z:6:ARG:NH1	2.29	0.79
22:H:270:ILE:CG2	22:H:337:GLU:HB3	2.12	0.79
12:AB:140:PRO:CG	30:P:6:ILE:HD11	2.13	0.79
50:j:4:LEU:HD23	50:j:29:VAL:HG11	1.65	0.79
9:9:3:LEU:H	9:9:3:LEU:HD12	1.46	0.79
11:AA:853:ASP:CA	16:AG:105:ILE:CG2	2.59	0.79
14:AE:144:TYR:HE1	14:AE:162:GLU:OE2	1.64	0.79
16:AG:381:LEU:CA	16:AG:384:LEU:HD12	2.08	0.79
41:a:1406:U:O2'	41:a:1407:G:P	2.41	0.79
41:a:2189:U:OP1	41:a:2189:U:O4'	2.00	0.79
10:A:70:G:H2'	10:A:71:C:C5'	2.11	0.79
12:AB:114:ARG:HE	12:AB:114:ARG:C	1.91	0.79
24:J:162:ALA:HA	24:J:165:ARG:NH2	1.96	0.79
24:J:162:ALA:HB2	24:J:165:ARG:HH22	1.47	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:g:16:CYS:HB2	47:g:37:CYS:HB3	1.63	0.79
10:A:22:G:H2'	10:A:23:C:C6	2.16	0.78
10:A:76:A:H2'	41:a:2394:C:H42	1.47	0.78
12:AB:19:GLU:CG	12:AB:44:VAL:HG13	2.09	0.78
16:AG:434:LEU:CD2	16:AG:456:LEU:N	2.46	0.78
10:B:58:A:O2'	10:B:59:A:H3'	1.82	0.78
8:7:3:G:C5'	18:D:1500:A:N6	2.42	0.78
9:9:78:GLY:N	9:9:79:PRO:HD2	1.97	0.78
10:B:5:G:H2'	10:B:6:G:H5'	1.66	0.78
21:G:35:ARG:HD2	22:H:14:LYS:HD3	1.66	0.78
13:AD:309:SER:CB	16:AG:40:GLU:OE1	2.31	0.78
14:AE:1075:ARG:NH2	14:AE:1168:GLU:OE2	2.17	0.78
16:AG:355:ALA:HB1	16:AG:382:GLU:CD	1.94	0.78
10:B:18:G:N2	10:B:58:A:C5	2.51	0.78
12:AB:64:PHE:HA	12:AB:66:PRO:HD3	1.64	0.78
16:AG:284:VAL:HG12	16:AG:296:ILE:HD13	1.66	0.78
10:A:15:G:N1	10:A:20:U:O2	2.17	0.78
12:AB:165:PHE:CA	30:P:88:MET:HA	2.14	0.78
10:A:18:G:C5	10:A:57:A:C6	2.72	0.78
11:AA:900:LYS:HD2	16:AG:11:ALA:HB1	1.65	0.78
16:AG:189:GLU:HB3	16:AG:194:GLN:HG3	1.64	0.78
18:D:1358:U:C4	18:D:1363:A:N1	2.52	0.77
21:G:16:PHE:CZ	22:H:41:GLY:O	2.36	0.77
22:H:19:ARG:HD3	22:H:73:ASP:CG	2.09	0.77
16:AG:354:ALA:HA	16:AG:357:ASP:CB	2.14	0.77
39:Y:32:VAL:HG13	39:Y:60:VAL:HG21	1.65	0.77
16:AG:402:THR:O	16:AG:405:ALA:HB3	1.84	0.77
10:B:15:G:N1	10:B:20:U:O2	2.17	0.77
10:B:18:G:C5	10:B:57:A:C6	2.72	0.77
11:AA:894:GLN:NE2	11:AA:894:GLN:O	2.17	0.77
14:AE:90:VAL:HG13	14:AE:90:VAL:O	1.82	0.77
16:AG:434:LEU:HD11	16:AG:455:THR:O	1.85	0.77
41:a:1406:U:O2'	41:a:1407:G:O5'	2.01	0.77
9:9:11:ILE:HD11	9:9:62:ARG:HA	1.65	0.77
11:AA:888:THR:HB	11:AA:889:PRO:HD2	1.65	0.77
11:AA:894:GLN:HE21	11:AA:894:GLN:H	1.32	0.77
14:AE:186:GLN:HG3	14:AE:238:ILE:HG13	1.65	0.77
10:B:68:C:C3'	10:B:69:C:H5"	2.15	0.77
41:a:2756:U:N3	41:a:2758:A:C6	2.53	0.77
12:AB:135:ARG:HG2	12:AB:135:ARG:HH11	1.50	0.77
16:AG:235:LYS:HD3	16:AG:327:LEU:HG	1.65	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:a:2756:U:N3	41:a:2758:A:N6	2.32	0.77
10:A:33:U:O3'	27:M:84:THR:OG1	2.02	0.77
12:AB:165:PHE:N	30:P:88:MET:CG	2.41	0.77
14:AE:123:ARG:HG3	14:AE:1337:VAL:HG11	1.67	0.77
16:AG:287:ALA:HB1	16:AG:331:LEU:HD12	1.62	0.77
13:AD:308:ALA:O	16:AG:96:GLN:OE1	1.96	0.77
12:AB:44:VAL:CG2	12:AB:69:VAL:HG13	2.15	0.77
22:H:305:HIS:CD2	22:H:306:VAL:N	2.53	0.77
12:AB:43:MET:HG2	12:AB:115:LEU:HD22	1.66	0.76
12:AB:64:PHE:CB	14:AE:285:LEU:HD21	2.15	0.76
12:AB:64:PHE:HB2	14:AE:285:LEU:CD2	2.15	0.76
12:AB:165:PHE:CE1	30:P:91:ASP:CA	2.68	0.76
16:AG:354:ALA:O	16:AG:356:ILE:N	2.18	0.76
16:AG:354:ALA:C	16:AG:356:ILE:N	2.43	0.76
9:9:60:LEU:HD23	9:9:64:VAL:HG21	1.67	0.76
10:A:5:G:H2'	10:A:6:G:H5'	1.65	0.76
10:A:68:C:C3'	10:A:69:C:H5"	2.15	0.76
12:AB:66:PRO:HG2	14:AE:281:ARG:HH22	1.48	0.76
9:9:31:ARG:NE	41:a:1054:A:C4'	2.48	0.76
12:AB:155:LYS:HE2	18:D:1277:C:P	2.26	0.76
16:AG:307:ILE:HB	16:AG:338:VAL:HA	1.66	0.76
16:AG:412:ASN:O	16:AG:416:THR:HG23	1.84	0.76
16:AG:233:ARG:HB2	16:AG:327:LEU:HD23	1.66	0.76
16:AG:283:PHE:CZ	16:AG:331:LEU:O	2.39	0.76
16:AG:425:LEU:HD23	16:AG:429:LYS:NZ	1.99	0.76
16:AG:451:ARG:CZ	16:AG:470:ILE:HG13	2.16	0.76
17:C:44:ILE:CD1	22:H:339:ARG:CG	2.62	0.76
25:K:137:VAL:O	25:K:140:THR:OG1	2.04	0.76
7:6:15:DC:C4	7:6:16:DC:N4	2.53	0.76
16:AG:248:VAL:HG22	16:AG:273:ILE:HG22	1.68	0.76
16:AG:425:LEU:CB	16:AG:429:LYS:HE3	2.16	0.76
16:AG:228:ARG:HD2	16:AG:236:ILE:HB	1.68	0.76
4:3:36:VAL:HG11	4:3:39:ILE:HD12	1.68	0.76
11:AA:903:ARG:CB	11:AA:903:ARG:HH11	1.99	0.76
12:AB:140:PRO:HB2	30:P:84:VAL:CG2	2.16	0.76
16:AG:240:THR:CG2	16:AG:247:PRO:HG3	2.16	0.76
16:AG:371:THR:O	16:AG:375:GLU:HG3	1.86	0.76
16:AG:434:LEU:CD2	16:AG:455:THR:C	2.58	0.76
9:9:52:MET:HG3	9:9:95:LEU:HD11	1.68	0.75
16:AG:393:LEU:CD2	16:AG:398:LEU:CG	2.58	0.75
22:H:109:THR:HA	22:H:153:GLU:HA	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:155:LYS:CE	18:D:1277:C:O5'	2.34	0.75
14:AE:202:ARG:HG2	14:AE:202:ARG:NH1	1.99	0.75
41:a:1021:A:H61	41:a:1141:U:H3	1.29	0.75
9:9:27:VAL:HG23	9:9:83:ALA:HB3	1.67	0.75
9:9:97:LYS:HD3	9:9:127:ALA:HA	1.68	0.75
11:AA:903:ARG:NH1	11:AA:903:ARG:O	2.20	0.75
16:AG:201:LYS:HD2	16:AG:201:LYS:N	2.01	0.75
18:D:197:A:N6	18:D:221:C:H4'	2.01	0.75
11:AA:855:PRO:HB3	16:AG:109:THR:HG21	1.67	0.75
39:Y:74:PRO:HG2	39:Y:77:VAL:HB	1.67	0.75
12:AB:23:ALA:CB	12:AB:44:VAL:CG2	2.59	0.75
12:AB:65:PHE:CD1	14:AE:285:LEU:HD23	2.21	0.75
11:AA:853:ASP:OD2	16:AG:103:ASP:C	2.29	0.75
11:AA:857:VAL:CG1	11:AA:862:LEU:CD1	2.65	0.75
16:AG:131:ARG:HA	16:AG:186:VAL:HG11	1.68	0.75
16:AG:365:ILE:HG23	16:AG:409:ARG:HH11	1.51	0.75
10:A:41:C:H1'	27:M:143:ARG:HH12	1.52	0.75
12:AB:165:PHE:CZ	30:P:91:ASP:CA	2.69	0.75
21:G:35:ARG:HG3	22:H:10:GLU:OE2	1.87	0.75
41:a:1021:A:N1	41:a:1141:U:C4	2.55	0.75
41:a:2298:A:C4	41:a:2321:U:H5	2.04	0.75
64:x:31:THR:O	64:x:102:ARG:NH1	2.19	0.75
16:AG:354:ALA:O	16:AG:355:ALA:C	2.26	0.74
10:B:18:G:H1'	10:B:58:A:C2	2.23	0.74
22:H:131:LEU:CB	22:H:166:VAL:C	2.60	0.74
10:A:18:G:H1'	10:A:58:A:C2	2.23	0.74
10:A:70:G:C3'	10:A:71:C:H5"	2.18	0.74
22:H:109:THR:CA	22:H:153:GLU:HA	2.18	0.74
47:g:18:CYS:CB	47:g:40:CYS:HB3	2.16	0.74
7:6:18:DC:N3	8:7:53:G:N2	2.31	0.74
14:AE:110:PRO:HG2	14:AE:183:GLU:HG3	1.68	0.74
16:AG:413:ALA:O	16:AG:416:THR:OG1	2.05	0.74
39:Y:85:ILE:H	39:Y:85:ILE:HD12	1.52	0.74
12:AB:139:GLY:HA3	30:P:102:LEU:HD11	1.67	0.74
16:AG:62:TRP:HB3	16:AG:75:ILE:HD11	1.69	0.74
11:AA:864:LYS:HE3	11:AA:877:VAL:HG12	1.70	0.74
16:AG:385:ALA:HB3	16:AG:411:LYS:HE2	1.68	0.74
16:AG:393:LEU:C	16:AG:398:LEU:HD23	2.13	0.74
10:B:76:A:H2'	10:B:76:A:N3	2.02	0.74
22:H:304:VAL:HG12	22:H:309:MET:SD	2.28	0.74
12:AB:155:LYS:CB	18:D:1277:C:OP2	2.33	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:44:ILE:HD12	14:AE:252:LEU:CD2	2.18	0.74
16:AG:354:ALA:C	16:AG:356:ILE:H	1.93	0.74
18:D:1228:C:OP1	38:X:107:ARG:NH1	2.21	0.74
9:9:78:GLY:N	9:9:79:PRO:CD	2.50	0.74
16:AG:313:ASN:N	16:AG:313:ASN:OD1	2.19	0.74
16:AG:429:LYS:H	16:AG:429:LYS:HD2	1.52	0.74
10:B:18:G:O2'	10:B:60:U:C2	2.41	0.74
8:7:50:U:H4'	14:AE:322:ARG:CD	2.18	0.74
10:A:41:C:O4'	27:M:143:ARG:NH1	2.20	0.74
12:AB:165:PHE:CZ	30:P:91:ASP:HB2	2.23	0.74
16:AG:219:GLU:HA	16:AG:219:GLU:OE2	1.87	0.74
11:AA:853:ASP:OD2	16:AG:103:ASP:CB	2.36	0.73
16:AG:365:ILE:CG2	16:AG:409:ARG:HH11	2.01	0.73
10:B:70:G:C3'	10:B:71:C:H5"	2.17	0.73
21:G:19:GLN:CG	22:H:76:GLU:HB2	2.18	0.73
11:AA:853:ASP:OD1	16:AG:105:ILE:CG2	2.20	0.73
12:AB:103:ILE:HD12	12:AB:107:GLU:OE2	1.87	0.73
16:AG:363:LEU:CD1	16:AG:410:ALA:HB2	2.17	0.73
16:AG:365:ILE:HG23	16:AG:409:ARG:NH1	2.02	0.73
16:AG:486:ARG:O	16:AG:490:TRP:CD1	2.41	0.73
22:H:110:GLY:CA	22:H:153:GLU:O	2.36	0.73
12:AB:140:PRO:HG3	30:P:6:ILE:HD11	1.69	0.73
10:B:6:G:O2'	10:B:7:G:O5'	2.05	0.73
30:P:102:LEU:HG	30:P:102:LEU:O	1.89	0.73
10:A:32:C:C1'	27:M:144:MET:HE1	2.16	0.73
14:AE:120:LEU:O	14:AE:1330:ARG:NH1	2.21	0.73
14:AE:211:GLU:HG2	14:AE:215:LYS:HE3	1.70	0.73
22:H:19:ARG:HB2	22:H:73:ASP:OD2	1.88	0.73
14:AE:105:ILE:HD12	14:AE:242:LEU:HD22	1.71	0.73
12:AB:138:ASP:HB3	12:AB:177:GLN:CA	2.18	0.73
16:AG:425:LEU:O	16:AG:429:LYS:HE3	1.87	0.73
16:AG:442:ARG:HB3	16:AG:446:PHE:HE2	1.53	0.73
10:B:70:G:H2'	10:B:71:C:C5'	2.11	0.73
18:D:517:G:O2'	18:D:530:G:H4'	1.88	0.73
39:Y:36:GLU:OE1	39:Y:36:GLU:HA	1.87	0.73
6:5:115:DA:OP1	14:AE:1148:ARG:NE	2.21	0.73
17:C:44:ILE:HD13	22:H:339:ARG:HG3	1.69	0.73
14:AE:157:GLN:OE1	14:AE:157:GLN:HA	1.89	0.73
14:AE:210:SER:HB3	14:AE:213:LYS:HB2	1.70	0.73
10:A:6:G:O2'	10:A:7:G:O5'	2.05	0.73
12:AB:128:PHE:HZ	12:AB:175:PHE:CA	2.02	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:285:ILE:HG13	16:AG:293:VAL:HG13	1.71	0.73
41:a:67:U:C4	41:a:74:A:N6	2.57	0.73
16:AG:198:THR:HB	16:AG:201:LYS:HD3	1.70	0.73
10:A:18:G:O2'	10:A:60:U:C2	2.41	0.72
8:7:9:U:N3	18:D:1196:A:C8	2.57	0.72
12:AB:167:ARG:HG2	12:AB:167:ARG:NH2	2.04	0.72
14:AE:1143:ASP:OD1	14:AE:1148:ARG:NH1	2.21	0.72
10:B:76:A:H1'	41:a:2494:G:OP1	1.88	0.72
10:A:33:U:H5"	27:M:84:THR:CG2	2.18	0.72
14:AE:107:LEU:HD11	14:AE:242:LEU:HB2	1.70	0.72
22:H:267:TRP:CE3	22:H:340:ARG:CG	2.72	0.72
12:AB:133:MET:HE2	12:AB:133:MET:N	2.05	0.72
14:AE:142:GLU:HG3	14:AE:142:GLU:O	1.89	0.72
16:AG:365:ILE:HD13	16:AG:406:LEU:HD21	1.70	0.72
17:C:12:ARG:HB2	22:H:264:GLU:CB	2.19	0.72
41:a:1839:G:C1'	41:a:1927:A:C1'	2.67	0.72
41:a:1913:A:OP2	41:a:1913:A:H3'	1.89	0.72
9:9:77:VAL:HG12	9:9:82:ILE:HG21	1.71	0.72
16:AG:127:VAL:HG22	16:AG:192:GLY:C	2.15	0.72
16:AG:223:ILE:O	16:AG:223:ILE:HD13	1.89	0.72
10:B:46:G:H1'	10:B:47:U:C5	2.25	0.72
12:AB:164:ILE:HD11	12:AB:169:THR:HB	1.72	0.72
16:AG:451:ARG:HE	16:AG:470:ILE:HG13	1.51	0.72
22:H:70:VAL:HA	22:H:85:SER:CB	2.20	0.72
14:AE:68:TYR:C	14:AE:75:TYR:CE2	2.65	0.72
29:O:84:THR:HG21	29:O:103:PHE:HB3	1.71	0.72
10:A:72:A:C3'	10:A:73:A:H5"	2.20	0.72
11:AA:854:ILE:CG1	11:AA:855:PRO:HD2	2.19	0.72
16:AG:434:LEU:CD2	16:AG:459:LEU:CD1	2.54	0.72
6:5:100:DA:OP1	12:AB:16:SER:C	2.33	0.72
16:AG:434:LEU:HG	16:AG:455:THR:C	2.14	0.72
7:6:21:DA:C6	8:7:51:G:N2	2.58	0.72
9:9:18:VAL:HA	9:9:86:MET:HE2	1.71	0.72
14:AE:220:ARG:HG2	14:AE:220:ARG:HH11	1.55	0.72
32:R:86:ARG:HG3	32:R:86:ARG:O	1.89	0.72
11:AA:901:LEU:HD11	16:AG:8:VAL:HG13	0.72	0.71
12:AB:44:VAL:HG22	12:AB:69:VAL:CG1	2.20	0.71
16:AG:393:LEU:HD23	16:AG:398:LEU:CD1	2.19	0.71
10:B:72:A:C3'	10:B:73:A:H5"	2.20	0.71
47:g:18:CYS:CB	47:g:40:CYS:CB	2.68	0.71
8:7:21:U:P	23:I:80:LYS:HA	2.29	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:853:ASP:CA	16:AG:105:ILE:HG23	2.21	0.71
16:AG:279:ASN:CB	16:AG:280:PRO:CD	2.66	0.71
16:AG:434:LEU:CA	16:AG:456:LEU:CD2	2.58	0.71
18:D:827:U:H3	18:D:872:A:N6	1.87	0.71
22:H:267:TRP:CE3	22:H:340:ARG:HG2	2.25	0.71
38:X:96:PRO:HG2	38:X:102:THR:CG2	2.21	0.71
10:A:18:G:C5	10:A:57:A:N6	2.59	0.71
16:AG:352:ALA:O	16:AG:356:ILE:HG22	1.90	0.71
21:G:16:PHE:CB	22:H:43:LYS:HA	2.20	0.71
41:a:2314:A:C1'	54:n:155:THR:HG21	2.21	0.71
16:AG:262:VAL:HA	16:AG:265:GLU:HB2	1.72	0.71
18:D:1308:U:O5'	38:X:98:ARG:HG3	1.91	0.71
22:H:86:ARG:O	22:H:89:ALA:HB3	1.90	0.71
9:9:3:LEU:HD12	9:9:3:LEU:N	2.05	0.71
10:A:46:G:H1'	10:A:47:U:C5	2.25	0.71
14:AE:44:ILE:HD12	14:AE:252:LEU:HD21	1.71	0.71
16:AG:422:GLU:CB	16:AG:426:GLY:HA3	2.21	0.71
12:AB:140:PRO:HB2	30:P:84:VAL:HG21	1.71	0.71
12:AB:164:ILE:HA	30:P:88:MET:SD	2.30	0.71
18:D:1227:A:H5'	38:X:110:LYS:HZ1	1.53	0.71
16:AG:220:VAL:O	16:AG:240:THR:HG22	1.90	0.71
16:AG:285:ILE:CG1	16:AG:293:VAL:CG1	2.54	0.71
16:AG:389:MET:O	16:AG:404:GLU:OE2	2.09	0.71
41:a:742:A:H2'	41:a:743:A:C8	2.26	0.71
16:AG:362:TYR:CA	16:AG:413:ALA:CB	2.69	0.70
10:B:76:A:H2'	41:a:2493:U:H5"	1.72	0.70
16:AG:297:VAL:HG23	16:AG:306:ASP:HB2	1.71	0.70
16:AG:403:VAL:HG22	16:AG:406:LEU:HD12	1.72	0.70
10:B:18:G:C5	10:B:57:A:N6	2.59	0.70
16:AG:282:GLN:NE2	16:AG:282:GLN:HA	2.05	0.70
16:AG:433:ASP:C	16:AG:456:LEU:CG	2.64	0.70
22:H:70:VAL:HA	22:H:85:SER:CA	2.22	0.70
18:D:1308:U:C3'	38:X:98:ARG:HH21	1.92	0.70
8:7:9:U:O4	18:D:1196:A:N9	2.24	0.70
16:AG:434:LEU:HD21	16:AG:456:LEU:N	2.03	0.70
18:D:915:A:N6	18:D:916:U:C4	2.60	0.70
22:H:19:ARG:HD3	22:H:73:ASP:OD1	1.92	0.70
16:AG:353:HIS:HA	16:AG:356:ILE:CG2	2.21	0.70
10:A:16:C:O2	41:a:2181:U:C5'	2.40	0.70
10:A:32:C:C1'	27:M:144:MET:CE	2.69	0.70
10:A:41:C:C1'	27:M:143:ARG:NH1	2.55	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:167:MET:HE1	16:AG:199:ARG:HG3	1.72	0.70
16:AG:279:ASN:CB	16:AG:280:PRO:HD2	2.22	0.70
22:H:267:TRP:CZ2	22:H:340:ARG:CG	2.68	0.70
16:AG:422:GLU:CA	16:AG:426:GLY:CA	2.65	0.70
10:A:15:G:H2'	10:A:15:G:N3	2.06	0.70
18:D:972:C:O2'	30:P:57:VAL:HG23	1.92	0.70
39:Y:21:PRO:CB	39:Y:22:PRO:HD3	2.22	0.70
10:A:11:A:H2'	10:A:12:G:O4'	1.92	0.69
11:AA:849:GLU:HG2	16:AG:104:ARG:HH11	0.66	0.69
14:AE:54:ASP:OD1	14:AE:54:ASP:N	2.24	0.69
16:AG:434:LEU:CA	16:AG:456:LEU:HD21	2.12	0.69
22:H:19:ARG:HD3	22:H:73:ASP:OD2	1.92	0.69
11:AA:65:ASN:HB3	11:AA:105:TYR:HB2	1.73	0.69
12:AB:96:THR:HB	14:AE:162:GLU:CG	2.23	0.69
10:B:11:A:H2'	10:B:12:G:O4'	1.92	0.69
11:AA:855:PRO:HB3	16:AG:109:THR:HG23	1.73	0.69
18:D:1309:G:H8	38:X:98:ARG:NH2	1.89	0.69
1:0:80:ARG:NH2	41:a:572:A:OP2	2.25	0.69
9:9:58:THR:HG21	9:9:81:LEU:HG	1.74	0.69
14:AE:39:LYS:O	14:AE:273:ILE:CG2	2.41	0.69
16:AG:434:LEU:HD11	16:AG:455:THR:C	2.17	0.69
8:7:50:U:H4'	14:AE:322:ARG:HD2	1.73	0.69
10:A:32:C:C4'	27:M:144:MET:CE	2.66	0.69
11:AA:905:ILE:HD12	16:AG:8:VAL:HG11	1.74	0.69
11:AA:1332:SER:O	14:AE:243:PRO:HG2	1.93	0.69
16:AG:60:ARG:HG3	16:AG:98:GLU:HG3	1.74	0.69
16:AG:171:GLU:OE1	16:AG:267:GLY:HA3	1.92	0.69
16:AG:321:ASN:OD1	16:AG:321:ASN:N	2.25	0.69
16:AG:393:LEU:CD2	16:AG:398:LEU:HD13	2.19	0.69
16:AG:425:LEU:CB	16:AG:429:LYS:CE	2.71	0.69
21:G:19:GLN:CD	22:H:76:GLU:HB2	2.08	0.69
22:H:117:LYS:CB	22:H:279:LYS:O	2.41	0.69
41:a:1596:A:H2'	41:a:1597:A:C8	2.28	0.69
41:a:1839:G:H1'	41:a:1927:A:N9	2.03	0.69
12:AB:95:GLY:O	14:AE:162:GLU:HG3	1.92	0.69
16:AG:235:LYS:HZ2	16:AG:331:LEU:HG	1.58	0.69
16:AG:355:ALA:C	16:AG:380:THR:HG21	2.18	0.69
18:D:563:A:N1	18:D:884:U:C4	2.61	0.69
41:a:1021:A:H3'	41:a:1021:A:N3	2.07	0.69
10:B:15:G:H2'	10:B:15:G:N3	2.06	0.69
41:a:927:A:H2'	41:a:928:A:C8	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:a:2310:C:O2'	54:n:74:VAL:CG1	2.40	0.69
18:D:13:U:O4	18:D:21:G:C2	2.46	0.68
9:9:118:ILE:HB	9:9:119:PRO:HD3	1.75	0.68
14:AE:128:LEU:HD11	14:AE:189:LEU:HG	1.74	0.68
14:AE:161:THR:HG22	14:AE:164:GLN:HB2	1.75	0.68
16:AG:239:LYS:HG3	16:AG:276:TRP:HB3	1.75	0.68
16:AG:285:ILE:CD1	16:AG:293:VAL:HG11	2.22	0.68
48:h:146:MET:HE3	48:h:154:LEU:HD21	1.74	0.68
12:AB:149:GLU:N	12:AB:149:GLU:OE1	2.27	0.68
12:AB:167:ARG:HH11	23:I:62:LYS:CB	2.06	0.68
16:AG:462:GLN:OE1	16:AG:467:LEU:HD21	1.93	0.68
41:a:1839:G:C4	41:a:1927:A:C4	2.81	0.68
7:6:8:DC:C6	7:6:9:DT:H72	2.28	0.68
14:AE:832:LYS:C	14:AE:1242:ARG:HH12	2.01	0.68
16:AG:266:LEU:H	16:AG:266:LEU:CD2	2.06	0.68
16:AG:433:ASP:O	16:AG:437:LEU:HG	1.93	0.68
41:a:2310:C:O2'	54:n:74:VAL:HG12	1.94	0.68
13:AC:232:VAL:C	13:AD:221:ALA:HB1	2.15	0.68
14:AE:94:GLN:HB2	14:AE:97:VAL:HG23	1.76	0.68
16:AG:355:ALA:CB	16:AG:382:GLU:OE1	2.18	0.68
16:AG:440:VAL:HG23	16:AG:481:LEU:HD22	1.76	0.68
22:H:110:GLY:HA3	22:H:153:GLU:O	1.93	0.68
38:X:96:PRO:CG	38:X:102:THR:CG2	2.71	0.68
9:9:50:VAL:HG13	39:Y:119:ALA:CB	2.22	0.68
11:AA:902:LEU:O	11:AA:902:LEU:HD22	1.94	0.68
11:AA:1268:GLN:HE22	14:AE:352:ARG:HD2	1.57	0.68
14:AE:117:LEU:HD12	14:AE:117:LEU:O	1.94	0.68
14:AE:141:PHE:CD2	14:AE:293:ARG:O	2.47	0.68
16:AG:168:LEU:HB2	16:AG:171:GLU:HB2	1.76	0.68
41:a:2756:U:C4	41:a:2758:A:N6	2.61	0.68
11:AA:902:LEU:O	11:AA:902:LEU:HD13	1.94	0.68
12:AB:155:LYS:CE	18:D:1277:C:H3'	2.23	0.68
16:AG:453:VAL:CG2	16:AG:462:GLN:NE2	2.56	0.68
7:6:21:DA:C2	8:7:51:G:N2	2.61	0.68
12:AB:19:GLU:C	12:AB:44:VAL:CG1	2.66	0.68
16:AG:102:PHE:HB2	16:AG:106:THR:HG21	1.75	0.68
16:AG:107:THR:HA	16:AG:110:ALA:HB3	1.74	0.68
16:AG:323:GLN:HA	16:AG:323:GLN:HE21	1.59	0.68
10:A:5:G:H2'	10:A:6:G:C5'	2.24	0.68
13:AD:48:LEU:HB2	13:AD:183:ILE:HD11	1.76	0.68
14:AE:395:LYS:HZ2	14:AE:399:LYS:CD	2.06	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:228:ARG:HA	16:AG:327:LEU:CD1	2.22	0.68
16:AG:429:LYS:CD	16:AG:429:LYS:H	2.05	0.68
41:a:1153:C:OP1	66:z:92:ARG:NH1	2.27	0.68
41:a:1779:U:H5	41:a:1784:A:N7	1.92	0.68
41:a:1839:G:C8	41:a:1927:A:C1'	2.74	0.68
9:9:31:ARG:HD2	41:a:1054:A:C5'	2.22	0.67
10:A:19:G:N2	41:a:2112:G:C8	2.62	0.67
16:AG:171:GLU:OE2	16:AG:267:GLY:CA	2.41	0.67
16:AG:253:GLY:HA3	16:AG:258:ARG:HD2	1.76	0.67
39:Y:14:ALA:HB2	39:Y:54:ILE:HD12	1.76	0.67
12:AB:95:GLY:O	14:AE:162:GLU:CG	2.42	0.67
12:AB:123:ARG:HB3	12:AB:127:LEU:HB2	1.76	0.67
16:AG:453:VAL:HG13	16:AG:458:ASP:HB3	1.77	0.67
9:9:73:LYS:HB2	9:9:117:LEU:HD21	1.75	0.67
12:AB:128:PHE:CE1	12:AB:175:PHE:HD1	2.12	0.67
16:AG:207:GLU:HA	16:AG:210:ARG:HB2	1.76	0.67
22:H:267:TRP:CD2	22:H:340:ARG:CG	2.76	0.67
23:I:75:ILE:O	23:I:75:ILE:HD13	1.94	0.67
33:S:47:LYS:O	33:S:50:THR:OG1	2.12	0.67
11:AA:900:LYS:CD	16:AG:11:ALA:HB1	2.25	0.67
12:AB:165:PHE:HA	30:P:88:MET:C	2.20	0.67
16:AG:298:VAL:HA	16:AG:303:HIS:HD1	1.58	0.67
11:AA:858:GLY:C	11:AA:861:ALA:H	2.03	0.67
14:AE:984:LEU:HB3	14:AE:993:GLU:HB2	1.77	0.67
16:AG:448:LEU:CD2	16:AG:473:LEU:HD12	2.24	0.67
9:9:43:LYS:HD2	9:9:43:LYS:O	1.94	0.67
12:AB:140:PRO:CB	30:P:84:VAL:CG2	2.73	0.67
9:9:50:VAL:CG2	39:Y:119:ALA:CB	2.59	0.67
16:AG:353:HIS:C	16:AG:357:ASP:H	2.01	0.67
36:V:25:ILE:HD11	36:V:61:ILE:HD11	1.77	0.67
9:9:11:ILE:CD1	9:9:62:ARG:HD3	2.24	0.67
14:AE:108:ALA:CB	14:AE:279:LEU:HD22	2.25	0.67
10:B:5:G:H2'	10:B:6:G:C5'	2.24	0.67
10:B:21:A:H4'	10:B:21:A:OP1	1.95	0.67
22:H:110:GLY:N	22:H:153:GLU:C	2.53	0.67
22:H:110:GLY:H	22:H:153:GLU:CA	2.08	0.67
16:AG:363:LEU:CD2	16:AG:409:ARG:CA	2.71	0.67
39:Y:116:MET:HB3	39:Y:124:MET:HG2	1.76	0.67
56:p:24:ILE:HD13	56:p:72:LEU:HD21	1.77	0.67
14:AE:108:ALA:HB3	14:AE:279:LEU:HD22	1.77	0.66
18:D:37:U:H3	18:D:397:A:N6	1.90	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:X:96:PRO:CG	38:X:102:THR:HG22	2.25	0.66
9:9:67:THR:N	9:9:68:PRO:CD	2.57	0.66
41:a:1920:C:O5'	41:a:1920:C:H6	1.77	0.66
16:AG:123:ARG:HG2	16:AG:191:ARG:O	1.96	0.66
16:AG:385:ALA:HB2	16:AG:411:LYS:HE3	1.70	0.66
12:AB:165:PHE:H	30:P:88:MET:CB	2.09	0.66
41:a:1923:U:H2'	41:a:1923:U:OP2	1.96	0.66
8:7:15:U:OP1	23:I:136:ARG:NH2	2.28	0.66
9:9:50:VAL:CG1	39:Y:119:ALA:HB3	2.26	0.66
11:AA:853:ASP:HA	16:AG:105:ILE:CG2	2.26	0.66
16:AG:284:VAL:CG1	16:AG:296:ILE:HD13	2.25	0.66
10:B:56:C:H5'	54:n:80:ARG:NH2	2.11	0.66
18:D:1358:U:O4	18:D:1363:A:C2	2.47	0.66
41:a:2013:A:N6	41:a:2613:U:N3	2.33	0.66
16:AG:232:SER:HB2	16:AG:323:GLN:OE1	1.96	0.66
39:Y:58:ILE:HD13	39:Y:58:ILE:N	2.10	0.66
16:AG:355:ALA:CB	16:AG:382:GLU:CG	2.54	0.66
16:AG:380:THR:O	16:AG:384:LEU:HD12	1.95	0.66
10:B:66:C:H5'	10:B:66:C:H6	1.60	0.66
22:H:70:VAL:HA	22:H:85:SER:HA	1.77	0.66
59:s:114:LEU:HG	59:s:118:MET:HE3	1.78	0.66
11:AA:894:GLN:HE21	11:AA:894:GLN:N	1.94	0.66
12:AB:165:PHE:HD1	30:P:88:MET:O	1.78	0.66
22:H:162:LYS:CB	22:H:298:GLU:OE1	2.44	0.66
12:AB:165:PHE:HZ	30:P:91:ASP:HB2	1.58	0.66
38:X:96:PRO:HG3	38:X:102:THR:HG22	1.78	0.66
8:7:9:U:O4	18:D:1196:A:O4'	2.13	0.66
12:AB:133:MET:H	12:AB:133:MET:CE	2.08	0.66
14:AE:1355:ARG:NH1	14:AE:1369:ARG:HH12	1.93	0.66
16:AG:235:LYS:NZ	16:AG:331:LEU:HG	2.11	0.66
16:AG:308:ALA:HB2	16:AG:344:LEU:HD11	1.77	0.66
16:AG:353:HIS:HA	16:AG:356:ILE:HG23	1.78	0.66
16:AG:363:LEU:CD2	16:AG:409:ARG:CB	2.62	0.66
16:AG:393:LEU:O	16:AG:398:LEU:HD23	1.95	0.66
10:B:37:A:H3'	10:B:37:A:OP2	1.96	0.66
22:H:270:ILE:HG23	22:H:337:GLU:HB3	1.77	0.66
16:AG:183:LEU:HA	16:AG:197:VAL:HA	1.78	0.65
18:D:1308:U:H5"	38:X:98:ARG:HG2	1.78	0.65
9:9:61:ARG:NH1	41:a:1047:G:N7	2.44	0.65
14:AE:193:ASP:HB3	14:AE:196:GLN:HB2	1.78	0.65
12:AB:163:SER:O	30:P:88:MET:SD	2.54	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:142:THR:HG21	40:Z:7:ILE:CD1	2.26	0.65
16:AG:422:GLU:CA	16:AG:426:GLY:H	2.08	0.65
18:D:197:A:C6	18:D:221:C:C4'	2.80	0.65
22:H:267:TRP:CE2	22:H:340:ARG:CG	2.72	0.65
10:A:6:G:HO2'	10:A:7:G:H8	1.44	0.65
12:AB:128:PHE:CZ	12:AB:175:PHE:O	2.49	0.65
12:AB:141:PHE:HE2	12:AB:171:VAL:HG11	1.57	0.65
14:AE:978:ARG:HG2	14:AE:1197:ASN:HD21	1.60	0.65
16:AG:361:LYS:CD	16:AG:417:ILE:CG1	2.75	0.65
10:A:3:C:H2'	10:A:4:G:H8	1.62	0.65
10:A:66:C:H6	10:A:66:C:H5'	1.60	0.65
14:AE:68:TYR:HB3	14:AE:75:TYR:CE2	2.32	0.65
14:AE:1037:PHE:HB3	14:AE:1040:MET:HB2	1.77	0.65
16:AG:447:LYS:O	16:AG:470:ILE:HD13	1.95	0.65
18:D:827:U:N3	18:D:872:A:N6	2.45	0.65
10:B:76:A:H1'	41:a:2493:U:O3'	1.97	0.65
9:9:78:GLY:H	9:9:79:PRO:CD	2.10	0.65
10:A:21:A:H4'	10:A:21:A:OP1	1.95	0.65
12:AB:161:SER:HA	12:AB:170:PRO:HA	1.79	0.65
14:AE:141:PHE:HD2	14:AE:293:ARG:O	1.80	0.65
16:AG:227:ALA:HB3	16:AG:331:LEU:HA	1.78	0.65
41:a:1082:U:N3	41:a:1086:A:N6	2.45	0.65
7:6:16:DC:H1'	14:AE:426:ALA:HB1	1.77	0.65
9:9:11:ILE:HG13	9:9:65:GLU:HB3	1.79	0.65
14:AE:111:THR:CG2	14:AE:300:GLN:CD	2.66	0.65
16:AG:349:GLN:C	16:AG:351:GLU:H	2.05	0.65
16:AG:393:LEU:HD23	16:AG:398:LEU:HD13	1.78	0.65
22:H:52:GLN:O	22:H:53:PHE:CD1	2.50	0.65
56:p:121:ILE:HD12	56:p:141:ILE:HG22	1.79	0.65
10:A:18:G:C8	10:A:57:A:C6	2.85	0.64
10:A:56:C:C5	41:a:2168:G:C6	2.84	0.64
10:B:75:C:OP1	41:a:2602:A:N9	2.30	0.64
8:7:8:U:OP2	18:D:1397:C:N3	2.30	0.64
10:A:41:C:C4'	27:M:143:ARG:NH1	2.61	0.64
14:AE:245:LEU:HG	14:AE:246:PRO:HD2	1.79	0.64
16:AG:133:HIS:ND1	16:AG:136:GLU:CD	2.55	0.64
10:B:3:C:H2'	10:B:4:G:H8	1.62	0.64
39:Y:116:MET:HE2	39:Y:116:MET:HA	1.79	0.64
9:9:29:ASP:HB2	9:9:56:ARG:HD3	1.79	0.64
9:9:57:ASN:CG	9:9:62:ARG:CG	2.68	0.64
12:AB:152:ASP:HB2	12:AB:157:ARG:HB3	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:67:ASP:OD1	14:AE:95:THR:OG1	2.15	0.64
16:AG:226:ALA:O	16:AG:228:ARG:HD3	1.97	0.64
16:AG:425:LEU:HG	16:AG:429:LYS:HE2	1.66	0.64
21:G:18:HIS:HA	22:H:43:LYS:CD	2.28	0.64
11:AA:898:GLU:HA	11:AA:898:GLU:OE2	1.96	0.64
55:o:26:HIS:CE1	55:o:48:ALA:HB2	2.32	0.64
2:1:36:LEU:HD13	2:1:48:LYS:HA	1.80	0.64
11:AA:900:LYS:HZ1	16:AG:13:SER:N	1.95	0.64
11:AA:913:VAL:CG2	16:AG:108:GLN:HE21	1.94	0.64
14:AE:84:ILE:O	14:AE:84:ILE:HG13	1.96	0.64
14:AE:162:GLU:OE1	14:AE:162:GLU:HA	1.97	0.64
16:AG:64:VAL:HG22	16:AG:75:ILE:HD12	1.78	0.64
16:AG:205:LEU:HA	16:AG:208:LEU:HB2	1.80	0.64
16:AG:213:VAL:HG22	16:AG:216:ILE:HG13	1.78	0.64
16:AG:433:ASP:O	16:AG:456:LEU:CG	2.45	0.64
10:B:18:G:C8	10:B:57:A:C6	2.85	0.64
22:H:85:SER:O	22:H:88:LYS:CB	2.45	0.64
41:a:1909:C:O5'	41:a:1909:C:H6	1.81	0.64
8:7:9:U:N3	18:D:1196:A:N7	2.44	0.64
11:AA:314:ASN:HD21	11:AA:348:SER:HA	1.62	0.64
14:AE:975:ILE:HG22	14:AE:977:SER:H	1.62	0.64
16:AG:425:LEU:O	16:AG:429:LYS:CE	2.45	0.64
16:AG:254:MET:HG2	16:AG:257:ALA:HB3	1.77	0.64
16:AG:302:LYS:H	16:AG:302:LYS:CE	2.00	0.64
41:a:1839:G:H8	41:a:1927:A:H1'	1.54	0.64
41:a:2303:G:N3	41:a:2314:A:C2	2.66	0.64
8:7:14:U:H5'	23:I:132:ARG:CZ	2.26	0.64
13:AD:285:THR:CB	16:AG:82:TYR:HD1	2.08	0.64
14:AE:136:GLU:CD	14:AE:312:ARG:HH22	2.06	0.64
16:AG:131:ARG:HG2	16:AG:186:VAL:HG12	1.80	0.64
16:AG:254:MET:HG3	16:AG:257:ALA:HB2	1.74	0.64
10:B:22:G:H2'	10:B:23:C:H6	1.62	0.64
18:D:1227:A:OP2	38:X:110:LYS:NZ	2.29	0.64
9:9:11:ILE:HD12	9:9:62:ARG:HD3	1.80	0.64
9:9:60:LEU:HA	9:9:64:VAL:HB	1.77	0.64
16:AG:63:LEU:HD22	16:AG:92:TYR:HD1	1.63	0.64
16:AG:425:LEU:HG	16:AG:429:LYS:HD3	1.79	0.64
11:AA:854:ILE:HG12	11:AA:855:PRO:HD3	1.77	0.64
12:AB:140:PRO:CD	30:P:102:LEU:CD1	2.67	0.64
10:B:50:U:H2'	10:B:51:C:C6	2.33	0.64
22:H:267:TRP:CE3	22:H:340:ARG:HG3	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:813:GLU:HB2	14:AE:461:PHE:HD2	1.63	0.63
12:AB:138:ASP:CB	12:AB:177:GLN:HA	2.20	0.63
12:AB:156:SER:O	12:AB:156:SER:OG	2.16	0.63
16:AG:354:ALA:CA	16:AG:357:ASP:H	2.10	0.63
16:AG:363:LEU:HD21	16:AG:410:ALA:N	1.79	0.63
18:D:1329:A:P	38:X:28:THR:CB	2.83	0.63
22:H:49:PRO:CD	22:H:84:LEU:HD11	2.29	0.63
9:9:18:VAL:HG13	9:9:71:CYS:HB2	1.81	0.63
10:A:50:U:H2'	10:A:51:C:C6	2.33	0.63
16:AG:354:ALA:HA	16:AG:357:ASP:CA	2.28	0.63
18:D:1059:C:O2	30:P:55:PRO:HG3	1.99	0.63
41:a:1839:G:O4'	41:a:1927:A:H1'	1.97	0.63
16:AG:174:ARG:HB3	16:AG:175:PRO:CD	2.25	0.63
16:AG:266:LEU:H	16:AG:266:LEU:HD23	1.64	0.63
17:C:44:ILE:CD1	22:H:339:ARG:HG2	2.12	0.63
18:D:1308:U:O5'	38:X:98:ARG:CG	2.45	0.63
22:H:280:LEU:N	22:H:330:VAL:O	2.32	0.63
10:A:69:C:H2'	10:A:70:G:O4'	1.99	0.63
14:AE:44:ILE:CD1	14:AE:252:LEU:HD21	2.29	0.63
16:AG:422:GLU:HG2	16:AG:426:GLY:HA3	1.80	0.63
16:AG:434:LEU:HD12	16:AG:454:CYS:C	2.22	0.63
30:P:17:LEU:HD11	30:P:94:ALA:O	1.98	0.63
41:a:1789:A:OP2	48:h:221:ARG:NH1	2.32	0.63
10:A:31:G:O2'	27:M:144:MET:SD	2.56	0.63
11:AA:120:GLN:NE2	11:AA:490:GLN:OE1	2.32	0.63
16:AG:162:ILE:HD11	16:AG:199:ARG:HD2	1.80	0.63
16:AG:389:MET:HE3	16:AG:407:ARG:HD2	1.81	0.63
12:AB:96:THR:CB	14:AE:162:GLU:HG3	2.29	0.63
14:AE:92:VAL:O	14:AE:92:VAL:HG12	1.99	0.63
21:G:35:ARG:HH21	22:H:10:GLU:HG2	1.62	0.63
41:a:2297:A:C2	41:a:2321:U:C4	2.86	0.63
10:A:37:A:O2'	10:A:38:A:H5'	1.99	0.63
11:AA:862:LEU:HD22	11:AA:862:LEU:N	2.14	0.63
16:AG:323:GLN:HE21	16:AG:323:GLN:CA	2.12	0.63
21:G:16:PHE:HZ	22:H:41:GLY:O	1.77	0.63
22:H:162:LYS:CB	22:H:298:GLU:OE2	2.45	0.63
39:Y:32:VAL:HA	39:Y:60:VAL:HG11	1.81	0.63
9:9:57:ASN:OD1	9:9:62:ARG:HD2	1.98	0.63
14:AE:395:LYS:HZ2	14:AE:399:LYS:HD3	1.63	0.63
16:AG:258:ARG:HG2	16:AG:258:ARG:NH1	1.99	0.63
18:D:13:U:O4	18:D:20:U:C4	2.52	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:98:DA:C2'	6:5:99:DT:H72	2.28	0.63
10:A:41:C:C1'	27:M:143:ARG:HH12	2.12	0.63
11:AA:853:ASP:OD2	16:AG:104:ARG:N	2.32	0.63
16:AG:233:ARG:CB	16:AG:327:LEU:HD23	2.28	0.63
21:G:19:GLN:CG	22:H:76:GLU:CB	2.76	0.63
22:H:119:GLY:CA	22:H:131:LEU:O	2.46	0.63
6:5:101:DT:OP2	14:AE:275:ARG:NH2	2.31	0.62
11:AA:853:ASP:HA	16:AG:105:ILE:HG21	1.80	0.62
14:AE:201:LEU:HB2	14:AE:221:ILE:HD13	1.80	0.62
16:AG:424:SER:C	16:AG:429:LYS:CG	2.72	0.62
18:D:1309:G:C8	38:X:98:ARG:NH2	2.66	0.62
21:G:19:GLN:CG	22:H:75:VAL:CG2	2.70	0.62
30:P:87:LEU:CD2	30:P:100:ILE:CD1	2.71	0.62
11:AA:908:GLU:OE1	16:AG:104:ARG:HG2	1.99	0.62
12:AB:128:PHE:HZ	12:AB:175:PHE:HB3	1.61	0.62
16:AG:393:LEU:CB	16:AG:398:LEU:HD22	1.90	0.62
16:AG:433:ASP:C	16:AG:456:LEU:CD1	2.72	0.62
21:G:19:GLN:CD	22:H:75:VAL:HG22	2.24	0.62
27:M:23:LEU:O	27:M:27:VAL:HG13	1.99	0.62
41:a:2189:U:O4'	41:a:2189:U:P	2.57	0.62
6:5:100:DA:OP1	12:AB:16:SER:CB	2.48	0.62
10:A:42:G:H2'	10:A:43:A:H8	1.65	0.62
13:AD:211:ILE:HG12	13:AD:219:ARG:HH12	1.65	0.62
16:AG:301:ASP:OD1	16:AG:301:ASP:N	2.32	0.62
18:D:37:U:O2	18:D:548:G:C2	2.52	0.62
18:D:1358:U:H3	18:D:1363:A:N6	1.96	0.62
22:H:332:VAL:HG12	22:H:334:ASP:H	1.62	0.62
9:9:57:ASN:CG	9:9:62:ARG:HG2	2.24	0.62
12:AB:177:GLN:HE22	30:P:103:GLY:HA3	1.65	0.62
16:AG:353:HIS:CA	16:AG:356:ILE:CG2	2.76	0.62
16:AG:434:LEU:CD1	16:AG:454:CYS:C	2.72	0.62
16:AG:440:VAL:HG23	16:AG:481:LEU:CD2	2.29	0.62
3:2:50:LEU:HD23	45:e:26:PHE:CE1	2.35	0.62
9:9:92:ALA:HB3	9:9:129:LEU:HB2	1.81	0.62
11:AA:1101:LEU:HD23	14:AE:725:MET:SD	2.40	0.62
12:AB:93:ILE:HG21	14:AE:291:ILE:HA	1.80	0.62
14:AE:1355:ARG:NH1	14:AE:1369:ARG:NH1	2.47	0.62
16:AG:223:ILE:HA	16:AG:238:VAL:HG12	1.80	0.62
18:D:1358:U:N3	18:D:1363:A:N6	2.46	0.62
22:H:270:ILE:HG21	22:H:337:GLU:HB3	1.80	0.62
8:7:7:U:H6	8:7:7:U:H5"	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:1287:LEU:HD13	14:AE:1357:ILE:HD11	1.81	0.62
14:AE:111:THR:CG2	14:AE:300:GLN:NE2	2.62	0.62
16:AG:187:ARG:CB	16:AG:188:PRO:HD3	2.20	0.62
16:AG:453:VAL:HG21	16:AG:462:GLN:CD	2.25	0.62
21:G:38:VAL:HG22	22:H:75:VAL:CG2	2.25	0.62
41:a:1839:G:N9	41:a:1927:A:N9	2.48	0.62
10:A:56:C:O2	41:a:2112:G:C4	2.52	0.62
12:AB:155:LYS:NZ	18:D:1277:C:C3'	2.44	0.62
10:B:69:C:H2'	10:B:70:G:O4'	1.99	0.62
11:AA:1280:ALA:HB1	14:AE:918:ILE:HG22	1.79	0.62
41:a:754:U:H2'	41:a:755:U:C6	2.35	0.62
41:a:2683:C:OP1	65:y:51:ARG:NH2	2.32	0.62
7:6:15:DC:N4	7:6:16:DC:H41	1.96	0.62
12:AB:42:VAL:HG13	12:AB:42:VAL:O	2.00	0.62
14:AE:395:LYS:NZ	14:AE:399:LYS:HD3	2.15	0.62
10:B:65:C:H2'	10:B:66:C:H5'	1.82	0.62
22:H:118:GLY:C	22:H:133:GLY:CA	2.68	0.62
14:AE:68:TYR:HB3	14:AE:75:TYR:CZ	2.35	0.62
16:AG:127:VAL:CG2	16:AG:192:GLY:CA	2.78	0.62
16:AG:285:ILE:CG2	16:AG:293:VAL:HG11	2.28	0.62
16:AG:380:THR:C	16:AG:384:LEU:HD11	2.24	0.62
16:AG:428:ASN:O	16:AG:428:ASN:ND2	2.32	0.62
17:C:29:LEU:O	17:C:33:ILE:HG23	2.00	0.62
30:P:57:VAL:O	30:P:58:ASN:CG	2.43	0.62
41:a:1998:A:OP2	50:j:141:ARG:NH2	2.32	0.62
8:7:11:U:O2'	25:K:33:PHE:HE1	1.76	0.61
10:A:3:C:H2'	10:A:4:G:C8	2.35	0.61
10:A:65:C:H2'	10:A:66:C:H5'	1.82	0.61
11:AA:901:LEU:CG	16:AG:8:VAL:CG1	2.70	0.61
10:B:42:G:H2'	10:B:43:A:H8	1.65	0.61
24:J:162:ALA:CB	24:J:165:ARG:HH22	2.08	0.61
38:X:101:ARG:O	38:X:101:ARG:HD3	2.00	0.61
8:7:53:G:OP2	11:AA:540:ARG:NH1	2.33	0.61
10:A:33:U:H4'	27:M:84:THR:HB	1.82	0.61
11:AA:896:THR:HB	11:AA:897:PRO:HD2	1.82	0.61
12:AB:128:PHE:CZ	12:AB:175:PHE:CA	2.83	0.61
14:AE:24:LEU:CG	14:AE:232:ASN:ND2	2.63	0.61
16:AG:433:ASP:C	16:AG:456:LEU:HD11	2.23	0.61
22:H:135:LEU:CA	22:H:157:ILE:CB	2.74	0.61
40:Z:7:ILE:HG23	40:Z:7:ILE:O	2.00	0.61
10:A:54:U:N3	10:A:58:A:N6	2.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AD:112:ALA:HB3	13:AD:126:PRO:HA	1.83	0.61
16:AG:288:MET:SD	16:AG:293:VAL:N	2.72	0.61
21:G:19:GLN:HG3	22:H:76:GLU:HB2	1.82	0.61
22:H:19:ARG:O	22:H:72:LEU:CB	2.40	0.61
22:H:305:HIS:O	22:H:306:VAL:HB	2.00	0.61
1:0:40:MET:HE1	66:z:105:ALA:HB1	1.81	0.61
11:AA:905:ILE:HD12	16:AG:8:VAL:HG21	1.82	0.61
16:AG:421:GLN:O	16:AG:425:LEU:N	2.34	0.61
11:AA:905:ILE:HG23	11:AA:905:ILE:O	2.00	0.61
16:AG:279:ASN:HB3	16:AG:280:PRO:HD2	1.83	0.61
22:H:110:GLY:N	22:H:153:GLU:O	2.32	0.61
22:H:270:ILE:CG2	22:H:337:GLU:CB	2.77	0.61
9:9:62:ARG:CG	9:9:62:ARG:HH21	2.14	0.61
12:AB:159:LYS:O	12:AB:159:LYS:HG2	2.00	0.61
14:AE:128:LEU:HA	14:AE:192:MET:HE1	1.81	0.61
14:AE:223:LEU:HG	14:AE:223:LEU:O	2.00	0.61
9:9:23:LEU:HB3	9:9:92:ALA:HA	1.81	0.61
12:AB:127:LEU:O	12:AB:127:LEU:HG	2.00	0.61
16:AG:285:ILE:HD13	16:AG:285:ILE:N	2.15	0.61
10:B:54:U:N3	10:B:58:A:N6	2.47	0.61
10:B:56:C:C4'	54:n:80:ARG:NH2	2.63	0.61
22:H:84:LEU:HD22	22:H:84:LEU:N	2.15	0.61
14:AE:154:LEU:HD21	14:AE:160:LEU:HD21	1.83	0.61
14:AE:1161:GLY:HA3	14:AE:1179:PRO:HA	1.83	0.61
16:AG:451:ARG:CZ	16:AG:469:ASP:HB2	2.30	0.61
18:D:13:U:C5	18:D:20:U:O4	2.53	0.61
41:a:2885:G:N7	49:i:40:ARG:NH2	2.46	0.61
12:AB:96:THR:HB	14:AE:162:GLU:CB	2.31	0.61
16:AG:63:LEU:HG	16:AG:73:LYS:HB3	1.83	0.61
16:AG:402:THR:O	16:AG:406:LEU:N	2.33	0.61
22:H:72:LEU:HD12	22:H:72:LEU:N	2.10	0.61
7:6:15:DC:C4	7:6:16:DC:C4	2.89	0.61
12:AB:129:GLU:H	12:AB:180:LYS:HD2	1.66	0.61
12:AB:133:MET:HE2	12:AB:133:MET:O	2.01	0.61
14:AE:67:ASP:OD1	14:AE:67:ASP:N	2.34	0.61
16:AG:287:ALA:HB1	16:AG:331:LEU:HB3	1.81	0.61
8:7:14:U:OP1	23:I:132:ARG:NH1	2.34	0.60
9:9:6:GLN:OE1	9:9:6:GLN:HA	2.00	0.60
12:AB:155:LYS:HE2	18:D:1277:C:O5'	2.01	0.60
16:AG:27:LEU:HD22	16:AG:114:ILE:HG23	1.82	0.60
16:AG:303:HIS:HB3	16:AG:334:TRP:HZ3	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:320:ARG:CG	16:AG:320:ARG:HH11	2.14	0.60
22:H:304:VAL:HG12	22:H:304:VAL:O	1.99	0.60
12:AB:145:ASN:N	12:AB:145:ASN:OD1	2.34	0.60
16:AG:434:LEU:CD1	16:AG:455:THR:C	2.74	0.60
10:B:3:C:H2'	10:B:4:G:C8	2.36	0.60
22:H:305:HIS:CD2	22:H:307:SER:H	2.19	0.60
41:a:2297:A:C2	41:a:2321:U:C5	2.89	0.60
11:AA:618:GLN:CG	14:AE:770:LEU:HD13	2.32	0.60
12:AB:46:THR:HG22	12:AB:46:THR:O	2.00	0.60
12:AB:128:PHE:HZ	12:AB:175:PHE:O	1.81	0.60
12:AB:155:LYS:HG3	12:AB:155:LYS:O	2.00	0.60
18:D:658:C:H1'	34:T:22:THR:HG21	1.83	0.60
11:AA:55:SER:OG	11:AA:465:ARG:NH1	2.33	0.60
11:AA:903:ARG:HH11	11:AA:903:ARG:CA	2.15	0.60
16:AG:240:THR:OG1	16:AG:247:PRO:HG2	2.01	0.60
17:C:44:ILE:CD1	22:H:339:ARG:HG3	2.28	0.60
35:U:21:VAL:HG21	35:U:60:TRP:CD1	2.36	0.60
11:AA:862:LEU:HD22	11:AA:862:LEU:H	1.66	0.60
41:a:1406:U:HO2'	41:a:1407:G:C5'	2.07	0.60
10:A:41:C:H4'	27:M:143:ARG:CZ	2.32	0.60
11:AA:528:ARG:NH2	11:AA:576:SER:O	2.30	0.60
12:AB:103:ILE:HD12	12:AB:107:GLU:OE1	2.00	0.60
12:AB:165:PHE:HA	30:P:88:MET:HA	1.83	0.60
14:AE:118:LYS:HD2	14:AE:312:ARG:NH2	2.17	0.60
14:AE:951:GLN:NE2	14:AE:1014:GLY:O	2.35	0.60
16:AG:212:GLU:HB3	16:AG:258:ARG:HB3	1.84	0.60
16:AG:434:LEU:HG	16:AG:456:LEU:N	2.16	0.60
21:G:19:GLN:HG3	22:H:75:VAL:CG2	2.24	0.60
22:H:284:VAL:HG12	22:H:294:VAL:HB	1.84	0.60
13:AC:45:ARG:HD3	13:AD:38:THR:HB	1.82	0.60
14:AE:342:LEU:HD23	14:AE:1352:ILE:HG23	1.83	0.60
16:AG:168:LEU:HD21	16:AG:230:PRO:O	2.00	0.60
16:AG:424:SER:C	16:AG:429:LYS:HG3	2.26	0.60
18:D:1218:C:H2'	18:D:1219:A:C8	2.36	0.60
22:H:71:ALA:O	22:H:72:LEU:CD1	2.42	0.60
27:M:69:VAL:HG23	27:M:100:ALA:HB1	1.83	0.60
41:a:2720:U:OP1	65:y:53:ARG:NH2	2.34	0.60
16:AG:425:LEU:O	16:AG:429:LYS:NZ	2.33	0.60
16:AG:437:LEU:CD2	16:AG:456:LEU:HD11	2.27	0.60
9:9:47:GLU:HG3	9:9:95:LEU:HD21	1.83	0.60
10:A:22:G:H2'	10:A:23:C:H6	1.62	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:34:C:P	27:M:84:THR:OG1	2.60	0.60
11:AA:1072:ASN:ND2	11:AA:1111:GLN:OE1	2.34	0.60
12:AB:66:PRO:CG	14:AE:281:ARG:NH2	2.53	0.60
12:AB:128:PHE:CE1	12:AB:175:PHE:CD1	2.89	0.60
14:AE:514:THR:HG21	14:AE:596:LEU:HD12	1.84	0.60
16:AG:197:VAL:HG11	16:AG:199:ARG:HH21	1.66	0.60
35:U:4:ILE:HG12	35:U:21:VAL:HG22	1.84	0.60
12:AB:23:ALA:CB	12:AB:44:VAL:CB	2.64	0.60
9:9:19:ALA:HA	9:9:70:GLU:HG2	1.84	0.59
14:AE:90:VAL:O	14:AE:90:VAL:CG1	2.48	0.59
16:AG:233:ARG:HG2	16:AG:270:ARG:HB2	1.83	0.59
46:f:24:LEU:HD11	46:f:54:MET:HE2	1.84	0.59
6:5:100:DA:P	12:AB:16:SER:OG	2.48	0.59
16:AG:202:PRO:O	16:AG:205:LEU:HD12	2.02	0.59
39:Y:54:ILE:O	39:Y:54:ILE:HG22	2.00	0.59
41:a:1921:G:O5'	41:a:1921:G:H8	1.84	0.59
11:AA:857:VAL:CG1	11:AA:862:LEU:HD13	2.30	0.59
41:a:1021:A:C2	41:a:1141:U:O4	2.51	0.59
12:AB:135:ARG:HH11	12:AB:135:ARG:CG	2.14	0.59
14:AE:416:ILE:HG13	14:AE:441:LEU:HD11	1.83	0.59
18:D:1225:A:H4'	37:W:78:ARG:NH1	2.17	0.59
22:H:331:MET:N	22:H:331:MET:SD	2.75	0.59
11:AA:549:ASP:OD2	14:AE:750:PRO:CB	2.44	0.59
14:AE:97:VAL:HG11	14:AE:101:ARG:NH2	2.18	0.59
16:AG:10:GLU:HA	16:AG:12:VAL:HG22	1.83	0.59
16:AG:240:THR:CB	16:AG:247:PRO:HG3	2.32	0.59
16:AG:434:LEU:N	16:AG:456:LEU:HG	2.17	0.59
10:B:47:U:O2'	10:B:50:U:P	2.61	0.59
4:3:36:VAL:CG1	4:3:39:ILE:HD12	2.32	0.59
9:9:136:ILE:HD12	9:9:139:LEU:HD12	1.83	0.59
10:A:47:U:O2'	10:A:50:U:P	2.61	0.59
16:AG:433:ASP:HB3	16:AG:456:LEU:HD12	1.83	0.59
22:H:117:LYS:CB	22:H:278:THR:HG23	2.32	0.59
11:AA:1142:ARG:NH1	11:AA:1161:LEU:O	2.36	0.59
16:AG:354:ALA:CA	16:AG:357:ASP:HB3	2.32	0.59
16:AG:437:LEU:HD22	16:AG:488:ILE:CD1	2.33	0.59
18:D:13:U:C2	18:D:915:A:N6	2.70	0.59
20:F:4:ILE:CD1	20:F:19:PHE:HA	2.33	0.59
25:K:107:ALA:HB2	25:K:125:ALA:HB3	1.83	0.59
9:9:77:VAL:HG12	9:9:77:VAL:O	2.01	0.59
14:AE:201:LEU:HD11	14:AE:220:ARG:HH11	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:412:LEU:HD22	14:AE:441:LEU:HD21	1.84	0.59
18:D:404:G:N7	24:J:2:ALA:HB3	2.17	0.59
21:G:35:ARG:HD2	22:H:14:LYS:CD	2.32	0.59
41:a:1590:A:H2'	41:a:1591:A:C8	2.38	0.59
10:A:34:C:P	27:M:84:THR:HG1	2.26	0.59
14:AE:144:TYR:CE1	14:AE:162:GLU:OE2	2.51	0.59
14:AE:275:ARG:NH1	14:AE:278:ARG:NH1	2.51	0.59
14:AE:926:PRO:HG2	14:AE:1248:ILE:HD11	1.84	0.59
22:H:270:ILE:HG21	22:H:337:GLU:CB	2.32	0.59
40:Z:20:VAL:O	40:Z:20:VAL:HG12	2.02	0.59
11:AA:707:ALA:O	11:AA:711:ASP:HB2	2.03	0.59
14:AE:370:LYS:HG2	14:AE:441:LEU:HD23	1.84	0.59
41:a:70:G:H4'	41:a:71:A:OP1	2.02	0.59
41:a:2314:A:O2'	54:n:155:THR:CG2	2.51	0.59
53:m:31:LEU:HD22	53:m:42:LEU:HD13	1.84	0.59
8:7:10:U:H5"	8:7:10:U:O2	2.03	0.58
11:AA:845:LEU:O	11:AA:845:LEU:HG	2.03	0.58
12:AB:44:VAL:HG12	12:AB:44:VAL:O	2.02	0.58
16:AG:254:MET:HB2	16:AG:257:ALA:HB2	1.85	0.58
16:AG:318:ILE:HG12	16:AG:338:VAL:HG11	1.85	0.58
16:AG:453:VAL:HG11	16:AG:459:LEU:HG	1.84	0.58
18:D:1308:U:C5'	38:X:98:ARG:HG2	2.32	0.58
38:X:104:THR:O	38:X:104:THR:HG22	2.03	0.58
10:A:18:G:C8	10:A:57:A:N6	2.69	0.58
11:AA:838:CYS:HB2	11:AA:918:LEU:HD22	1.85	0.58
11:AA:1282:GLY:HA3	15:AF:17:PHE:HE1	1.67	0.58
14:AE:161:THR:HG23	14:AE:164:GLN:H	1.68	0.58
14:AE:241:VAL:HG12	14:AE:241:VAL:O	2.04	0.58
16:AG:139:THR:HG22	16:AG:180:ARG:HB3	1.83	0.58
16:AG:254:MET:HG3	16:AG:257:ALA:CB	2.30	0.58
16:AG:354:ALA:HA	16:AG:357:ASP:N	2.18	0.58
16:AG:363:LEU:HG	16:AG:410:ALA:N	2.16	0.58
21:G:217:VAL:O	21:G:220:THR:HG22	2.02	0.58
22:H:119:GLY:HA3	22:H:132:PRO:C	2.28	0.58
6:5:99:DT:H2"	6:5:100:DA:H5"	1.85	0.58
14:AE:99:ARG:HG3	14:AE:99:ARG:NH1	2.17	0.58
16:AG:130:PHE:C	16:AG:186:VAL:HG11	2.28	0.58
16:AG:287:ALA:CB	16:AG:331:LEU:HB3	2.33	0.58
18:D:563:A:N6	18:D:884:U:N3	2.51	0.58
41:a:2245:U:O2'	41:a:2436:G:OP2	2.22	0.58
14:AE:124:ILE:HG22	14:AE:124:ILE:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:127:VAL:HG21	16:AG:192:GLY:HA2	1.84	0.58
16:AG:413:ALA:HA	16:AG:416:THR:OG1	2.03	0.58
19:E:25:ARG:HA	19:E:66:LEU:HD21	1.85	0.58
22:H:36:VAL:HB	22:H:48:ILE:HB	1.84	0.58
22:H:110:GLY:H	22:H:153:GLU:C	2.12	0.58
10:A:58:A:H1'	10:A:60:U:C5	2.38	0.58
11:AA:69:GLN:HE21	11:AA:101:ARG:HD2	1.67	0.58
11:AA:858:GLY:O	11:AA:861:ALA:HB3	2.04	0.58
12:AB:140:PRO:CA	30:P:84:VAL:HG21	2.34	0.58
12:AB:165:PHE:CD1	30:P:88:MET:O	2.56	0.58
16:AG:63:LEU:HD23	16:AG:63:LEU:H	1.69	0.58
39:Y:78:LEU:HD13	39:Y:108:ILE:HG22	1.85	0.58
8:7:9:U:O4	18:D:1196:A:C1'	2.52	0.58
12:AB:165:PHE:CZ	30:P:91:ASP:CB	2.87	0.58
16:AG:25:GLU:HG3	16:AG:49:ILE:HD11	1.85	0.58
16:AG:31:LEU:HD23	16:AG:110:ALA:HB1	1.85	0.58
16:AG:353:HIS:O	16:AG:356:ILE:C	2.43	0.58
22:H:291:GLY:HA2	22:H:305:HIS:HA	1.86	0.58
8:7:7:U:H5"	8:7:7:U:C6	2.39	0.58
12:AB:155:LYS:HE3	18:D:1277:C:O5'	2.03	0.58
16:AG:33:THR:HG23	16:AG:43:ILE:HD11	1.85	0.58
16:AG:361:LYS:CE	16:AG:417:ILE:CG1	2.74	0.58
41:a:2572:A:C8	50:j:149:ASN:OD1	2.56	0.58
9:9:52:MET:HE3	9:9:52:MET:O	2.03	0.58
11:AA:1328:LYS:HE2	14:AE:100:GLU:HA	1.85	0.58
12:AB:128:PHE:HE1	12:AB:175:PHE:HB3	1.59	0.58
12:AB:133:MET:N	12:AB:133:MET:SD	2.77	0.58
12:AB:140:PRO:CG	30:P:102:LEU:CB	2.82	0.58
13:AC:82:LEU:HD11	13:AC:171:LEU:HD23	1.86	0.58
16:AG:266:LEU:HD23	16:AG:266:LEU:N	2.19	0.58
39:Y:7:TYR:HB2	39:Y:57:VAL:HG22	1.86	0.58
10:A:35:A:H2'	10:A:36:U:C6	2.38	0.58
10:A:60:U:P	10:A:61:C:H41	2.27	0.58
12:AB:128:PHE:HZ	12:AB:175:PHE:CB	2.13	0.58
12:AB:157:ARG:HD2	12:AB:172:GLU:HB3	1.86	0.58
16:AG:162:ILE:HD13	16:AG:167:MET:HE2	1.86	0.58
16:AG:434:LEU:HD22	16:AG:459:LEU:CG	2.31	0.58
25:K:56:VAL:O	25:K:60:ILE:HG23	2.04	0.58
41:a:84:A:N1	41:a:98:G:O2'	2.33	0.58
41:a:1839:G:N9	41:a:1927:A:C4	2.72	0.58
11:AA:13:LYS:HB2	11:AA:1180:MET:HE2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:167:ARG:HH11	23:I:62:LYS:CA	2.17	0.58
16:AG:137:ILE:O	16:AG:137:ILE:HG22	2.03	0.58
16:AG:233:ARG:O	16:AG:327:LEU:HD21	2.04	0.58
21:G:19:GLN:NE2	22:H:75:VAL:HG22	2.19	0.58
11:AA:888:THR:CB	11:AA:889:PRO:HD2	2.34	0.57
10:B:58:A:H1'	10:B:60:U:C5	2.38	0.57
18:D:1329:A:P	38:X:28:THR:OG1	2.62	0.57
22:H:290:TYR:C	22:H:305:HIS:O	2.47	0.57
38:X:17:ILE:O	38:X:20:THR:OG1	2.22	0.57
47:g:16:CYS:HB3	47:g:37:CYS:HB3	1.87	0.57
11:AA:853:ASP:C	16:AG:105:ILE:CB	2.71	0.57
16:AG:440:VAL:HG22	16:AG:481:LEU:CD2	2.34	0.57
50:j:33:ARG:NH1	50:j:53:GLY:O	2.36	0.57
9:9:61:ARG:CZ	41:a:1047:G:N7	2.67	0.57
14:AE:438:GLU:HG3	14:AE:485:MET:HE1	1.84	0.57
14:AE:491:LEU:HB2	14:AE:904:ALA:HA	1.86	0.57
16:AG:233:ARG:HH12	16:AG:324:ASN:N	2.02	0.57
16:AG:367:GLU:O	16:AG:371:THR:HG23	2.04	0.57
16:AG:392:LEU:CD2	16:AG:395:ILE:HD11	2.35	0.57
16:AG:422:GLU:CG	16:AG:426:GLY:HA3	2.35	0.57
18:D:321:A:N7	18:D:328:C:O2'	2.34	0.57
22:H:267:TRP:CH2	22:H:340:ARG:CB	2.86	0.57
39:Y:77:VAL:O	39:Y:77:VAL:HG12	2.05	0.57
12:AB:140:PRO:HG3	30:P:6:ILE:CG1	2.35	0.57
14:AE:615:LYS:HG2	15:AF:5:THR:HG21	1.85	0.57
16:AG:453:VAL:CG2	16:AG:462:GLN:CD	2.76	0.57
18:D:439:U:O2	18:D:440:C:C6	2.56	0.57
18:D:496:A:N3	18:D:496:A:H2'	2.19	0.57
22:H:49:PRO:HD3	22:H:84:LEU:HD11	1.86	0.57
8:7:12:U:H5"	25:K:56:VAL:HG21	1.86	0.57
9:9:54:VAL:O	9:9:54:VAL:HG22	2.03	0.57
14:AE:510:LEU:HD22	14:AE:601:ILE:HD12	1.86	0.57
16:AG:352:ALA:O	16:AG:356:ILE:CG2	2.51	0.57
16:AG:379:SER:HG	16:AG:384:LEU:HD21	1.69	0.57
10:B:56:C:C5'	54:n:80:ARG:NH2	2.68	0.57
22:H:110:GLY:N	22:H:153:GLU:CA	2.67	0.57
2:1:93:ALA:HB2	41:a:1614:A:C2	2.40	0.57
6:5:115:DA:OP2	14:AE:1148:ARG:HG3	2.04	0.57
11:AA:849:GLU:HB2	11:AA:887:VAL:HG13	1.86	0.57
14:AE:102:MET:HG2	14:AE:246:PRO:HG3	1.87	0.57
16:AG:131:ARG:CA	16:AG:186:VAL:HG11	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:1227:A:H5'	38:X:110:LYS:HZ3	1.66	0.57
22:H:332:VAL:CG1	22:H:335:ILE:HG13	2.33	0.57
61:u:77:ILE:HD11	61:u:108:ALA:HB1	1.87	0.57
8:7:9:U:O4	18:D:1196:A:C8	2.57	0.57
9:9:34:THR:HG22	9:9:38:MET:HE3	1.85	0.57
11:AA:901:LEU:HD11	16:AG:8:VAL:CB	2.32	0.57
11:AA:1122:LYS:NZ	11:AA:1126:ASP:OD1	2.38	0.57
14:AE:160:LEU:HD22	14:AE:164:GLN:HB3	1.86	0.57
14:AE:343:LEU:HD11	14:AE:1324:SER:HB3	1.87	0.57
16:AG:130:PHE:HB3	16:AG:186:VAL:HG22	1.86	0.57
2:1:20:VAL:HG11	2:1:44:ALA:HA	1.86	0.57
16:AG:221:ILE:HD13	16:AG:247:PRO:HA	1.85	0.57
16:AG:283:PHE:CE2	16:AG:331:LEU:O	2.58	0.57
18:D:1526:G:OP2	20:F:42:THR:HG23	2.04	0.57
8:7:56:G:OP1	11:AA:1073:LYS:NZ	2.26	0.57
14:AE:247:PRO:HA	14:AE:250:ARG:HG3	1.87	0.57
16:AG:9:VAL:HA	16:AG:24:PHE:CZ	2.40	0.57
16:AG:302:LYS:NZ	16:AG:302:LYS:HB2	2.20	0.57
43:c:31:PRO:HG2	43:c:33:LEU:HD13	1.87	0.57
8:7:1:A:H2'	8:7:2:U:H6	1.70	0.57
8:7:21:U:H5'	23:I:80:LYS:CE	2.35	0.57
10:A:76:A:C2'	41:a:2394:C:H42	2.16	0.57
14:AE:638:SER:OG	14:AE:639:VAL:N	2.36	0.57
16:AG:210:ARG:HE	16:AG:216:ILE:HG22	1.69	0.57
10:B:11:A:H2'	10:B:12:G:C8	2.39	0.57
39:Y:96:LYS:HE3	39:Y:136:GLY:HA3	1.87	0.57
10:A:50:U:H2'	10:A:51:C:H6	1.70	0.56
11:AA:839:VAL:HG12	11:AA:1049:ILE:HG12	1.87	0.56
12:AB:133:MET:HE2	12:AB:133:MET:CA	2.32	0.56
12:AB:165:PHE:HE1	30:P:91:ASP:CA	2.17	0.56
12:AB:173:LEU:HD12	30:P:102:LEU:CD2	2.30	0.56
14:AE:130:MET:HE2	14:AE:135:ILE:HG12	1.87	0.56
16:AG:434:LEU:HD11	16:AG:455:THR:N	2.19	0.56
21:G:148:LEU:HD22	21:G:151:ILE:HD11	1.86	0.56
22:H:118:GLY:C	22:H:133:GLY:HA2	2.28	0.56
47:g:16:CYS:CB	47:g:37:CYS:CB	2.82	0.56
8:7:9:U:C4	18:D:1196:A:C8	2.93	0.56
9:9:31:ARG:HH11	9:9:31:ARG:CG	2.14	0.56
12:AB:165:PHE:HZ	30:P:91:ASP:CB	2.18	0.56
16:AG:334:TRP:N	16:AG:334:TRP:CD1	2.73	0.56
30:P:6:ILE:HG23	30:P:100:ILE:HG23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:l:104:ALA:O	52:l:108:ILE:HG23	2.05	0.56
1:0:51:VAL:HG23	66:z:86:ALA:O	2.05	0.56
12:AB:103:ILE:CD1	12:AB:107:GLU:OE2	2.52	0.56
12:AB:126:THR:O	12:AB:126:THR:HG22	2.04	0.56
12:AB:164:ILE:C	30:P:88:MET:HG3	2.27	0.56
12:AB:165:PHE:HA	30:P:88:MET:CA	2.34	0.56
14:AE:171:GLU:HA	14:AE:171:GLU:OE1	2.06	0.56
14:AE:1046:ILE:HD12	14:AE:1059:LEU:HB3	1.86	0.56
14:AE:1167:LYS:HZ2	14:AE:1170:LYS:HB2	1.70	0.56
16:AG:434:LEU:HD23	16:AG:456:LEU:CG	2.35	0.56
21:G:18:HIS:CA	22:H:43:LYS:HD2	2.29	0.56
41:a:580:U:O3'	66:z:31:VAL:HG13	2.05	0.56
7:6:21:DA:N6	8:7:51:G:H1	2.04	0.56
11:AA:854:ILE:H	16:AG:105:ILE:HG23	1.60	0.56
12:AB:134:VAL:HG12	12:AB:180:LYS:HA	1.87	0.56
12:AB:172:GLU:HB2	30:P:101:SER:OG	2.06	0.56
16:AG:362:TYR:CZ	16:AG:382:GLU:HG2	2.40	0.56
10:B:32:C:OP2	29:O:130:ARG:NH2	2.38	0.56
39:Y:137:LEU:N	39:Y:137:LEU:HD23	2.19	0.56
7:6:18:DC:N4	8:7:53:G:H1	1.99	0.56
11:AA:900:LYS:HZ2	16:AG:11:ALA:HB1	1.44	0.56
16:AG:61:ARG:HD2	16:AG:73:LYS:HD3	1.86	0.56
16:AG:307:ILE:HD11	16:AG:336:LEU:HB2	1.87	0.56
18:D:927:G:O2'	18:D:1503:A:N7	2.36	0.56
31:Q:67:ALA:HB2	31:Q:96:THR:HG23	1.86	0.56
12:AB:165:PHE:CA	30:P:88:MET:HG3	2.33	0.56
16:AG:320:ARG:HB2	16:AG:323:GLN:HB2	1.88	0.56
10:B:6:G:HO2'	10:B:7:G:H8	1.54	0.56
10:B:60:U:P	10:B:61:C:H41	2.27	0.56
22:H:267:TRP:CH2	22:H:340:ARG:HB3	2.41	0.56
41:a:1818:U:OP2	48:h:156:ARG:NH1	2.38	0.56
9:9:17:GLU:HB3	9:9:86:MET:HB2	1.87	0.56
16:AG:380:THR:C	16:AG:384:LEU:CD1	2.79	0.56
16:AG:392:LEU:HD22	16:AG:395:ILE:HD11	1.87	0.56
10:A:11:A:H2'	10:A:12:G:C8	2.40	0.56
10:A:11:A:O5'	10:A:11:A:H8	1.89	0.56
12:AB:93:ILE:HG22	14:AE:290:ILE:HG22	1.88	0.56
14:AE:741:ALA:O	14:AE:762:ASN:ND2	2.38	0.56
16:AG:63:LEU:HD23	16:AG:63:LEU:N	2.21	0.56
16:AG:162:ILE:HG22	16:AG:162:ILE:O	2.06	0.56
16:AG:457:GLU:HG2	16:AG:489:CYS:SG	2.45	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:50:U:H2'	10:B:51:C:H6	1.70	0.56
10:A:56:C:C6	41:a:2168:G:C6	2.94	0.56
11:AA:818:VAL:HG22	11:AA:1096:ILE:HG12	1.87	0.56
14:AE:74:LYS:HD2	14:AE:85:CYS:SG	2.45	0.56
16:AG:49:ILE:HG22	16:AG:49:ILE:O	2.04	0.56
18:D:1308:U:H2'	38:X:98:ARG:HH22	1.62	0.56
22:H:330:VAL:HB	22:H:344:LEU:HD23	1.86	0.56
28:N:10:MET:HE3	28:N:61:LEU:HD11	1.87	0.56
39:Y:112:LYS:HZ2	39:Y:112:LYS:HB3	1.71	0.56
41:a:2249:U:H3'	41:a:2250:G:C5'	2.36	0.56
41:a:2314:A:O2'	54:n:155:THR:HG21	2.06	0.56
10:A:76:A:H2'	41:a:2394:C:N4	2.11	0.56
14:AE:1175:LEU:HD22	14:AE:1190:ILE:HD11	1.88	0.56
16:AG:173:PHE:N	16:AG:173:PHE:CD2	2.73	0.56
10:B:11:A:H8	10:B:11:A:O5'	1.89	0.56
39:Y:59:THR:HG22	39:Y:61:TYR:HE1	1.69	0.56
41:a:2303:G:C4	41:a:2314:A:C2	2.94	0.56
11:AA:913:VAL:N	16:AG:108:GLN:HG2	2.20	0.55
12:AB:140:PRO:HG3	30:P:6:ILE:CD1	2.33	0.55
16:AG:287:ALA:HB1	16:AG:331:LEU:CB	2.36	0.55
16:AG:354:ALA:HA	16:AG:357:ASP:H	1.70	0.55
16:AG:447:LYS:O	16:AG:470:ILE:HD11	2.05	0.55
10:B:60:U:O2'	10:B:61:C:OP1	2.23	0.55
39:Y:21:PRO:HB2	39:Y:22:PRO:CD	2.30	0.55
62:v:66:ARG:NH1	62:v:104:GLU:OE1	2.39	0.55
16:AG:365:ILE:HD11	16:AG:406:LEU:HD22	1.87	0.55
16:AG:448:LEU:HD22	16:AG:467:LEU:HD22	1.89	0.55
52:l:130:LYS:HB2	52:l:133:LEU:HD12	1.89	0.55
8:7:12:U:H3'	8:7:12:U:H6	1.70	0.55
11:AA:895:LEU:HD23	11:AA:895:LEU:N	2.12	0.55
11:AA:1070:HIS:NE2	11:AA:1114:GLU:OE1	2.36	0.55
12:AB:63:LYS:O	12:AB:63:LYS:HG2	2.07	0.55
13:AC:28:LEU:HD22	13:AC:201:LEU:HD23	1.88	0.55
14:AE:833:GLU:HB2	14:AE:1242:ARG:NH1	2.22	0.55
16:AG:362:TYR:CA	16:AG:413:ALA:HB1	2.31	0.55
37:W:15:LEU:HD13	37:W:33:THR:HG21	1.88	0.55
52:l:108:ILE:HD11	52:l:180:LEU:HD13	1.89	0.55
12:AB:65:PHE:CD2	12:AB:111:ILE:CD1	2.71	0.55
16:AG:133:HIS:CE1	16:AG:136:GLU:OE1	2.59	0.55
16:AG:285:ILE:O	16:AG:288:MET:CE	2.54	0.55
22:H:305:HIS:HD2	22:H:306:VAL:H	1.50	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:8:U:H5'	18:D:1397:C:N3	2.22	0.55
9:9:35:VAL:HA	9:9:38:MET:HB2	1.88	0.55
12:AB:165:PHE:HZ	30:P:91:ASP:HA	1.62	0.55
13:AD:308:ALA:HB1	16:AG:60:ARG:HD3	1.89	0.55
14:AE:144:TYR:HE1	14:AE:162:GLU:CD	2.14	0.55
22:H:154:PHE:CB	22:H:168:VAL:CB	2.85	0.55
34:T:5:THR:O	34:T:8:THR:OG1	2.18	0.55
41:a:404:A:O2'	41:a:405:U:OP2	2.22	0.55
8:7:11:U:O2	8:7:11:U:H2'	2.06	0.55
11:AA:806:PRO:O	14:AE:633:ALA:HA	2.06	0.55
14:AE:37:GLU:O	14:AE:61:ILE:CD1	2.52	0.55
16:AG:220:VAL:HG12	16:AG:245:ILE:HG21	1.88	0.55
16:AG:437:LEU:HD22	16:AG:488:ILE:HD12	1.88	0.55
8:7:1:A:C4	8:7:2:U:C5	2.95	0.55
11:AA:633:LEU:HD13	11:AA:644:LEU:HD23	1.89	0.55
11:AA:850:ILE:O	11:AA:850:ILE:HG22	2.05	0.55
11:AA:1142:ARG:NH2	11:AA:1166:ASP:OD1	2.38	0.55
12:AB:140:PRO:CG	30:P:102:LEU:HB2	2.36	0.55
16:AG:46:ARG:HH11	16:AG:61:ARG:HB3	1.71	0.55
16:AG:425:LEU:N	16:AG:429:LYS:HG3	2.20	0.55
18:D:563:A:N6	18:D:884:U:H3	2.05	0.55
18:D:1227:A:P	38:X:110:LYS:HZ1	2.29	0.55
22:H:45:GLU:OE1	22:H:45:GLU:N	2.40	0.55
6:5:110:DA:N7	11:AA:183:TRP:CH2	2.75	0.55
10:A:38:A:H2'	10:A:39:C:H5'	1.88	0.55
11:AA:516:ASP:OD1	11:AA:516:ASP:O	2.23	0.55
14:AE:198:CYS:HA	14:AE:221:ILE:HD11	1.87	0.55
18:D:1515:G:H2'	18:D:1516:G:H8	1.72	0.55
22:H:52:GLN:OE1	22:H:86:ARG:CB	2.55	0.55
8:7:3:G:H5"	18:D:1501:C:N4	2.21	0.55
8:7:21:U:C5'	23:I:80:LYS:HG2	2.37	0.55
13:AD:308:ALA:HB1	16:AG:96:GLN:CB	2.23	0.55
14:AE:903:LEU:HD21	14:AE:1249:ASN:HD22	1.70	0.55
14:AE:1155:ILE:HG13	14:AE:1210:ILE:HB	1.89	0.55
16:AG:130:PHE:O	16:AG:186:VAL:HG11	2.07	0.55
16:AG:168:LEU:CD2	16:AG:230:PRO:O	2.55	0.55
16:AG:355:ALA:HB1	16:AG:382:GLU:CB	2.36	0.55
21:G:38:VAL:CG2	22:H:75:VAL:CG2	2.77	0.55
22:H:22:SER:N	22:H:69:ASP:OD2	2.40	0.55
22:H:84:LEU:HD22	22:H:84:LEU:H	1.72	0.55
22:H:332:VAL:O	22:H:334:ASP:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:a:2000:C:OP1	63:w:5:LYS:NZ	2.36	0.55
16:AG:327:LEU:HD12	16:AG:327:LEU:O	2.07	0.55
7:6:26:DT:H2"	7:6:27:DG:H5'	1.88	0.54
12:AB:47:GLU:HB2	12:AB:63:LYS:HB2	1.87	0.54
14:AE:1166:GLY:HA3	14:AE:1174:ARG:HB2	1.88	0.54
3:2:50:LEU:HD23	45:e:26:PHE:CZ	2.42	0.54
12:AB:148:VAL:HG13	12:AB:148:VAL:O	2.06	0.54
14:AE:99:ARG:HH11	14:AE:99:ARG:CG	2.18	0.54
16:AG:320:ARG:NH1	16:AG:320:ARG:HG2	2.22	0.54
30:P:8:ILE:HD12	30:P:25:ILE:HD11	1.89	0.54
41:a:811:U:H2'	61:u:21:ARG:HA	1.89	0.54
64:x:35:ILE:HG21	64:x:71:ALA:HA	1.89	0.54
8:7:3:G:C3'	18:D:1500:A:N6	2.71	0.54
11:AA:360:LEU:HD13	11:AA:378:ARG:HH11	1.72	0.54
11:AA:855:PRO:HB2	16:AG:109:THR:CG2	2.30	0.54
16:AG:223:ILE:HD13	16:AG:223:ILE:C	2.32	0.54
16:AG:285:ILE:HD12	16:AG:293:VAL:HG11	1.88	0.54
11:AA:29:SER:O	11:AA:33:ASP:HB2	2.07	0.54
11:AA:143:ARG:NH2	11:AA:512:SER:O	2.40	0.54
11:AA:840:SER:HB2	11:AA:850:ILE:HD11	1.89	0.54
14:AE:39:LYS:O	14:AE:273:ILE:HG23	2.08	0.54
14:AE:46:TYR:CD1	14:AE:46:TYR:C	2.85	0.54
14:AE:145:VAL:HG23	14:AE:159:ILE:HG22	1.89	0.54
16:AG:387:VAL:HB	16:AG:388:PRO:HD2	1.85	0.54
22:H:279:LYS:HA	22:H:331:MET:CB	2.34	0.54
41:a:2192:U:H2'	41:a:2193:G:C8	2.43	0.54
47:g:18:CYS:HB3	47:g:40:CYS:HB2	1.88	0.54
11:AA:811:ASN:HA	11:AA:815:SER:HB2	1.90	0.54
12:AB:167:ARG:NH1	23:I:61:ALA:O	2.41	0.54
18:D:13:U:C2	18:D:915:A:C6	2.95	0.54
18:D:769:G:H4'	18:D:1513:A:H4'	1.88	0.54
18:D:1228:C:OP2	38:X:110:LYS:NZ	2.41	0.54
39:Y:116:MET:HG3	39:Y:124:MET:HB3	1.89	0.54
40:Z:2:ILE:HB	40:Z:5:ASP:HB3	1.89	0.54
52:l:131:THR:HG22	52:l:160:ALA:O	2.08	0.54
8:7:11:U:O2'	25:K:33:PHE:CZ	2.52	0.54
11:AA:243:PRO:HB2	11:AA:274:ILE:HG23	1.90	0.54
14:AE:30:ILE:HG21	14:AE:241:VAL:O	2.08	0.54
16:AG:254:MET:HG2	16:AG:257:ALA:HB2	1.60	0.54
16:AG:336:LEU:HD12	16:AG:336:LEU:N	2.01	0.54
18:D:439:U:O2	18:D:440:C:C5	2.61	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:961:U:O4	18:D:974:A:N1	2.40	0.54
22:H:321:VAL:HG13	22:H:322:VAL:HG23	1.90	0.54
7:6:2:DC:H2"	7:6:3:DC:C5	2.43	0.54
9:9:31:ARG:HD2	41:a:1054:A:C4'	2.29	0.54
10:A:12:G:H2'	10:A:13:C:OP1	2.08	0.54
13:AC:100:LEU:HD23	13:AC:115:ILE:HG21	1.90	0.54
14:AE:814:CYS:SG	14:AE:883:ARG:NH2	2.81	0.54
16:AG:131:ARG:HA	16:AG:186:VAL:CG1	2.38	0.54
16:AG:235:LYS:HG2	16:AG:235:LYS:O	2.07	0.54
16:AG:305:MET:HG3	16:AG:336:LEU:HB3	1.89	0.54
58:r:58:LEU:O	58:r:61:VAL:HG22	2.08	0.54
10:A:56:C:C2	41:a:2112:G:C8	2.96	0.54
14:AE:39:LYS:O	14:AE:273:ILE:HG21	2.06	0.54
16:AG:448:LEU:HD11	16:AG:481:LEU:HD13	1.89	0.54
11:AA:985:GLU:HB3	11:AA:988:LYS:HB2	1.89	0.54
14:AE:58:CYS:SG	14:AE:59:ALA:N	2.80	0.54
16:AG:288:MET:HE2	16:AG:293:VAL:HB	1.89	0.54
10:B:12:G:H2'	10:B:13:C:OP1	2.08	0.54
18:D:945:G:C2	18:D:946:A:C8	2.96	0.54
32:R:80:ILE:HD12	32:R:97:THR:HG22	1.89	0.54
39:Y:116:MET:HE2	39:Y:117:THR:H	1.73	0.54
42:b:37:ILE:HD11	42:b:82:ILE:HD11	1.90	0.54
8:7:21:U:P	23:I:80:LYS:HG2	2.48	0.54
9:9:43:LYS:HG2	9:9:98:GLU:HG2	1.90	0.54
11:AA:895:LEU:H	11:AA:895:LEU:CD2	2.07	0.54
11:AA:901:LEU:HD12	16:AG:8:VAL:HG13	1.68	0.54
14:AE:26:SER:HB2	14:AE:236:TRP:CE2	2.42	0.54
14:AE:124:ILE:HG23	14:AE:128:LEU:HD12	1.90	0.54
16:AG:434:LEU:CD2	16:AG:455:THR:O	2.50	0.54
10:B:76:A:N3	41:a:2493:U:H4'	2.24	0.54
22:H:116:VAL:C	22:H:279:LYS:HB2	2.33	0.54
39:Y:19:PRO:HG2	39:Y:24:GLY:H	1.73	0.54
41:a:1906:G:H5"	41:a:1906:G:H8	1.73	0.54
41:a:523:C:O2	41:a:554:U:O2'	2.25	0.53
41:a:1056:G:O2'	41:a:1103:A:N6	2.41	0.53
9:9:51:TYR:CD1	9:9:51:TYR:C	2.85	0.53
9:9:125:ARG:HA	9:9:125:ARG:CZ	2.38	0.53
12:AB:148:VAL:HA	12:AB:160:VAL:HA	1.90	0.53
14:AE:111:THR:HG22	14:AE:300:GLN:NE2	2.23	0.53
18:D:528:C:H6	18:D:528:C:H5"	1.71	0.53
22:H:135:LEU:CB	22:H:167:VAL:CA	2.86	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:K:94:VAL:HG13	25:K:111:MET:HE1	1.91	0.53
9:9:139:LEU:HD11	40:Z:11:VAL:HG13	1.90	0.53
11:AA:903:ARG:HH11	11:AA:903:ARG:C	2.16	0.53
13:AD:16:ILE:HG23	13:AD:26:VAL:HG22	1.91	0.53
14:AE:56:LEU:CD1	14:AE:273:ILE:HD12	2.39	0.53
14:AE:136:GLU:OE1	14:AE:312:ARG:CZ	2.55	0.53
16:AG:213:VAL:HG22	16:AG:213:VAL:O	2.08	0.53
16:AG:434:LEU:CG	16:AG:456:LEU:N	2.71	0.53
64:x:27:VAL:HG21	64:x:40:ILE:HD12	1.89	0.53
7:6:22:DC:H4'	11:AA:508:SER:OG	2.07	0.53
12:AB:140:PRO:HD2	30:P:102:LEU:CD2	2.38	0.53
14:AE:68:TYR:CA	14:AE:75:TYR:HE2	2.22	0.53
16:AG:374:VAL:O	16:AG:374:VAL:HG12	2.08	0.53
22:H:267:TRP:CZ3	22:H:340:ARG:HG3	2.43	0.53
25:K:99:ALA:HB1	25:K:103:THR:HG21	1.89	0.53
8:7:3:G:C4'	18:D:1500:A:H62	2.21	0.53
8:7:51:G:H2'	8:7:52:A:C8	2.43	0.53
10:A:6:G:O2'	10:A:7:G:H8	1.92	0.53
11:AA:900:LYS:HZ3	16:AG:11:ALA:HB1	1.72	0.53
14:AE:759:ILE:HG23	14:AE:771:GLN:HB3	1.89	0.53
16:AG:299:ASP:HB2	16:AG:303:HIS:HA	1.89	0.53
8:7:53:G:H2'	8:7:54:A:C8	2.44	0.53
9:9:58:THR:HG21	9:9:81:LEU:HA	1.90	0.53
9:9:62:ARG:HG2	9:9:62:ARG:NH2	2.20	0.53
10:A:17:C:O2	10:A:17:C:H2'	2.08	0.53
11:AA:628:HIS:HB3	11:AA:647:ARG:HH21	1.73	0.53
11:AA:684:ASN:OD1	11:AA:687:ARG:NH2	2.41	0.53
11:AA:888:THR:HB	11:AA:889:PRO:CD	2.37	0.53
18:D:13:U:C4	18:D:21:G:C2	2.96	0.53
22:H:84:LEU:H	22:H:84:LEU:CD2	2.21	0.53
39:Y:57:VAL:O	39:Y:57:VAL:HG12	2.07	0.53
39:Y:109:ALA:HB2	39:Y:128:ILE:HG13	1.89	0.53
9:9:123:ILE:O	9:9:123:ILE:HG12	2.08	0.53
11:AA:853:ASP:CG	16:AG:103:ASP:HB2	2.33	0.53
11:AA:1268:GLN:HE21	14:AE:352:ARG:HD2	1.66	0.53
12:AB:141:PHE:HB3	12:AB:144:PHE:HB2	1.91	0.53
12:AB:167:ARG:NH1	23:I:62:LYS:CB	2.71	0.53
10:B:18:G:C2	10:B:58:A:C5	2.97	0.53
39:Y:12:VAL:HG12	39:Y:23:VAL:HG21	1.90	0.53
39:Y:138:VAL:HG12	39:Y:138:VAL:O	2.08	0.53
8:7:3:G:H3'	18:D:1500:A:N6	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:78:GLY:H	9:9:79:PRO:HD2	1.68	0.53
14:AE:209:ASN:HA	14:AE:214:ARG:HH21	1.74	0.53
14:AE:785:ASP:O	14:AE:789:LYS:HB2	2.08	0.53
14:AE:802:ASP:OD1	14:AE:1348:LYS:NZ	2.31	0.53
10:B:17:C:O2	10:B:17:C:H2'	2.08	0.53
10:B:18:G:C8	10:B:57:A:N6	2.69	0.53
18:D:767:A:H2'	18:D:768:A:O4'	2.08	0.53
4:3:13:VAL:CG2	4:3:39:ILE:HD13	2.38	0.53
9:9:71:CYS:HA	9:9:117:LEU:HD13	1.91	0.53
11:AA:1284:ALA:HB3	14:AE:1361:THR:HB	1.90	0.53
14:AE:205:LEU:HG	14:AE:217:LEU:HB3	1.90	0.53
14:AE:746:LEU:HG	14:AE:758:PRO:HG3	1.90	0.53
10:B:6:G:O2'	10:B:7:G:H8	1.92	0.53
39:Y:37:PHE:CZ	39:Y:56:VAL:HG11	2.44	0.53
2:1:59:GLU:CG	2:1:66:ILE:HD11	2.38	0.53
9:9:93:ALA:O	9:9:129:LEU:HD13	2.06	0.53
10:A:18:G:C2	10:A:58:A:C5	2.96	0.53
10:A:38:A:C2'	10:A:39:C:H5'	2.39	0.53
16:AG:9:VAL:HG22	16:AG:24:PHE:CE2	2.44	0.53
16:AG:363:LEU:CG	16:AG:410:ALA:CB	2.71	0.53
22:H:135:LEU:CB	22:H:157:ILE:CB	2.87	0.53
8:7:56:G:O2'	14:AE:425:ARG:NH2	2.40	0.52
10:A:22:G:O2'	10:A:23:C:P	2.67	0.52
10:A:72:A:H2'	10:A:73:A:C5'	2.32	0.52
11:AA:143:ARG:NH1	11:AA:507:GLY:O	2.32	0.52
11:AA:1117:LEU:HD12	11:AA:1195:ILE:HG12	1.90	0.52
13:AC:43:LEU:HD13	13:AC:217:ILE:HD11	1.90	0.52
13:AD:28:LEU:HD12	13:AD:201:LEU:HD23	1.91	0.52
16:AG:63:LEU:HA	16:AG:92:TYR:HA	1.91	0.52
16:AG:179:VAL:HB	16:AG:199:ARG:HH11	1.73	0.52
16:AG:362:TYR:CE1	16:AG:414:LEU:HD21	2.43	0.52
10:B:72:A:H2'	10:B:73:A:C5'	2.33	0.52
22:H:19:ARG:O	22:H:72:LEU:HD22	2.09	0.52
22:H:49:PRO:HD2	22:H:84:LEU:CD1	2.39	0.52
10:A:16:C:O2	10:A:16:C:H2'	2.09	0.52
11:AA:103:VAL:HB	11:AA:114:VAL:HG11	1.89	0.52
16:AG:233:ARG:C	16:AG:327:LEU:HD21	2.34	0.52
14:AE:78:LEU:O	14:AE:78:LEU:HD13	2.08	0.52
16:AG:285:ILE:HD12	16:AG:293:VAL:HG21	1.92	0.52
10:B:16:C:O2	10:B:16:C:H2'	2.09	0.52
10:B:22:G:O2'	10:B:23:C:P	2.67	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:n:8:TYR:HA	54:n:12:VAL:HB	1.91	0.52
10:A:56:C:C3'	10:A:57:A:H5"	2.40	0.52
12:AB:141:PHE:HE2	12:AB:171:VAL:CG1	2.23	0.52
14:AE:99:ARG:HG3	14:AE:99:ARG:HH11	1.74	0.52
16:AG:11:ALA:HB3	16:AG:12:VAL:HA	1.92	0.52
16:AG:398:LEU:HG	16:AG:398:LEU:O	2.09	0.52
17:C:61:ARG:NH2	18:D:736:C:OP1	2.43	0.52
18:D:1329:A:OP1	38:X:28:THR:N	2.42	0.52
11:AA:714:VAL:HB	11:AA:787:PRO:HD2	1.92	0.52
11:AA:857:VAL:CG1	11:AA:861:ALA:CB	2.71	0.52
11:AA:894:GLN:NE2	11:AA:894:GLN:H	2.04	0.52
14:AE:215:LYS:HA	14:AE:218:THR:HG22	1.91	0.52
14:AE:291:ILE:HG22	14:AE:292:VAL:HG13	1.91	0.52
23:I:77:ILE:HA	23:I:84:VAL:HG23	1.91	0.52
39:Y:33:ASN:H	39:Y:66:PHE:HE1	1.56	0.52
41:a:1980:G:O2'	41:a:1982:U:OP2	2.28	0.52
13:AD:100:LEU:HD21	13:AD:121:VAL:HG11	1.90	0.52
14:AE:144:TYR:CE1	14:AE:162:GLU:CD	2.88	0.52
16:AG:244:ARG:CD	16:AG:244:ARG:N	2.73	0.52
22:H:119:GLY:CA	22:H:133:GLY:CA	2.74	0.52
39:Y:27:LEU:HD12	39:Y:27:LEU:C	2.35	0.52
41:a:639:U:H2'	41:a:640:C:C6	2.45	0.52
8:7:17:U:H2'	8:7:18:U:H5"	1.90	0.52
8:7:47:U:C2	11:AA:1253:LEU:HD12	2.37	0.52
10:A:12:G:C2'	10:A:13:C:OP1	2.58	0.52
11:AA:618:GLN:HG3	14:AE:770:LEU:CD1	2.38	0.52
11:AA:855:PRO:HG3	16:AG:108:GLN:OE1	2.10	0.52
16:AG:254:MET:H	16:AG:257:ALA:HB3	1.74	0.52
10:B:56:C:C5'	54:n:80:ARG:CZ	2.76	0.52
18:D:673:A:H2'	18:D:674:G:C8	2.44	0.52
21:G:35:ARG:NH2	22:H:10:GLU:HG2	2.25	0.52
4:3:94:ARG:HB3	4:3:103:ILE:HD12	1.92	0.52
18:D:60:A:N1	18:D:107:G:O2'	2.42	0.52
18:D:864:A:C2	18:D:865:A:C2	2.98	0.52
41:a:2298:A:C5	41:a:2321:U:O4	2.62	0.52
60:t:7:MET:HE1	60:t:44:LYS:HD2	1.91	0.52
8:7:14:U:H3'	8:7:14:U:H6	1.75	0.52
9:9:3:LEU:HD13	9:9:5:LEU:H	1.75	0.52
10:A:60:U:O2'	10:A:61:C:OP1	2.23	0.52
12:AB:23:ALA:HB2	12:AB:44:VAL:CG1	2.39	0.52
12:AB:63:LYS:HG2	12:AB:66:PRO:HB3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:140:PRO:HB2	30:P:84:VAL:CG1	2.39	0.52
15:AF:3:ARG:NH1	15:AF:55:GLU:OE2	2.40	0.52
16:AG:139:THR:HA	16:AG:180:ARG:HA	1.92	0.52
16:AG:360:THR:HG22	16:AG:360:THR:O	2.10	0.52
22:H:24:VAL:HG12	22:H:69:ASP:H	1.74	0.52
63:w:38:LEU:N	63:w:39:PRO:CD	2.73	0.52
8:7:3:G:C4'	18:D:1500:A:N6	2.73	0.52
8:7:51:G:H2'	8:7:52:A:H8	1.75	0.52
9:9:41:LEU:HD12	39:Y:117:THR:HG22	1.92	0.52
11:AA:125:GLY:HA2	11:AA:499:SER:HB2	1.92	0.52
12:AB:106:LYS:HA	12:AB:109:ASP:HB2	1.92	0.52
13:AD:205:MET:HE3	13:AD:213:PRO:HB3	1.91	0.52
16:AG:285:ILE:CD1	16:AG:285:ILE:N	2.73	0.52
16:AG:442:ARG:C	16:AG:446:PHE:HD2	2.15	0.52
10:B:12:G:C2'	10:B:13:C:OP1	2.57	0.52
39:Y:112:LYS:NZ	39:Y:112:LYS:CB	2.73	0.52
41:a:587:C:OP2	61:u:21:ARG:NH1	2.43	0.52
41:a:929:U:H1'	46:f:26:GLY:O	2.10	0.52
60:t:71:ARG:NH2	60:t:123:LEU:O	2.42	0.52
4:3:12:ILE:HG21	4:3:80:ALA:HB2	1.92	0.51
9:9:11:ILE:CD1	9:9:11:ILE:N	2.73	0.51
9:9:23:LEU:HA	9:9:118:ILE:HG13	1.92	0.51
11:AA:853:ASP:CA	16:AG:105:ILE:HG21	2.37	0.51
11:AA:901:LEU:HG	16:AG:8:VAL:CG1	2.39	0.51
12:AB:44:VAL:CG2	12:AB:69:VAL:CG1	2.83	0.51
14:AE:99:ARG:HA	14:AE:248:ASP:HB2	1.92	0.51
14:AE:390:LEU:N	14:AE:390:LEU:CD1	2.73	0.51
14:AE:804:ALA:O	14:AE:806:ASP:N	2.41	0.51
14:AE:850:LYS:HB2	14:AE:857:LEU:HB2	1.92	0.51
16:AG:282:GLN:NE2	16:AG:282:GLN:CA	2.73	0.51
16:AG:440:VAL:HG21	16:AG:481:LEU:HD22	1.88	0.51
10:B:15:G:H22	10:B:20:U:H3	1.58	0.51
25:K:81:LEU:HD13	25:K:123:VAL:HG12	1.92	0.51
11:AA:93:SER:HA	11:AA:128:PRO:HA	1.93	0.51
14:AE:112:ALA:HA	14:AE:238:ILE:HA	1.91	0.51
16:AG:362:TYR:CE2	16:AG:382:GLU:HG2	2.45	0.51
16:AG:453:VAL:HG11	16:AG:459:LEU:CD2	2.41	0.51
10:B:56:C:C3'	10:B:57:A:H5"	2.40	0.51
17:C:30:LYS:HA	17:C:33:ILE:HD13	1.91	0.51
18:D:1308:U:P	38:X:98:ARG:HG3	2.50	0.51
22:H:49:PRO:HD2	22:H:84:LEU:HD11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:a:523:C:H4'	41:a:540:C:O2	2.09	0.51
41:a:1693:U:O2'	48:h:14:ARG:NH2	2.43	0.51
11:AA:246:LEU:HB3	11:AA:269:ILE:HD13	1.92	0.51
11:AA:255:ILE:HB	11:AA:263:VAL:HB	1.93	0.51
14:AE:832:LYS:HB3	14:AE:1242:ARG:NH1	2.24	0.51
16:AG:444:LEU:HD22	16:AG:473:LEU:HD21	1.92	0.51
22:H:332:VAL:C	22:H:334:ASP:H	2.18	0.51
41:a:2328:A:H2'	41:a:2329:U:C6	2.44	0.51
10:A:19:G:C5	41:a:2112:G:H4'	2.44	0.51
14:AE:975:ILE:HD11	14:AE:1003:LEU:HD11	1.91	0.51
16:AG:254:MET:H	16:AG:257:ALA:CB	2.23	0.51
16:AG:402:THR:HA	16:AG:405:ALA:HB3	1.91	0.51
41:a:1266:G:OP2	49:i:17:ARG:NE	2.43	0.51
59:s:17:VAL:HG23	59:s:137:PRO:HB2	1.92	0.51
12:AB:172:GLU:N	12:AB:172:GLU:OE1	2.44	0.51
41:a:2315:G:O2'	54:n:125:ARG:HD3	2.09	0.51
2:1:93:ALA:HB2	41:a:1614:A:N1	2.25	0.51
8:7:52:A:H2'	8:7:53:G:C8	2.46	0.51
9:9:125:ARG:O	9:9:125:ARG:HG3	2.10	0.51
11:AA:524:ILE:HG21	11:AA:708:VAL:HG13	1.92	0.51
12:AB:93:ILE:HG21	14:AE:291:ILE:CA	2.40	0.51
16:AG:233:ARG:NH1	16:AG:324:ASN:HB2	2.25	0.51
16:AG:422:GLU:CA	16:AG:426:GLY:N	2.62	0.51
39:Y:59:THR:HG22	39:Y:61:TYR:CE1	2.45	0.51
6:5:101:DT:H72	14:AE:271:ARG:CZ	2.41	0.51
8:7:2:U:H2'	8:7:3:G:C8	2.45	0.51
13:AC:140:ILE:HD12	13:AC:142:MET:HE3	1.92	0.51
14:AE:24:LEU:CB	14:AE:232:ASN:OD1	2.54	0.51
14:AE:437:PHE:HZ	14:AE:453:VAL:HG11	1.76	0.51
10:B:15:G:N3	10:B:15:G:C2'	2.73	0.51
22:H:308:GLU:O	22:H:310:ASP:N	2.44	0.51
34:T:40:GLN:CA	34:T:40:GLN:HE21	2.23	0.51
41:a:1141:U:O2	41:a:1142:A:N6	2.44	0.51
9:9:31:ARG:HG3	9:9:31:ARG:NH1	2.17	0.51
10:A:18:G:C2	10:A:58:A:C6	2.99	0.51
14:AE:88:CYS:HB3	14:AE:90:VAL:HG12	1.92	0.51
16:AG:329:SER:HA	16:AG:336:LEU:HG	1.92	0.51
18:D:1276:G:O5'	18:D:1276:G:H8	1.93	0.51
18:D:1499:A:O2'	18:D:1500:A:H5'	2.10	0.51
41:a:1964:G:H4'	41:a:1965:C:OP2	2.11	0.51
10:A:48:C:H2'	10:A:48:C:O2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:974:ARG:HD2	11:AA:1014:LEU:HD21	1.92	0.51
12:AB:167:ARG:NH2	12:AB:167:ARG:CG	2.73	0.51
14:AE:201:LEU:HD12	14:AE:224:LEU:HD12	1.92	0.51
16:AG:12:VAL:HG23	16:AG:16:LYS:HE2	1.92	0.51
18:D:1404:C:H2'	18:D:1404:C:O2	2.10	0.51
2:1:24:ILE:HD13	2:1:36:LEU:HD11	1.93	0.51
10:A:76:A:O2'	41:a:2395:C:C2	2.64	0.51
11:AA:400:VAL:HG21	11:AA:452:ARG:HE	1.76	0.51
12:AB:68:TYR:CE2	14:AE:291:ILE:HG23	2.46	0.51
12:AB:71:VAL:HG12	12:AB:73:MET:HB2	1.93	0.51
18:D:1228:C:OP1	38:X:107:ARG:CZ	2.58	0.51
41:a:1869:G:N2	41:a:1871:A:O2'	2.44	0.51
41:a:1910:G:O5'	41:a:1910:G:H8	1.92	0.51
41:a:2243:U:H2'	41:a:2244:U:C6	2.46	0.51
66:z:58:ARG:HA	66:z:61:TRP:CE3	2.45	0.51
10:A:56:C:H2'	10:A:57:A:C5'	2.27	0.50
18:D:1410:A:C2	18:D:1491:G:C2	2.99	0.50
39:Y:100:ILE:HB	39:Y:105:LEU:HD11	1.92	0.50
1:0:14:VAL:HG21	1:0:98:ILE:HG13	1.93	0.50
2:1:59:GLU:HG3	2:1:66:ILE:HD11	1.92	0.50
11:AA:400:VAL:HG11	11:AA:452:ARG:HD2	1.94	0.50
11:AA:411:ARG:NH2	11:AA:427:ASP:OD2	2.44	0.50
12:AB:167:ARG:NH1	23:I:62:LYS:C	2.58	0.50
16:AG:5:ILE:HA	16:AG:8:VAL:HB	1.93	0.50
16:AG:65:VAL:HG12	16:AG:66:ASP:H	1.76	0.50
10:B:18:G:C2	10:B:58:A:C6	2.99	0.50
29:O:98:LEU:HB3	29:O:104:VAL:HG13	1.92	0.50
41:a:118:A:C8	41:a:119:A:C8	2.99	0.50
41:a:995:C:O2	59:s:3:THR:OG1	2.24	0.50
2:1:55:ILE:HG23	2:1:66:ILE:HD12	1.93	0.50
9:9:50:VAL:HG13	39:Y:119:ALA:HB3	1.88	0.50
10:A:56:C:C5	41:a:2168:G:O6	2.65	0.50
14:AE:683:ILE:HD12	14:AE:754:ILE:HG21	1.93	0.50
16:AG:384:LEU:O	16:AG:387:VAL:HG23	2.11	0.50
18:D:108:G:H5"	18:D:108:G:N3	2.27	0.50
53:m:31:LEU:HD22	53:m:42:LEU:CD1	2.40	0.50
11:AA:146:VAL:HG21	11:AA:513:GLN:HE21	1.77	0.50
16:AG:21:GLU:HB3	16:AG:49:ILE:HD12	1.91	0.50
11:AA:845:LEU:HD23	11:AA:889:PRO:HB2	1.93	0.50
11:AA:1101:LEU:HD21	14:AE:508:LEU:HD22	1.92	0.50
12:AB:129:GLU:H	12:AB:180:LYS:CD	2.24	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:421:VAL:O	14:AE:436:ALA:HA	2.12	0.50
18:D:1366:C:O2'	30:P:62:ARG:NH2	2.45	0.50
60:t:43:ILE:HD12	60:t:56:ASP:HB2	1.93	0.50
9:9:51:TYR:CG	9:9:89:PRO:HD2	2.47	0.50
10:A:15:G:N3	10:A:15:G:C2'	2.73	0.50
11:AA:562:GLU:OE1	11:AA:662:SER:OG	2.28	0.50
14:AE:749:LYS:HB3	14:AE:755:ILE:HD11	1.94	0.50
16:AG:448:LEU:CG	16:AG:473:LEU:HD11	2.42	0.50
22:H:117:LYS:CB	22:H:278:THR:CG2	2.90	0.50
30:P:57:VAL:O	30:P:57:VAL:HG13	2.10	0.50
53:m:22:MET:O	53:m:28:ARG:NH1	2.45	0.50
59:s:32:LEU:CD2	59:s:54:ILE:HG21	2.42	0.50
63:w:55:ALA:HA	63:w:80:PHE:CE1	2.47	0.50
12:AB:11:VAL:CG2	12:AB:103:ILE:HD13	2.38	0.50
16:AG:285:ILE:HD13	16:AG:285:ILE:H	1.76	0.50
10:B:34:C:O2	10:B:34:C:H2'	2.11	0.50
41:a:1824:G:O2'	48:h:252:THR:HG21	2.11	0.50
44:d:106:G:H2'	44:d:107:G:O4'	2.10	0.50
50:j:25:THR:HG21	50:j:193:VAL:HG22	1.94	0.50
8:7:6:U:C2	18:D:1493:A:C2	3.00	0.50
10:A:56:C:H1'	41:a:2112:G:C5	2.46	0.50
12:AB:167:ARG:NE	23:I:61:ALA:C	2.53	0.50
16:AG:216:ILE:HG12	16:AG:221:ILE:HB	1.93	0.50
10:B:24:U:O2'	41:a:1922:G:O3'	2.29	0.50
18:D:1208:C:H2'	18:D:1209:C:C6	2.47	0.50
28:N:3:MET:HA	28:N:3:MET:HE3	1.94	0.50
34:T:4:SER:O	34:T:8:THR:HG23	2.12	0.50
6:5:96:DT:H2"	6:5:97:DC:C5	2.46	0.50
9:9:44:ALA:HB1	9:9:52:MET:HB3	1.94	0.50
10:A:37:A:H2'	10:A:38:A:H8	1.77	0.50
10:A:41:C:H4'	27:M:143:ARG:NH1	2.26	0.50
11:AA:232:ILE:HG12	11:AA:237:LEU:HG	1.94	0.50
16:AG:183:LEU:HD23	16:AG:197:VAL:HG22	1.94	0.50
10:B:47:U:H2'	10:B:48:C:H4'	1.93	0.50
41:a:2093:G:O2'	41:a:2198:A:N1	2.41	0.50
41:a:2557:G:H2'	41:a:2558:C:C6	2.46	0.50
41:a:2646:C:O5'	41:a:2646:C:H6	1.95	0.50
44:d:5:U:OP1	44:d:61:G:O2'	2.26	0.50
48:h:107:PRO:HD2	48:h:110:LEU:HD22	1.94	0.50
56:p:121:ILE:HD12	56:p:141:ILE:CG2	2.40	0.50
10:A:11:A:H2'	10:A:12:G:C1'	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:529:ARG:HH11	11:AA:572:ILE:HG22	1.77	0.49
14:AE:275:ARG:HH12	14:AE:278:ARG:NH1	2.09	0.49
14:AE:972:LYS:HD2	14:AE:1004:ALA:HA	1.93	0.49
16:AG:123:ARG:NH1	16:AG:123:ARG:HG2	2.26	0.49
16:AG:305:MET:HG2	16:AG:336:LEU:HA	1.94	0.49
18:D:872:A:H2'	18:D:872:A:N3	2.27	0.49
54:n:127:ASN:ND2	54:n:127:ASN:N	2.59	0.49
8:7:2:U:OP2	18:D:926:G:N2	2.45	0.49
10:A:28:C:H2'	10:A:29:G:H8	1.76	0.49
11:AA:857:VAL:HB	11:AA:862:LEU:HD11	1.93	0.49
11:AA:1336:ASN:ND2	14:AE:29:MET:HG2	2.27	0.49
12:AB:103:ILE:CG1	12:AB:107:GLU:OE2	2.60	0.49
14:AE:145:VAL:HG12	14:AE:184:ALA:HB1	1.94	0.49
16:AG:171:GLU:OE2	16:AG:267:GLY:C	2.54	0.49
16:AG:283:PHE:CE2	16:AG:332:SER:HA	2.47	0.49
16:AG:422:GLU:O	16:AG:427:ASP:N	2.45	0.49
16:AG:429:LYS:HD2	16:AG:429:LYS:N	2.24	0.49
16:AG:433:ASP:O	16:AG:456:LEU:HD21	2.12	0.49
10:B:48:C:O2	10:B:48:C:H2'	2.11	0.49
22:H:132:PRO:N	22:H:167:VAL:CB	2.75	0.49
41:a:464:U:O3'	53:m:12:ARG:NH2	2.45	0.49
41:a:742:A:C2	41:a:743:A:C6	3.00	0.49
41:a:1814:G:H4'	48:h:51:THR:HG21	1.93	0.49
63:w:67:PHE:O	63:w:71:ARG:N	2.45	0.49
66:z:47:TYR:CD1	66:z:47:TYR:C	2.90	0.49
9:9:52:MET:HE3	9:9:52:MET:CA	2.42	0.49
11:AA:18:ARG:HE	11:AA:620:ASN:HA	1.77	0.49
11:AA:896:THR:HG23	11:AA:899:GLU:HG2	1.94	0.49
13:AD:309:SER:CB	16:AG:40:GLU:CD	2.85	0.49
14:AE:799:ARG:HG2	14:AE:1325:PHE:HZ	1.77	0.49
14:AE:1371:ARG:HE	14:AE:1372:ARG:NH1	2.10	0.49
18:D:1499:A:H3'	18:D:1499:A:OP2	2.12	0.49
20:F:4:ILE:HD12	20:F:19:PHE:HA	1.93	0.49
39:Y:80:LYS:HG3	39:Y:86:LYS:HA	1.93	0.49
60:t:113:MET:O	60:t:116:ILE:HG13	2.11	0.49
6:5:108:DT:H73	11:AA:199:ASP:HB3	1.94	0.49
11:AA:862:LEU:O	11:AA:862:LEU:HD23	2.11	0.49
16:AG:64:VAL:HA	16:AG:75:ILE:HB	1.94	0.49
24:J:61:VAL:HG21	24:J:200:ILE:CD1	2.35	0.49
41:a:565:C:H2'	41:a:566:U:O4'	2.13	0.49
16:AG:130:PHE:C	16:AG:186:VAL:CG1	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:358:THR:O	16:AG:358:THR:OG1	2.25	0.49
22:H:318:PRO:HA	22:H:321:VAL:HG12	1.95	0.49
41:a:2297:A:C6	41:a:2321:U:O4	2.65	0.49
56:p:35:ARG:HD3	56:p:71:LEU:HD13	1.94	0.49
8:7:8:U:H5'	18:D:1397:C:C2	2.48	0.49
10:A:76:A:C2'	41:a:2394:C:N4	2.75	0.49
12:AB:140:PRO:CG	30:P:102:LEU:HB3	2.42	0.49
14:AE:800:LEU:HB3	14:AE:920:ALA:HB1	1.95	0.49
16:AG:393:LEU:CG	16:AG:398:LEU:HD22	2.22	0.49
16:AG:399:ASP:OD2	16:AG:399:ASP:N	2.39	0.49
41:a:2303:G:C6	41:a:2314:A:N1	2.81	0.49
10:A:49:G:H8	10:A:49:G:O5'	1.96	0.49
14:AE:152:THR:HB	14:AE:172:PHE:CZ	2.48	0.49
14:AE:550:VAL:O	14:AE:569:LEU:HA	2.13	0.49
16:AG:453:VAL:HG11	16:AG:459:LEU:CG	2.42	0.49
58:r:3:VAL:HG22	58:r:36:ALA:HB1	1.95	0.49
8:7:6:U:C2	18:D:1493:A:H2	2.31	0.49
11:AA:900:LYS:HD2	16:AG:11:ALA:CB	2.37	0.49
12:AB:167:ARG:HE	23:I:62:LYS:HB2	1.77	0.49
16:AG:440:VAL:HG22	16:AG:481:LEU:HD21	1.95	0.49
16:AG:453:VAL:HG11	16:AG:459:LEU:HD23	1.95	0.49
18:D:1356:G:H2'	18:D:1357:A:C8	2.47	0.49
41:a:1412:U:C4	41:a:1413:A:N7	2.81	0.49
6:5:98:DA:N9	6:5:99:DT:H72	2.27	0.49
6:5:110:DA:N7	11:AA:183:TRP:HH2	2.11	0.49
8:7:8:U:OP2	18:D:1397:C:C2	2.66	0.49
9:9:31:ARG:HD2	41:a:1054:A:H5'	1.80	0.49
11:AA:900:LYS:HZ3	16:AG:11:ALA:C	2.20	0.49
11:AA:903:ARG:HH11	11:AA:903:ARG:HB3	1.77	0.49
14:AE:201:LEU:HD11	14:AE:220:ARG:HG2	1.95	0.49
16:AG:285:ILE:HG23	16:AG:293:VAL:HG11	1.82	0.49
10:B:76:A:N3	10:B:76:A:C2'	2.74	0.49
18:D:5:U:O2	18:D:5:U:O4'	2.29	0.49
18:D:974:A:OP1	33:S:69:ARG:NH1	2.46	0.49
18:D:1311:A:OP1	47:g:59:ARG:NH1	2.45	0.49
30:P:6:ILE:HG23	30:P:100:ILE:CG2	2.43	0.49
41:a:2038:G:H2'	41:a:2039:U:O4'	2.12	0.49
7:6:21:DA:N6	8:7:51:G:N1	2.61	0.49
10:A:42:G:H2'	10:A:43:A:C8	2.47	0.49
11:AA:812:PHE:HA	14:AE:505:ASP:OD2	2.13	0.49
11:AA:862:LEU:C	11:AA:862:LEU:CD2	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AD:100:LEU:HB2	13:AD:144:ILE:HG23	1.94	0.49
16:AG:369:PHE:O	16:AG:373:LEU:HG	2.12	0.49
10:B:25:C:H2'	10:B:26:G:H5'	1.95	0.49
18:D:1017:U:O2'	18:D:1018:G:O4'	2.31	0.49
25:K:114:VAL:HG21	25:K:141:ILE:HD12	1.94	0.49
41:a:1433:A:H2'	41:a:1434:A:O4'	2.13	0.49
1:0:14:VAL:CG2	1:0:98:ILE:HG13	2.43	0.48
11:AA:9:LYS:HG2	11:AA:1171:ARG:HH12	1.77	0.48
11:AA:857:VAL:CB	11:AA:862:LEU:CD1	2.91	0.48
14:AE:67:ASP:CG	14:AE:95:THR:HG1	2.19	0.48
16:AG:240:THR:HG21	16:AG:247:PRO:HG3	1.92	0.48
16:AG:254:MET:C	16:AG:256:GLY:N	2.69	0.48
16:AG:277:ASP:HB2	16:AG:282:GLN:HG3	1.95	0.48
16:AG:296:ILE:HD11	16:AG:307:ILE:HD13	1.93	0.48
16:AG:444:LEU:HD22	16:AG:473:LEU:CD2	2.43	0.48
10:B:5:G:C2'	10:B:6:G:H5'	2.40	0.48
10:B:49:G:O5'	10:B:49:G:H8	1.96	0.48
34:T:21:ASP:O	34:T:22:THR:HG22	2.12	0.48
41:a:2298:A:N3	41:a:2321:U:C5	2.80	0.48
46:f:24:LEU:HD11	46:f:54:MET:CE	2.42	0.48
1:0:40:MET:HE3	1:0:49:ILE:CD1	2.43	0.48
9:9:8:LYS:NZ	41:a:1046:A:H61	2.11	0.48
10:A:47:U:H2'	10:A:48:C:H4'	1.94	0.48
11:AA:732:ILE:HD11	11:AA:769:PRO:HB3	1.95	0.48
11:AA:905:ILE:CD1	16:AG:8:VAL:HG11	2.43	0.48
14:AE:117:LEU:HG	14:AE:118:LYS:HG3	1.95	0.48
14:AE:809:VAL:HG21	14:AE:909:ILE:HG12	1.95	0.48
16:AG:148:ASP:HA	16:AG:164:ARG:CD	2.44	0.48
18:D:50:A:O2'	18:D:360:G:N2	2.45	0.48
36:V:75:LEU:C	36:V:75:LEU:HD12	2.38	0.48
42:b:37:ILE:HG21	42:b:80:ILE:HG21	1.95	0.48
53:m:24:THR:HG23	53:m:27:GLY:H	1.78	0.48
59:s:30:THR:HG22	59:s:31:GLU:N	2.27	0.48
16:AG:353:HIS:O	16:AG:356:ILE:CB	2.58	0.48
16:AG:448:LEU:HD23	16:AG:473:LEU:HD12	1.95	0.48
2:1:4:ILE:HG12	2:1:106:VAL:HG22	1.95	0.48
10:A:37:A:H2'	10:A:38:A:C8	2.48	0.48
11:AA:554:HIS:HD2	11:AA:558:VAL:HB	1.77	0.48
11:AA:900:LYS:CE	16:AG:11:ALA:HB1	2.43	0.48
14:AE:115:TRP:O	14:AE:1333:THR:HG21	2.13	0.48
16:AG:18:LEU:HB3	16:AG:19:PRO:HD2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:62:TRP:CD1	16:AG:95:ASP:HB2	2.49	0.48
16:AG:342:ASP:N	16:AG:342:ASP:OD1	2.45	0.48
10:B:11:A:C2'	10:B:12:G:O4'	2.60	0.48
18:D:1064:G:O2'	18:D:1190:G:N2	2.47	0.48
18:D:1169:A:H2'	18:D:1170:A:C8	2.48	0.48
22:H:23:ILE:N	22:H:69:ASP:OD2	2.47	0.48
26:L:18:VAL:N	26:L:19:PRO:CD	2.76	0.48
39:Y:77:VAL:HG13	39:Y:80:LYS:CE	2.44	0.48
9:9:51:TYR:CD1	9:9:88:HIS:HB2	2.49	0.48
10:A:25:C:H2'	10:A:26:G:H5'	1.94	0.48
10:A:76:A:N6	41:a:2422:C:O4'	2.46	0.48
11:AA:565:GLU:HA	11:AA:569:ILE:HG12	1.95	0.48
11:AA:903:ARG:HH11	11:AA:903:ARG:CG	2.25	0.48
14:AE:1261:LEU:HD12	14:AE:1304:ARG:HH21	1.78	0.48
16:AG:288:MET:O	16:AG:288:MET:HG2	2.13	0.48
22:H:120:PHE:CB	22:H:136:VAL:CB	2.90	0.48
41:a:2685:G:OP1	60:t:78:ARG:NH2	2.47	0.48
43:c:3:ARG:HD2	43:c:30:LEU:HD22	1.94	0.48
48:h:210:ALA:HA	48:h:213:TRP:CE3	2.48	0.48
50:j:121:THR:HB	50:j:127:PHE:CD2	2.49	0.48
2:1:25:ARG:NH1	2:1:74:ILE:O	2.46	0.48
4:3:7:ARG:HB2	41:a:85:G:OP2	2.13	0.48
8:7:21:U:P	23:I:81:GLY:N	2.86	0.48
10:A:18:G:C5	10:A:57:A:C5	3.01	0.48
11:AA:786:GLY:N	11:AA:789:THR:OG1	2.41	0.48
11:AA:1286:THR:O	11:AA:1290:MET:HB2	2.14	0.48
12:AB:11:VAL:HG11	14:AE:291:ILE:CG1	2.43	0.48
13:AD:182:ARG:O	13:AD:205:MET:HA	2.13	0.48
14:AE:1347:LEU:HG	14:AE:1357:ILE:HG23	1.96	0.48
16:AG:316:GLN:HE21	16:AG:316:GLN:HB2	1.49	0.48
16:AG:363:LEU:HD11	16:AG:410:ALA:HB2	1.92	0.48
10:B:18:G:C5	10:B:57:A:C5	3.01	0.48
50:j:4:LEU:HD23	50:j:29:VAL:CG1	2.39	0.48
10:A:15:G:C2	10:A:20:U:O2	2.66	0.48
10:A:59:A:H2'	10:A:60:U:H5'	1.94	0.48
12:AB:155:LYS:HE3	18:D:1277:C:H3'	1.93	0.48
14:AE:220:ARG:HG2	14:AE:220:ARG:NH1	2.26	0.48
16:AG:131:ARG:O	16:AG:134:GLU:CG	2.47	0.48
16:AG:243:LYS:O	16:AG:243:LYS:HD3	2.14	0.48
16:AG:320:ARG:CG	16:AG:320:ARG:NH1	2.73	0.48
16:AG:361:LYS:HD2	16:AG:417:ILE:HG12	1.92	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:39:C:O5'	10:B:39:C:H6	1.95	0.48
21:G:35:ARG:CD	22:H:14:LYS:HD3	2.40	0.48
22:H:72:LEU:CD1	22:H:72:LEU:N	2.72	0.48
50:j:156:PHE:CE1	59:s:81:ILE:HD13	2.48	0.48
10:A:18:G:N3	10:A:58:A:C6	2.82	0.48
12:AB:11:VAL:HG11	14:AE:291:ILE:HD11	1.96	0.48
12:AB:129:GLU:N	12:AB:180:LYS:HG3	2.29	0.48
18:D:13:U:C4	18:D:915:A:C6	2.92	0.48
18:D:911:U:H2'	18:D:912:C:C6	2.49	0.48
25:K:99:ALA:CB	25:K:103:THR:HG21	2.43	0.48
64:x:51:ALA:HB3	64:x:78:VAL:HB	1.94	0.48
8:7:7:U:C6	8:7:7:U:C3'	2.97	0.48
10:A:41:C:H5'	27:M:143:ARG:HD2	1.96	0.48
11:AA:363:LEU:HB3	11:AA:381:ALA:HB1	1.96	0.48
12:AB:68:TYR:CZ	14:AE:291:ILE:HG23	2.49	0.48
14:AE:47:ARG:CZ	14:AE:47:ARG:HB2	2.44	0.48
14:AE:53:ARG:HA	14:AE:54:ASP:HA	1.56	0.48
14:AE:102:MET:HG2	14:AE:246:PRO:HD3	1.95	0.48
16:AG:59:PHE:CD1	16:AG:97:ILE:HG23	2.48	0.48
16:AG:63:LEU:HD22	16:AG:92:TYR:CD1	2.47	0.48
10:B:59:A:H2'	10:B:60:U:H5'	1.94	0.48
10:B:68:C:C4	10:B:69:C:C5	3.02	0.48
18:D:35:G:N3	32:R:115:SER:OG	2.47	0.48
18:D:1174:G:H2'	18:D:1175:G:H5'	1.95	0.48
41:a:1588:G:C6	41:a:1589:U:O4	2.67	0.48
41:a:2303:G:C2	41:a:2314:A:N3	2.82	0.48
10:A:5:G:C2'	10:A:6:G:H5'	2.39	0.48
11:AA:836:LEU:HD13	11:AA:1054:LEU:HD13	1.95	0.48
12:AB:155:LYS:HA	18:D:1276:G:OP2	2.13	0.48
14:AE:103:GLY:H	14:AE:244:VAL:HG22	1.78	0.48
14:AE:891:ASP:OD2	14:AE:1290:ARG:NH2	2.47	0.48
14:AE:968:ASN:HA	14:AE:1117:SER:HB2	1.96	0.48
16:AG:248:VAL:HG21	16:AG:275:LEU:HG	1.94	0.48
16:AG:437:LEU:CG	16:AG:456:LEU:CD1	2.92	0.48
10:B:15:G:C2	10:B:20:U:O2	2.66	0.48
41:a:1993:U:H4'	50:j:133:THR:HG22	1.96	0.48
1:0:5:PHE:HB3	1:0:59:ILE:HD12	1.96	0.47
10:A:11:A:C2'	10:A:12:G:O4'	2.60	0.47
10:A:68:C:C4	10:A:69:C:C5	3.02	0.47
11:AA:1336:ASN:OD1	14:AE:33:TRP:HZ2	1.97	0.47
12:AB:47:GLU:H	12:AB:63:LYS:HG3	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:99:ARG:NH1	14:AE:99:ARG:CG	2.76	0.47
14:AE:123:ARG:HD3	14:AE:123:ARG:HA	1.48	0.47
14:AE:141:PHE:CE2	14:AE:296:LYS:CB	2.94	0.47
16:AG:61:ARG:HD2	16:AG:73:LYS:CD	2.44	0.47
10:B:11:A:H2'	10:B:12:G:C1'	2.43	0.47
18:D:13:U:O4	18:D:21:G:N3	2.46	0.47
18:D:604:G:H2'	18:D:605:U:O4'	2.14	0.47
36:V:48:ASP:HB3	36:V:75:LEU:HD23	1.94	0.47
41:a:1839:G:N9	41:a:1927:A:H1'	2.23	0.47
41:a:2168:G:H8	41:a:2168:G:OP1	1.97	0.47
9:9:23:LEU:HD22	9:9:92:ALA:HB1	1.95	0.47
10:A:14:A:H2'	10:A:14:A:N3	2.29	0.47
11:AA:857:VAL:HB	11:AA:862:LEU:CD1	2.43	0.47
16:AG:35:THR:HG21	16:AG:106:THR:HG22	1.96	0.47
16:AG:233:ARG:O	16:AG:327:LEU:CD2	2.62	0.47
16:AG:413:ALA:C	16:AG:416:THR:HG1	2.14	0.47
16:AG:467:LEU:HD12	16:AG:482:ILE:HD11	1.95	0.47
10:B:58:A:C8	10:B:58:A:OP2	2.67	0.47
18:D:13:U:O2	18:D:915:A:N7	2.47	0.47
45:e:18:LEU:HB2	45:e:53:VAL:HG11	1.95	0.47
9:9:48:ALA:HB3	9:9:51:TYR:CD2	2.50	0.47
11:AA:900:LYS:HZ3	16:AG:11:ALA:CB	2.23	0.47
12:AB:140:PRO:HD2	30:P:102:LEU:HD22	1.95	0.47
12:AB:140:PRO:CB	30:P:6:ILE:CD1	2.87	0.47
13:AD:59:VAL:HG22	13:AD:144:ILE:HA	1.96	0.47
14:AE:141:PHE:HE2	14:AE:296:LYS:CB	2.22	0.47
14:AE:1036:ARG:HE	14:AE:1081:VAL:HG11	1.79	0.47
16:AG:87:LEU:HD22	16:AG:93:VAL:HG21	1.96	0.47
16:AG:362:TYR:HA	16:AG:413:ALA:HB3	1.94	0.47
10:B:9:G:H5"	10:B:10:G:OP2	2.15	0.47
18:D:526:C:P	32:R:88:LYS:HE3	2.54	0.47
19:E:54:MET:O	19:E:57:ILE:HG22	2.15	0.47
41:a:1839:G:N9	41:a:1927:A:C1'	2.77	0.47
64:x:27:VAL:CG2	64:x:40:ILE:HD12	2.44	0.47
2:1:29:VAL:HB	2:1:55:ILE:HD11	1.96	0.47
9:9:17:GLU:HG2	9:9:88:HIS:NE2	2.29	0.47
11:AA:318:SER:OG	11:AA:320:ASP:OD1	2.31	0.47
14:AE:114:ILE:HG12	14:AE:311:ARG:HD2	1.95	0.47
14:AE:319:SER:HA	14:AE:320:ASN:HA	1.64	0.47
16:AG:200:SER:C	16:AG:230:PRO:HG2	2.38	0.47
16:AG:209:PHE:CE1	16:AG:262:VAL:HG21	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:o:13:ARG:HD3	61:u:58:TYR:O	2.14	0.47
3:2:61:LEU:C	3:2:61:LEU:HD12	2.39	0.47
10:A:60:U:H4'	10:A:61:C:OP2	2.14	0.47
11:AA:844:LYS:HD3	11:AA:844:LYS:HA	1.36	0.47
12:AB:167:ARG:NE	23:I:62:LYS:HB2	2.29	0.47
14:AE:288:PRO:HB2	14:AE:291:ILE:HD12	1.96	0.47
16:AG:26:ALA:HB1	16:AG:117:LYS:HG2	1.96	0.47
22:H:84:LEU:N	22:H:84:LEU:CD2	2.78	0.47
22:H:309:MET:HE2	22:H:318:PRO:HB3	1.97	0.47
24:J:162:ALA:O	24:J:165:ARG:O	2.33	0.47
30:P:6:ILE:CG2	30:P:100:ILE:HG23	2.43	0.47
41:a:517:C:OP2	49:i:10:ARG:NH2	2.48	0.47
10:A:9:G:H5"	10:A:10:G:OP2	2.15	0.47
11:AA:207:THR:OG1	11:AA:354:ASP:OD2	2.32	0.47
11:AA:618:GLN:CD	14:AE:770:LEU:HD13	2.40	0.47
13:AC:102:LEU:HD12	13:AC:115:ILE:HG12	1.96	0.47
13:AD:304:LYS:O	16:AG:96:GLN:HG2	2.14	0.47
14:AE:128:LEU:HD21	14:AE:188:LEU:HB3	1.97	0.47
14:AE:1060:VAL:HG13	14:AE:1106:ILE:HG12	1.96	0.47
14:AE:1146:GLU:OE2	14:AE:1310:THR:HG22	2.14	0.47
22:H:135:LEU:CB	22:H:167:VAL:O	2.63	0.47
22:H:330:VAL:HG12	22:H:345:GLY:O	2.14	0.47
28:N:102:ALA:HB3	28:N:113:ASP:HB3	1.96	0.47
29:O:81:HIS:O	29:O:84:THR:OG1	2.23	0.47
41:a:686:U:O4	53:m:12:ARG:HB2	2.15	0.47
9:9:1:MET:SD	9:9:2:ALA:N	2.88	0.47
9:9:31:ARG:HE	41:a:1054:A:C5'	2.19	0.47
9:9:43:LYS:HZ1	9:9:95:LEU:HD13	1.79	0.47
9:9:118:ILE:HB	9:9:119:PRO:CD	2.44	0.47
9:9:132:TYR:CE1	40:Z:19:VAL:HG22	2.50	0.47
10:A:32:C:O2'	27:M:86:GLN:CD	2.31	0.47
11:AA:689:ALA:HB2	11:AA:1233:LEU:HD23	1.97	0.47
11:AA:861:ALA:O	11:AA:882:ILE:HD13	2.14	0.47
12:AB:172:GLU:N	12:AB:172:GLU:CD	2.73	0.47
14:AE:833:GLU:N	14:AE:1242:ARG:HH12	2.12	0.47
14:AE:902:ASP:OD2	14:AE:905:ARG:HB2	2.15	0.47
14:AE:1027:VAL:HB	14:AE:1121:LEU:HB2	1.95	0.47
14:AE:1167:LYS:NZ	14:AE:1170:LYS:HB2	2.30	0.47
16:AG:36:LYS:HE3	16:AG:43:ILE:HG12	1.95	0.47
16:AG:207:GLU:HG3	16:AG:210:ARG:HB3	1.96	0.47
16:AG:220:VAL:CG1	16:AG:245:ILE:HG21	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:233:ARG:HG2	16:AG:270:ARG:CB	2.45	0.47
16:AG:285:ILE:O	16:AG:288:MET:HE3	2.14	0.47
16:AG:442:ARG:C	16:AG:446:PHE:CD2	2.85	0.47
39:Y:77:VAL:HG13	39:Y:80:LYS:HE3	1.95	0.47
39:Y:133:ARG:O	39:Y:133:ARG:HG2	2.14	0.47
40:Z:4:LYS:O	40:Z:4:LYS:HD2	2.15	0.47
41:a:1394:U:H4'	41:a:1603:A:H4'	1.97	0.47
10:A:15:G:H22	10:A:20:U:H3	1.59	0.47
10:A:29:G:H2'	10:A:30:G:O4'	2.15	0.47
10:A:58:A:OP2	10:A:58:A:C8	2.67	0.47
12:AB:96:THR:CA	14:AE:162:GLU:HG3	2.44	0.47
14:AE:526:VAL:HG12	14:AE:549:LYS:HB2	1.96	0.47
14:AE:1221:LEU:HD22	14:AE:1306:LEU:HB2	1.97	0.47
16:AG:1:MET:SD	16:AG:53:SER:HA	2.55	0.47
16:AG:168:LEU:CD2	16:AG:231:GLY:HA2	2.09	0.47
10:B:18:G:N3	10:B:58:A:C6	2.82	0.47
18:D:1329:A:OP1	38:X:28:THR:OG1	2.31	0.47
39:Y:79:LEU:HD13	39:Y:132:ALA:HA	1.97	0.47
60:t:18:ARG:HB2	60:t:45:GLU:HB3	1.97	0.47
11:AA:103:VAL:HG12	11:AA:117:ILE:HG22	1.97	0.47
11:AA:894:GLN:NE2	11:AA:894:GLN:N	2.61	0.47
14:AE:211:GLU:CG	14:AE:215:LYS:HE3	2.44	0.47
14:AE:842:ARG:HH22	14:AE:1250:ASP:HB2	1.80	0.47
16:AG:27:LEU:HD22	16:AG:114:ILE:HG12	1.96	0.47
16:AG:33:THR:CG2	16:AG:43:ILE:HD11	2.44	0.47
16:AG:138:ILE:HD12	16:AG:183:LEU:CD1	2.45	0.47
16:AG:349:GLN:C	16:AG:351:GLU:N	2.71	0.47
41:a:1021:A:N3	41:a:1021:A:C3'	2.78	0.47
50:j:152:PRO:HG3	50:j:156:PHE:CZ	2.50	0.47
7:6:21:DA:C6	8:7:51:G:C2	3.03	0.47
9:9:27:VAL:HG22	9:9:99:PHE:HE2	1.80	0.47
9:9:139:LEU:HD21	40:Z:11:VAL:HG22	1.97	0.47
12:AB:64:PHE:CZ	12:AB:114:ARG:HD2	2.50	0.47
16:AG:363:LEU:HG	16:AG:410:ALA:HA	1.94	0.47
18:D:526:C:OP2	32:R:88:LYS:HE3	2.15	0.47
26:L:67:PRO:O	26:L:70:VAL:HG22	2.15	0.47
41:a:1814:G:C4'	48:h:51:THR:HG21	2.44	0.47
41:a:2168:G:OP1	41:a:2168:G:C8	2.68	0.47
41:a:2756:U:C4	41:a:2759:G:C6	3.03	0.47
1:0:51:VAL:HG22	1:0:51:VAL:O	2.15	0.46
11:AA:400:VAL:HG22	11:AA:584:TYR:HB3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:1245:ALA:O	14:AE:375:GLU:HG2	2.15	0.46
16:AG:389:MET:HA	16:AG:407:ARG:NH1	2.29	0.46
41:a:2585:U:O2	41:a:2585:U:O4'	2.32	0.46
10:A:18:G:C8	10:A:57:A:N1	2.83	0.46
11:AA:858:GLY:O	11:AA:861:ALA:CB	2.62	0.46
12:AB:153:TYR:CD2	12:AB:153:TYR:N	2.81	0.46
14:AE:395:LYS:NZ	14:AE:399:LYS:CE	2.77	0.46
14:AE:1219:ASP:O	14:AE:1223:LEU:HB2	2.16	0.46
16:AG:183:LEU:CD2	16:AG:197:VAL:HG22	2.45	0.46
16:AG:299:ASP:CB	16:AG:303:HIS:HA	2.44	0.46
16:AG:434:LEU:HD22	16:AG:459:LEU:HD11	1.80	0.46
10:B:18:G:C6	10:B:57:A:N7	2.83	0.46
18:D:946:A:H2'	18:D:947:G:C8	2.50	0.46
18:D:1228:C:P	38:X:107:ARG:HH12	2.38	0.46
18:D:1308:U:OP1	38:X:100:GLN:OE1	2.22	0.46
8:7:14:U:C6	8:7:14:U:C3'	2.98	0.46
11:AA:900:LYS:HZ1	16:AG:13:SER:H	1.62	0.46
14:AE:43:THR:HG22	14:AE:57:PHE:HE1	1.80	0.46
16:AG:201:LYS:HB3	16:AG:201:LYS:HZ3	1.81	0.46
16:AG:434:LEU:HD11	16:AG:455:THR:CA	2.46	0.46
16:AG:479:GLY:O	16:AG:483:MET:HG2	2.15	0.46
10:B:60:U:H4'	10:B:61:C:OP2	2.14	0.46
18:D:371:A:H2'	18:D:372:C:O4'	2.14	0.46
18:D:373:A:C2	18:D:374:A:C8	3.03	0.46
22:H:316:ILE:HD11	22:H:321:VAL:HG11	1.97	0.46
23:I:75:ILE:HD13	23:I:75:ILE:C	2.40	0.46
36:V:8:LEU:HD23	36:V:25:ILE:HG21	1.97	0.46
41:a:2298:A:C6	41:a:2299:U:C2	3.04	0.46
41:a:2315:G:H5'	54:n:157:THR:HG23	1.97	0.46
9:9:43:LYS:NZ	9:9:95:LEU:HD13	2.30	0.46
9:9:58:THR:HB	9:9:82:ILE:H	1.80	0.46
10:A:6:G:O2'	10:A:7:G:C5'	2.63	0.46
10:A:18:G:C6	10:A:57:A:N7	2.83	0.46
10:A:33:U:H2'	10:A:35:A:OP2	2.14	0.46
10:A:58:A:C1'	10:A:60:U:C5	2.99	0.46
11:AA:902:LEU:HG	16:AG:111:LYS:HG2	1.97	0.46
14:AE:385:LEU:HD23	14:AE:390:LEU:HB2	1.98	0.46
16:AG:36:LYS:HB2	16:AG:101:THR:HG21	1.97	0.46
16:AG:228:ARG:HB3	16:AG:234:ALA:HA	1.98	0.46
10:B:14:A:N3	10:B:14:A:H2'	2.29	0.46
10:B:18:G:C8	10:B:57:A:N1	2.83	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:19:ARG:O	22:H:72:LEU:HD13	2.16	0.46
40:Z:29:LYS:HE2	40:Z:29:LYS:HB2	1.45	0.46
62:v:96:ILE:HG21	62:v:126:ILE:HD12	1.98	0.46
3:2:30:ILE:HD13	3:2:93:LEU:HD12	1.97	0.46
9:9:60:LEU:HB2	9:9:61:ARG:NH2	2.31	0.46
9:9:67:THR:H	9:9:68:PRO:HD3	1.80	0.46
10:A:14:A:H1'	10:A:22:G:N2	2.31	0.46
11:AA:230:PHE:HB2	11:AA:333:ILE:HB	1.97	0.46
11:AA:900:LYS:NZ	16:AG:11:ALA:HB3	2.09	0.46
11:AA:913:VAL:HG21	16:AG:108:GLN:HE22	1.65	0.46
12:AB:149:GLU:N	12:AB:149:GLU:CD	2.73	0.46
14:AE:420:PRO:HA	14:AE:437:PHE:O	2.15	0.46
14:AE:1150:PRO:HG3	14:AE:1214:PRO:HB2	1.96	0.46
16:AG:266:LEU:CD2	16:AG:266:LEU:N	2.73	0.46
10:B:42:G:H2'	10:B:43:A:C8	2.48	0.46
10:B:48:C:N4	10:B:59:A:C5	2.84	0.46
18:D:1176:A:H2'	18:D:1177:G:O4'	2.16	0.46
18:D:1308:U:P	38:X:98:ARG:CG	3.03	0.46
40:Z:18:ASP:HB3	40:Z:22:LEU:CD1	2.45	0.46
41:a:1020:A:C6	41:a:1141:U:O2	2.68	0.46
63:w:28:LEU:HD23	63:w:48:VAL:HG21	1.98	0.46
16:AG:320:ARG:HH11	16:AG:320:ARG:HG2	1.80	0.46
16:AG:353:HIS:O	16:AG:356:ILE:CA	2.63	0.46
18:D:429:U:N3	18:D:431:A:N6	2.63	0.46
18:D:1175:G:N3	18:D:1176:A:C8	2.83	0.46
21:G:114:LEU:HA	21:G:144:LEU:HD13	1.98	0.46
8:7:52:A:H2'	8:7:53:G:H8	1.80	0.46
12:AB:133:MET:HE2	12:AB:133:MET:C	2.40	0.46
15:AF:25:ARG:NH1	15:AF:61:ASN:OD1	2.49	0.46
18:D:1225:A:OP1	38:X:101:ARG:HB2	2.15	0.46
29:O:63:LEU:HD13	29:O:65:ILE:HD11	1.97	0.46
41:a:742:A:C2	41:a:755:U:N3	2.81	0.46
41:a:1209:U:O2'	41:a:1237:A:N1	2.40	0.46
41:a:1266:G:OP1	49:i:16:ARG:NE	2.45	0.46
41:a:1695:G:N7	48:h:14:ARG:NH2	2.63	0.46
41:a:2636:C:HO2'	50:j:45:TYR:HH	1.62	0.46
47:g:18:CYS:HB2	47:g:40:CYS:HB3	1.96	0.46
54:n:36:LEU:HB3	54:n:57:LEU:HD21	1.97	0.46
56:p:24:ILE:CD1	56:p:72:LEU:HD21	2.44	0.46
59:s:84:ILE:HG23	59:s:84:ILE:O	2.14	0.46
10:A:41:C:C5'	27:M:143:ARG:HD2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:60:U:OP2	10:A:61:C:N4	2.45	0.46
12:AB:63:LYS:CG	12:AB:66:PRO:HB3	2.46	0.46
12:AB:173:LEU:HD12	30:P:102:LEU:HG	1.97	0.46
13:AC:64:VAL:HG11	13:AC:78:ILE:HG21	1.97	0.46
16:AG:434:LEU:HD11	16:AG:454:CYS:C	2.39	0.46
16:AG:442:ARG:O	16:AG:446:PHE:CE2	2.63	0.46
18:D:1103:C:O2	21:G:106:THR:HG21	2.15	0.46
22:H:69:ASP:O	22:H:85:SER:CB	2.63	0.46
22:H:332:VAL:HG11	22:H:335:ILE:CG1	2.38	0.46
31:Q:34:ILE:HG12	31:Q:70:CYS:SG	2.56	0.46
39:Y:42:ASN:HA	39:Y:45:THR:HB	1.98	0.46
41:a:68:G:N2	41:a:74:A:OP2	2.49	0.46
41:a:631:A:N3	41:a:2415:G:O2'	2.48	0.46
41:a:2291:U:H2'	41:a:2292:U:C6	2.51	0.46
11:AA:28:LEU:HD21	11:AA:524:ILE:HG13	1.98	0.46
12:AB:155:LYS:HE3	18:D:1277:C:C6	2.50	0.46
13:AD:35:PHE:HA	13:AD:38:THR:HG22	1.97	0.46
16:AG:314:LEU:HB3	16:AG:318:ILE:HD12	1.97	0.46
16:AG:440:VAL:CG2	16:AG:481:LEU:HD21	2.42	0.46
10:B:6:G:O2'	10:B:7:G:C5'	2.63	0.46
10:B:58:A:C1'	10:B:60:U:C5	2.99	0.46
22:H:52:GLN:O	22:H:53:PHE:HD1	1.95	0.46
22:H:291:GLY:HA2	22:H:305:HIS:O	2.15	0.46
38:X:16:VAL:HG23	38:X:17:ILE:HD12	1.97	0.46
41:a:1720:U:H2'	41:a:1721:G:O4'	2.16	0.46
9:9:39:THR:HA	9:9:42:ARG:HH11	1.81	0.46
13:AD:15:ASP:OD1	13:AD:27:THR:OG1	2.30	0.46
14:AE:209:ASN:HA	14:AE:214:ARG:NH2	2.31	0.46
16:AG:288:MET:HE2	16:AG:288:MET:HB3	1.75	0.46
20:F:67:ARG:HD3	20:F:67:ARG:N	2.31	0.46
21:G:114:LEU:HD13	21:G:144:LEU:CB	2.46	0.46
41:a:998:C:OP2	66:z:58:ARG:NH2	2.49	0.46
9:9:24:SER:HB2	9:9:116:GLU:HG2	1.98	0.45
9:9:34:THR:HG22	9:9:38:MET:CE	2.46	0.45
10:A:5:G:C2'	10:A:6:G:C5'	2.93	0.45
11:AA:903:ARG:NH1	11:AA:903:ARG:C	2.73	0.45
11:AA:1268:GLN:NE2	14:AE:352:ARG:CD	2.67	0.45
12:AB:128:PHE:CZ	12:AB:175:PHE:C	2.74	0.45
12:AB:173:LEU:CD1	30:P:102:LEU:CG	2.94	0.45
14:AE:198:CYS:HA	14:AE:221:ILE:CD1	2.45	0.45
14:AE:847:ASP:OD1	14:AE:847:ASP:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:16:PHE:CD2	22:H:42:LEU:O	2.69	0.45
23:I:117:ALA:HB2	23:I:200:VAL:CG1	2.46	0.45
41:a:784:G:H5'	41:a:785:G:OP1	2.15	0.45
54:n:57:LEU:HD22	54:n:89:VAL:CG2	2.47	0.45
8:7:14:U:H3'	8:7:14:U:C6	2.52	0.45
8:7:50:U:H2'	8:7:51:G:C8	2.52	0.45
10:A:48:C:N4	10:A:59:A:C5	2.84	0.45
12:AB:165:PHE:CA	30:P:88:MET:CA	2.90	0.45
14:AE:395:LYS:NZ	14:AE:399:LYS:CD	2.74	0.45
16:AG:80:ALA:HB1	16:AG:87:LEU:HB2	1.98	0.45
16:AG:288:MET:HE3	16:AG:289:ALA:N	2.31	0.45
10:B:14:A:H1'	10:B:22:G:N2	2.31	0.45
18:D:868:C:H2'	18:D:869:G:O4'	2.15	0.45
18:D:1517:G:H1'	41:a:1919:A:O2'	2.16	0.45
39:Y:35:MET:HE3	39:Y:35:MET:HB3	1.90	0.45
39:Y:37:PHE:CE1	39:Y:56:VAL:HG11	2.51	0.45
41:a:39:G:H1'	52:l:43:THR:HG21	1.99	0.45
41:a:1406:U:HO2'	41:a:1407:G:P	2.27	0.45
41:a:1565:C:O2'	41:a:1567:G:N7	2.48	0.45
41:a:1906:G:H4'	41:a:1906:G:OP1	2.16	0.45
9:9:50:VAL:CG2	39:Y:120:ASP:N	2.79	0.45
11:AA:176:ILE:HD11	11:AA:428:VAL:HG21	1.98	0.45
12:AB:135:ARG:CG	12:AB:135:ARG:NH1	2.73	0.45
16:AG:61:ARG:HA	16:AG:94:GLU:HA	1.97	0.45
10:B:5:G:C2'	10:B:6:G:C5'	2.93	0.45
17:C:12:ARG:CZ	22:H:264:GLU:HA	2.46	0.45
7:6:15:DC:N3	7:6:16:DC:C4	2.84	0.45
7:6:18:DC:C2	8:7:53:G:N2	2.78	0.45
9:9:111:ALA:HB3	9:9:114:GLU:HG3	1.98	0.45
11:AA:1314:GLN:HB2	15:AF:28:ARG:HH12	1.81	0.45
12:AB:140:PRO:HB3	30:P:79:PRO:HB3	1.98	0.45
14:AE:201:LEU:CB	14:AE:221:ILE:HD13	2.47	0.45
17:C:33:ILE:O	17:C:33:ILE:HG12	2.15	0.45
18:D:915:A:C8	18:D:915:A:H3'	2.50	0.45
21:G:208:ARG:HH12	22:H:29:VAL:HG11	1.82	0.45
25:K:96:MET:CE	25:K:115:LEU:HD11	2.45	0.45
39:Y:125:THR:HA	39:Y:128:ILE:HG12	1.98	0.45
54:n:77:PHE:N	54:n:77:PHE:CD1	2.82	0.45
11:AA:694:ARG:HH22	13:AC:80:GLU:HG3	1.82	0.45
11:AA:887:VAL:HG21	11:AA:913:VAL:CG2	2.24	0.45
12:AB:70:LEU:HB3	12:AB:108:VAL:HG11	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:226:ALA:HB1	16:AG:228:ARG:HH11	1.81	0.45
16:AG:433:ASP:HB3	16:AG:456:LEU:CD1	2.47	0.45
16:AG:434:LEU:CD1	16:AG:455:THR:O	2.62	0.45
10:B:60:U:OP2	10:B:61:C:N4	2.45	0.45
18:D:1329:A:P	38:X:28:THR:HG1	2.38	0.45
41:a:930:G:H1'	46:f:25:LEU:HD11	1.98	0.45
41:a:1007:C:OP1	59:s:37:ARG:NH2	2.50	0.45
59:s:30:THR:CG2	59:s:31:GLU:N	2.79	0.45
4:3:94:ARG:CB	4:3:103:ILE:HD12	2.45	0.45
6:5:110:DA:N1	11:AA:536:GLY:O	2.49	0.45
6:5:114:DC:H5"	14:AE:1148:ARG:CZ	2.46	0.45
9:9:18:VAL:HA	9:9:86:MET:CE	2.44	0.45
11:AA:913:VAL:O	11:AA:913:VAL:HG12	2.17	0.45
13:AC:218:ARG:NH1	13:AD:231:PHE:O	2.50	0.45
16:AG:19:PRO:HG2	16:AG:19:PRO:O	2.17	0.45
16:AG:353:HIS:HA	16:AG:356:ILE:HG21	1.94	0.45
18:D:915:A:H8	18:D:915:A:O5'	2.00	0.45
25:K:111:MET:CE	25:K:125:ALA:HB1	2.39	0.45
27:M:27:VAL:HG12	27:M:43:VAL:HG11	1.98	0.45
38:X:106:ALA:HB3	38:X:110:LYS:HD2	1.98	0.45
6:5:108:DT:O4	11:AA:199:ASP:OD2	2.35	0.45
9:9:50:VAL:HG22	39:Y:119:ALA:C	2.41	0.45
9:9:139:LEU:CD2	40:Z:11:VAL:HG22	2.47	0.45
11:AA:712:SER:OG	11:AA:713:GLY:N	2.49	0.45
11:AA:735:LYS:HA	11:AA:748:ILE:HG22	1.98	0.45
11:AA:853:ASP:CG	16:AG:103:ASP:CB	2.89	0.45
11:AA:903:ARG:HD2	11:AA:903:ARG:HA	1.30	0.45
14:AE:26:SER:HB2	14:AE:236:TRP:CH2	2.51	0.45
16:AG:3:LYS:HB3	16:AG:6:LEU:HD12	1.99	0.45
18:D:17:U:H2'	18:D:18:C:C6	2.52	0.45
18:D:1240:U:OP1	27:M:116:MET:HB2	2.16	0.45
19:E:55:GLN:N	19:E:56:PRO:HD2	2.32	0.45
39:Y:21:PRO:CB	39:Y:22:PRO:CD	2.90	0.45
41:a:560:C:O2	66:z:48:ARG:NH1	2.41	0.45
41:a:2547:A:H2'	41:a:2548:U:C6	2.52	0.45
58:r:15:LEU:HD13	58:r:15:LEU:C	2.42	0.45
7:6:15:DC:C4	7:6:16:DC:C5	3.05	0.45
8:7:47:U:OP2	8:7:47:U:C4	2.70	0.45
9:9:57:ASN:CG	9:9:62:ARG:HG3	2.30	0.45
11:AA:854:ILE:CG1	11:AA:855:PRO:CD	2.78	0.45
13:AD:185:TYR:HA	13:AD:202:VAL:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AD:308:ALA:HB1	16:AG:60:ARG:CD	2.47	0.45
14:AE:515:ARG:NH2	14:AE:718:SER:O	2.48	0.45
16:AG:102:PHE:HB3	16:AG:103:ASP:CG	2.41	0.45
16:AG:142:VAL:HB	16:AG:175:PRO:HA	1.99	0.45
16:AG:323:GLN:CA	16:AG:323:GLN:NE2	2.75	0.45
16:AG:362:TYR:HE1	16:AG:414:LEU:HD21	1.80	0.45
16:AG:403:VAL:C	16:AG:405:ALA:N	2.73	0.45
17:C:61:ARG:HG2	26:L:88:MET:HE1	1.98	0.45
18:D:1493:A:C8	18:D:1493:A:OP1	2.70	0.45
21:G:114:LEU:HD13	21:G:144:LEU:HB3	1.99	0.45
22:H:294:VAL:HG21	22:H:330:VAL:HG21	1.99	0.45
38:X:106:ALA:HB3	38:X:110:LYS:CD	2.47	0.45
48:h:6:CYS:SG	48:h:13:ARG:NH1	2.89	0.45
48:h:76:ALA:HB2	48:h:96:TYR:CD1	2.51	0.45
52:l:149:ILE:CD1	52:l:188:MET:HE3	2.46	0.45
2:1:17:VAL:HG12	2:1:76:VAL:HG21	1.98	0.45
8:7:13:U:H6	8:7:13:U:H5"	1.81	0.45
11:AA:900:LYS:NZ	16:AG:13:SER:H	2.14	0.45
11:AA:1002:LEU:HD21	11:AA:1007:LYS:HB2	1.98	0.45
11:AA:1311:GLY:O	15:AF:31:GLN:NE2	2.49	0.45
16:AG:239:LYS:CG	16:AG:276:TRP:HB3	2.46	0.45
16:AG:314:LEU:HD22	16:AG:318:ILE:HD11	1.98	0.45
10:B:37:A:N3	10:B:37:A:H5"	2.32	0.45
10:B:58:A:HO2'	10:B:60:U:H5	1.62	0.45
22:H:332:VAL:HG13	22:H:342:ILE:HG23	1.98	0.45
23:I:155:GLY:HA2	23:I:163:ALA:HB1	1.99	0.45
30:P:8:ILE:HD12	30:P:25:ILE:CD1	2.46	0.45
30:P:99:GLN:O	30:P:99:GLN:HG2	2.16	0.45
9:9:31:ARG:NE	41:a:1054:A:O4'	2.46	0.45
10:A:48:C:C5	10:A:59:A:C8	3.05	0.45
11:AA:1247:SER:HB3	14:AE:375:GLU:O	2.17	0.45
11:AA:1332:SER:C	14:AE:243:PRO:HG2	2.42	0.45
14:AE:68:TYR:HB3	14:AE:75:TYR:HE2	1.80	0.45
14:AE:222:LYS:HD2	14:AE:222:LYS:HA	1.32	0.45
14:AE:978:ARG:HD3	14:AE:999:TYR:H	1.82	0.45
16:AG:143:LYS:HG3	16:AG:153:ASP:HB2	1.99	0.45
39:Y:23:VAL:HB	39:Y:24:GLY:H	1.65	0.45
39:Y:95:ASP:OD2	39:Y:95:ASP:N	2.50	0.45
64:x:18:LEU:HD23	64:x:25:ARG:HD2	1.99	0.45
10:A:25:C:C2'	10:A:26:G:H5'	2.47	0.44
11:AA:1334:GLY:O	14:AE:25:ALA:HB3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:105:ILE:HD12	14:AE:242:LEU:CD2	2.44	0.44
14:AE:108:ALA:HB1	14:AE:279:LEU:HD22	1.96	0.44
16:AG:282:GLN:HA	16:AG:282:GLN:HE21	1.82	0.44
46:f:25:LEU:C	46:f:25:LEU:HD13	2.41	0.44
50:j:186:LEU:HD21	65:y:4:ILE:HG21	1.98	0.44
8:7:53:G:H2'	8:7:54:A:H8	1.80	0.44
9:9:106:PHE:CD2	9:9:106:PHE:O	2.70	0.44
9:9:106:PHE:O	9:9:106:PHE:CG	2.69	0.44
9:9:127:ALA:O	9:9:130:PRO:HG2	2.16	0.44
10:A:76:A:C2	55:o:31:HIS:NE2	2.85	0.44
11:AA:674:ASP:OD2	11:AA:1070:HIS:ND1	2.50	0.44
11:AA:893:THR:HG22	11:AA:894:GLN:HG3	1.99	0.44
12:AB:141:PHE:CE2	12:AB:173:LEU:HD21	2.52	0.44
10:B:34:C:O5'	10:B:34:C:C6	2.70	0.44
10:B:48:C:C5	10:B:59:A:C8	3.05	0.44
18:D:109:A:C6	18:D:326:G:C6	3.05	0.44
18:D:198:G:OP2	18:D:198:G:C8	2.70	0.44
18:D:1340:A:H8	18:D:1340:A:O5'	1.99	0.44
20:F:21:ARG:HH22	22:H:341:ARG:HD2	1.82	0.44
21:G:76:ALA:CB	21:G:210:VAL:HG11	2.48	0.44
41:a:340:A:O2'	52:l:162:ARG:NH1	2.50	0.44
41:a:645:C:H2'	41:a:647:G:C8	2.52	0.44
41:a:1327:A:H2'	41:a:1328:A:O4'	2.17	0.44
41:a:2133:G:O2'	41:a:2157:G:N2	2.51	0.44
8:7:12:U:C3'	8:7:12:U:C6	3.00	0.44
9:9:62:ARG:CG	9:9:62:ARG:NH2	2.73	0.44
9:9:72:LEU:HD22	9:9:72:LEU:C	2.42	0.44
10:A:49:G:O5'	10:A:49:G:C8	2.71	0.44
14:AE:213:LYS:HA	14:AE:213:LYS:HE3	1.98	0.44
14:AE:388:ARG:HG2	14:AE:388:ARG:NH1	2.32	0.44
14:AE:926:PRO:HB2	14:AE:1241:TYR:HE1	1.82	0.44
14:AE:1158:GLU:HA	14:AE:1223:LEU:HD21	1.99	0.44
16:AG:252:VAL:HG13	16:AG:256:GLY:HA2	1.99	0.44
16:AG:339:MET:HE2	16:AG:343:ASP:HB3	1.98	0.44
10:B:25:C:C2'	10:B:26:G:H5'	2.47	0.44
39:Y:34:ILE:HG22	39:Y:34:ILE:O	2.18	0.44
45:e:59:GLU:O	45:e:63:ALA:HB3	2.18	0.44
58:r:55:GLU:HA	58:r:58:LEU:HD12	1.99	0.44
8:7:8:U:OP2	18:D:1397:C:O2	2.34	0.44
8:7:9:U:OP2	8:7:9:U:C6	2.70	0.44
8:7:21:U:OP1	23:I:81:GLY:CA	2.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:7:ASP:OD1	9:9:7:ASP:N	2.36	0.44
11:AA:1246:ARG:HH11	11:AA:1266:GLY:HA2	1.82	0.44
12:AB:140:PRO:HA	30:P:79:PRO:HB2	1.99	0.44
13:AD:212:ASP:OD1	13:AD:212:ASP:N	2.48	0.44
14:AE:26:SER:CB	14:AE:236:TRP:CZ2	2.95	0.44
14:AE:115:TRP:HB3	14:AE:1333:THR:CG2	2.46	0.44
14:AE:201:LEU:CD1	14:AE:224:LEU:HD12	2.47	0.44
14:AE:850:LYS:HB3	14:AE:855:ASP:HB2	2.00	0.44
16:AG:227:ALA:CB	16:AG:330:GLN:C	2.90	0.44
16:AG:402:THR:C	16:AG:405:ALA:HB3	2.41	0.44
16:AG:429:LYS:CB	16:AG:430:PRO:HD2	2.47	0.44
41:a:1047:G:N2	41:a:1110:G:O2'	2.50	0.44
41:a:2822:G:OP1	50:j:164:GLN:NE2	2.47	0.44
45:e:56:LEU:HD23	45:e:56:LEU:HA	1.87	0.44
6:5:115:DA:P	14:AE:1148:ARG:HG3	2.58	0.44
10:A:34:C:OP1	27:M:84:THR:OG1	2.35	0.44
10:A:56:C:OP1	41:a:2168:G:C4	2.71	0.44
11:AA:24:VAL:HG11	11:AA:704:MET:HE1	1.99	0.44
11:AA:148:GLN:NE2	11:AA:535:PRO:O	2.40	0.44
11:AA:805:MET:HE3	11:AA:805:MET:HB2	1.86	0.44
11:AA:1314:GLN:HA	15:AF:28:ARG:HH22	1.82	0.44
13:AD:78:ILE:HA	13:AD:81:ILE:HG22	2.00	0.44
14:AE:62:PHE:N	14:AE:62:PHE:CD1	2.86	0.44
14:AE:111:THR:HG21	14:AE:303:VAL:HB	2.00	0.44
14:AE:478:LEU:HD21	15:AF:47:THR:HG23	1.99	0.44
14:AE:824:PRO:HD3	14:AE:835:LEU:HD12	2.00	0.44
14:AE:1024:THR:HG23	14:AE:1123:ARG:HA	2.00	0.44
18:D:337:G:H2'	18:D:338:A:C8	2.52	0.44
39:Y:140:GLU:OE1	39:Y:140:GLU:N	2.50	0.44
41:a:1082:U:H3	41:a:1086:A:N6	2.15	0.44
41:a:1925:C:C5	41:a:1925:C:OP2	2.70	0.44
8:7:47:U:OP2	8:7:47:U:C5	2.71	0.44
9:9:43:LYS:C	9:9:43:LYS:CD	2.86	0.44
9:9:106:PHE:CD2	9:9:106:PHE:C	2.95	0.44
10:A:32:C:HO2'	27:M:86:GLN:HG3	1.79	0.44
11:AA:557:ARG:HB3	11:AA:587:LEU:HD13	2.00	0.44
11:AA:800:MET:HB2	11:AA:800:MET:HE3	1.69	0.44
14:AE:75:TYR:CD2	14:AE:75:TYR:O	2.70	0.44
14:AE:76:LYS:HB3	14:AE:76:LYS:NZ	2.32	0.44
14:AE:109:SER:HB2	14:AE:296:LYS:HG2	1.98	0.44
16:AG:167:MET:HE3	16:AG:173:PHE:CZ	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:318:ILE:CG1	16:AG:338:VAL:HG11	2.48	0.44
16:AG:365:ILE:CD1	16:AG:406:LEU:HD21	2.38	0.44
10:B:68:C:H3'	10:B:69:C:H5"	1.96	0.44
18:D:13:U:C2	18:D:915:A:C5	3.06	0.44
18:D:976:G:C8	18:D:1358:U:O2	2.71	0.44
21:G:16:PHE:CG	22:H:43:LYS:HA	2.53	0.44
22:H:38:VAL:HG22	22:H:48:ILE:HD11	1.99	0.44
41:a:813:U:H2'	41:a:814:C:C6	2.53	0.44
44:d:48:U:H2'	44:d:49:C:C6	2.52	0.44
10:A:22:G:H2'	10:A:23:C:C5	2.52	0.44
10:A:49:G:C2'	10:A:50:U:H5'	2.47	0.44
11:AA:557:ARG:NH2	11:AA:607:SER:O	2.50	0.44
11:AA:845:LEU:HD23	11:AA:889:PRO:CB	2.48	0.44
11:AA:1298:VAL:HG11	14:AE:96:LYS:NZ	2.33	0.44
13:AD:29:GLU:HB3	13:AD:200:LYS:HG3	1.99	0.44
13:AD:68:TYR:HE1	13:AD:79:LEU:HD13	1.82	0.44
14:AE:395:LYS:NZ	14:AE:399:LYS:HE2	2.32	0.44
14:AE:506:VAL:HG23	14:AE:628:GLY:HA3	1.98	0.44
16:AG:15:GLU:HA	16:AG:18:LEU:HB2	2.00	0.44
16:AG:104:ARG:N	16:AG:105:ILE:HG12	2.32	0.44
16:AG:431:ALA:O	16:AG:435:LEU:HG	2.18	0.44
10:B:34:C:C5	10:B:34:C:OP1	2.70	0.44
18:D:107:G:N7	19:E:10:ARG:NH2	2.60	0.44
38:X:75:MET:HA	38:X:75:MET:HE3	1.99	0.44
40:Z:7:ILE:HD12	40:Z:7:ILE:HA	1.77	0.44
41:a:1927:A:C8	41:a:1927:A:O5'	2.70	0.44
41:a:2070:A:H2'	41:a:2071:A:O4'	2.16	0.44
54:n:17:MET:HE2	54:n:25:VAL:HA	1.98	0.44
9:9:16:SER:HB2	9:9:20:LYS:NZ	2.33	0.44
10:A:26:G:N2	10:A:45:G:N2	2.66	0.44
11:AA:998:LEU:HG	11:AA:1011:LEU:HB3	1.99	0.44
12:AB:140:PRO:HB2	30:P:6:ILE:HD11	1.95	0.44
13:AD:192:VAL:HG12	13:AD:193:GLU:H	1.83	0.44
14:AE:1079:LYS:HD3	14:AE:1098:GLN:HB3	2.00	0.44
16:AG:316:GLN:H	16:AG:316:GLN:HG3	1.54	0.44
10:B:26:G:N2	10:B:45:G:N2	2.66	0.44
18:D:1397:C:O5'	18:D:1397:C:C6	2.70	0.44
24:J:165:ARG:NH1	24:J:165:ARG:HB2	2.32	0.44
24:J:197:GLU:HA	24:J:200:ILE:HD12	1.99	0.44
40:Z:1:SER:HB3	40:Z:2:ILE:H	1.61	0.44
9:9:42:ARG:H	9:9:42:ARG:HG3	1.62	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:67:THR:H	9:9:68:PRO:CD	2.29	0.44
11:AA:1157:GLN:HG3	11:AA:1159:VAL:HG13	2.00	0.44
12:AB:133:MET:N	12:AB:133:MET:CE	2.73	0.44
14:AE:224:LEU:HD23	14:AE:224:LEU:HA	1.89	0.44
14:AE:894:VAL:HG22	14:AE:1258:ARG:HH11	1.83	0.44
16:AG:227:ALA:HB2	16:AG:330:GLN:O	2.18	0.44
16:AG:320:ARG:HB2	16:AG:323:GLN:CB	2.48	0.44
16:AG:402:THR:C	16:AG:405:ALA:H	2.26	0.44
10:B:1:C:C5	10:B:2:G:N7	2.86	0.44
10:B:49:G:C2'	10:B:50:U:H5'	2.47	0.44
18:D:397:A:H3'	18:D:397:A:N3	2.33	0.44
18:D:552:U:O2'	32:R:83:ARG:O	2.27	0.44
53:m:12:ARG:HG3	53:m:44:VAL:HG11	1.99	0.44
54:n:29:PRO:HB2	54:n:169:LEU:HD22	1.99	0.44
8:7:1:A:H2'	8:7:2:U:C6	2.50	0.43
11:AA:11:ILE:HG22	11:AA:1172:LEU:HD11	1.99	0.43
12:AB:95:GLY:C	14:AE:162:GLU:HG3	2.43	0.43
14:AE:128:LEU:CD2	14:AE:188:LEU:HB3	2.47	0.43
18:D:1126:U:OP1	30:P:7:ARG:NH2	2.51	0.43
18:D:1371:G:O3'	29:O:71:GLY:HA3	2.18	0.43
22:H:302:GLY:HA3	22:H:344:LEU:HD13	2.00	0.43
23:I:58:GLU:OE1	30:P:94:ALA:HB3	2.18	0.43
39:Y:123:ALA:HA	39:Y:126:ARG:HG3	2.00	0.43
40:Z:23:ILE:HD12	40:Z:23:ILE:HA	1.78	0.43
41:a:299:A:N1	41:a:322:A:O2'	2.47	0.43
41:a:1385:A:O2'	41:a:1396:U:O2	2.35	0.43
7:6:12:DC:O5'	7:6:12:DC:H6	2.01	0.43
12:AB:64:PHE:O	12:AB:114:ARG:NH1	2.31	0.43
12:AB:152:ASP:HB2	12:AB:157:ARG:CB	2.46	0.43
14:AE:1046:ILE:HG22	14:AE:1061:VAL:HA	2.00	0.43
14:AE:1108:GLN:HG3	14:AE:1109:LEU:HD12	2.00	0.43
15:AF:58:LEU:HD12	15:AF:59:ILE:HG12	2.00	0.43
16:AG:123:ARG:HG2	16:AG:123:ARG:HH11	1.81	0.43
16:AG:126:VAL:HG13	16:AG:130:PHE:CE2	2.53	0.43
16:AG:429:LYS:HB2	16:AG:430:PRO:HD2	1.99	0.43
16:AG:440:VAL:HG13	16:AG:444:LEU:HB2	2.00	0.43
10:B:9:G:O2'	10:B:45:G:H2'	2.18	0.43
22:H:109:THR:C	22:H:153:GLU:HA	2.43	0.43
22:H:136:VAL:HA	22:H:168:VAL:O	2.18	0.43
27:M:24:ALA:O	27:M:27:VAL:HG22	2.16	0.43
39:Y:121:ILE:HA	39:Y:124:MET:SD	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:a:954:G:OP2	62:v:16:ARG:NH2	2.50	0.43
41:a:2252:G:O2'	41:a:2253:G:H5'	2.18	0.43
60:t:24:VAL:HG13	60:t:33:ALA:HB2	2.00	0.43
62:v:35:ALA:HB2	62:v:102:LEU:HD11	2.00	0.43
66:z:76:TYR:OH	66:z:92:ARG:NH1	2.51	0.43
4:3:36:VAL:HG11	4:3:39:ILE:CD1	2.44	0.43
6:5:116:DG:C6	6:5:117:DA:C6	3.06	0.43
11:AA:906:PHE:CD1	11:AA:906:PHE:O	2.71	0.43
12:AB:27:ARG:HG3	12:AB:42:VAL:HG11	2.00	0.43
14:AE:213:LYS:HE3	14:AE:213:LYS:CA	2.47	0.43
10:B:49:G:O5'	10:B:49:G:C8	2.71	0.43
18:D:376:G:C2	18:D:389:A:C2	3.05	0.43
38:X:23:TYR:CD2	38:X:69:LEU:HD23	2.53	0.43
39:Y:7:TYR:CD2	39:Y:7:TYR:O	2.70	0.43
41:a:1589:U:C2	41:a:1590:A:C8	3.06	0.43
59:s:73:VAL:HG11	59:s:75:TYR:CZ	2.53	0.43
4:3:12:ILE:CG2	4:3:80:ALA:HB2	2.49	0.43
10:A:9:G:O2'	10:A:45:G:H2'	2.18	0.43
11:AA:894:GLN:C	11:AA:894:GLN:CD	2.87	0.43
11:AA:1275:VAL:HG13	11:AA:1287:LEU:HD11	2.01	0.43
11:AA:1282:GLY:O	14:AE:1361:THR:OG1	2.33	0.43
14:AE:515:ARG:HH12	14:AE:724:MET:HG2	1.83	0.43
14:AE:1227:HIS:HA	14:AE:1230:THR:HG22	1.99	0.43
10:B:57:A:O5'	10:B:58:A:P	2.76	0.43
18:D:324:G:N2	18:D:327:A:C8	2.86	0.43
18:D:384:G:H2'	18:D:385:C:C6	2.54	0.43
23:I:50:ALA:HB2	23:I:75:ILE:HD12	2.00	0.43
41:a:74:A:N7	41:a:88:G:C5	2.86	0.43
41:a:1386:C:H2'	41:a:1387:A:C8	2.53	0.43
41:a:2395:C:H2'	41:a:2396:G:O4'	2.18	0.43
50:j:172:VAL:HG11	50:j:175:LEU:HD21	2.01	0.43
9:9:9:GLN:CD	9:9:9:GLN:C	2.85	0.43
11:AA:444:ASP:OD1	11:AA:444:ASP:N	2.51	0.43
11:AA:561:ILE:HG21	14:AE:772:TYR:HE2	1.82	0.43
11:AA:829:THR:HG23	11:AA:1059:ARG:HG2	2.00	0.43
16:AG:127:VAL:HG22	16:AG:192:GLY:CA	2.46	0.43
16:AG:224:LYS:HB2	16:AG:276:TRP:CH2	2.54	0.43
21:G:206:ALA:O	21:G:210:VAL:HG23	2.18	0.43
29:O:80:ARG:O	29:O:84:THR:HG23	2.17	0.43
39:Y:37:PHE:CD2	39:Y:37:PHE:O	2.70	0.43
39:Y:104:GLN:HB3	39:Y:105:LEU:H	1.74	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:a:1921:G:C2'	41:a:1922:G:H5'	2.49	0.43
9:9:31:ARG:CG	9:9:31:ARG:NH1	2.73	0.43
10:A:1:C:C5	10:A:2:G:N7	2.86	0.43
10:A:57:A:O5'	10:A:58:A:P	2.76	0.43
11:AA:746:ALA:O	11:AA:974:ARG:NH2	2.45	0.43
11:AA:858:GLY:C	11:AA:860:ALA:N	2.73	0.43
12:AB:141:PHE:CE2	12:AB:171:VAL:CG1	2.88	0.43
14:AE:58:CYS:SG	14:AE:60:ARG:HG2	2.59	0.43
14:AE:111:THR:CG2	14:AE:300:GLN:HA	2.48	0.43
14:AE:161:THR:H	14:AE:164:GLN:HB2	1.82	0.43
16:AG:183:LEU:HD22	16:AG:195:LEU:HD13	2.00	0.43
16:AG:343:ASP:HB3	16:AG:347:LYS:HE3	2.01	0.43
10:B:22:G:H2'	10:B:23:C:C5	2.52	0.43
35:U:6:LEU:HG	35:U:17:TYR:HB3	2.00	0.43
41:a:2006:C:O2'	41:a:2823:A:N3	2.47	0.43
41:a:2189:U:O2'	41:a:2190:G:O4'	2.36	0.43
8:7:21:U:C5'	23:I:80:LYS:CG	2.97	0.43
11:AA:27:LEU:O	11:AA:528:ARG:NH1	2.43	0.43
11:AA:300:ASP:OD1	11:AA:313:ALA:N	2.51	0.43
14:AE:568:SER:HB3	14:AE:570:LYS:NZ	2.34	0.43
14:AE:1033:GLY:HA3	14:AE:1081:VAL:O	2.18	0.43
16:AG:197:VAL:HG11	16:AG:199:ARG:NH2	2.30	0.43
16:AG:353:HIS:C	16:AG:357:ASP:HB2	2.43	0.43
16:AG:398:LEU:C	16:AG:398:LEU:HD12	2.44	0.43
16:AG:425:LEU:HD23	16:AG:429:LYS:HZ3	1.83	0.43
10:B:53:G:C2	10:B:54:U:C5	3.07	0.43
18:D:1499:A:O2'	18:D:1500:A:C5'	2.67	0.43
25:K:156:LYS:HG2	28:N:71:VAL:HG13	2.00	0.43
41:a:57:C:H2'	41:a:58:G:O4'	2.18	0.43
41:a:705:A:O4'	48:h:9:THR:HG21	2.19	0.43
41:a:819:A:C4	41:a:1189:A:C2	3.07	0.43
41:a:879:G:H2'	41:a:880:G:O4'	2.19	0.43
41:a:1095:A:H2'	41:a:1096:A:C8	2.53	0.43
41:a:1326:U:O2'	41:a:2010:G:O2'	2.35	0.43
41:a:1932:A:H2'	41:a:1933:G:O4'	2.19	0.43
54:n:123:ASP:C	54:n:123:ASP:OD1	2.62	0.43
9:9:86:MET:H	9:9:86:MET:HG2	1.59	0.43
12:AB:157:ARG:HD3	12:AB:157:ARG:HA	1.33	0.43
14:AE:107:LEU:HA	14:AE:276:ASN:ND2	2.33	0.43
14:AE:126:LEU:HD12	14:AE:223:LEU:HD22	1.99	0.43
14:AE:586:GLY:HA3	14:AE:612:LEU:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:37:LYS:HD3	16:AG:37:LYS:HA	1.67	0.43
16:AG:162:ILE:HD13	16:AG:167:MET:CE	2.49	0.43
16:AG:363:LEU:CD2	16:AG:409:ARG:N	2.81	0.43
10:B:18:G:N3	10:B:58:A:C5	2.87	0.43
10:B:46:G:O2'	10:B:47:U:H5"	2.19	0.43
18:D:1417:G:C6	18:D:1482:G:C6	3.06	0.43
21:G:47:VAL:N	21:G:48:PRO:HD2	2.34	0.43
21:G:208:ARG:NH1	22:H:29:VAL:HG11	2.34	0.43
22:H:335:ILE:HG12	22:H:342:ILE:HG23	2.00	0.43
39:Y:19:PRO:HG2	39:Y:24:GLY:N	2.32	0.43
41:a:126:A:O5'	53:m:19:ARG:HG3	2.19	0.43
52:l:170:ARG:NH2	52:l:176:ASP:OD1	2.49	0.43
60:t:76:VAL:HG12	65:y:73:VAL:HB	2.00	0.43
60:t:107:LEU:HD21	60:t:115:ILE:HG21	2.01	0.43
9:9:8:LYS:HZ1	41:a:1046:A:H61	1.67	0.43
10:A:53:G:C2	10:A:54:U:C5	3.07	0.43
11:AA:646:SER:OG	11:AA:647:ARG:N	2.52	0.43
11:AA:811:ASN:ND2	11:AA:1098:LEU:O	2.51	0.43
12:AB:64:PHE:N	12:AB:64:PHE:CD1	2.86	0.43
12:AB:128:PHE:HD2	12:AB:128:PHE:HA	1.73	0.43
12:AB:132:GLU:CB	12:AB:147:VAL:HG13	2.49	0.43
12:AB:140:PRO:HB2	30:P:84:VAL:HG11	2.00	0.43
12:AB:140:PRO:HB3	30:P:6:ILE:HD11	1.94	0.43
14:AE:51:PRO:HB2	14:AE:52:GLU:H	1.65	0.43
14:AE:102:MET:HG2	14:AE:246:PRO:CG	2.49	0.43
14:AE:220:ARG:NH1	14:AE:220:ARG:CG	2.82	0.43
14:AE:559:ALA:HB3	14:AE:562:GLU:HB3	2.01	0.43
16:AG:21:GLU:HB3	16:AG:49:ILE:CD1	2.49	0.43
18:D:684:U:H2'	18:D:685:G:O4'	2.18	0.43
18:D:1308:U:O5'	38:X:98:ARG:HG2	2.16	0.43
18:D:1515:G:H2'	18:D:1516:G:C8	2.52	0.43
22:H:76:GLU:HA	22:H:76:GLU:OE2	2.18	0.43
22:H:110:GLY:H	22:H:153:GLU:N	2.17	0.43
39:Y:124:MET:HE2	39:Y:124:MET:HB2	1.77	0.43
41:a:1067:A:O2'	41:a:1068:G:O4'	2.31	0.43
52:l:145:ASP:HA	52:l:166:LYS:HB3	2.01	0.43
6:5:98:DA:C2'	6:5:99:DT:C7	2.96	0.43
9:9:31:ARG:HD3	41:a:1054:A:H4'	1.96	0.43
9:9:71:CYS:CA	9:9:117:LEU:HD13	2.48	0.43
10:A:18:G:N3	10:A:58:A:C5	2.87	0.43
10:A:26:G:H1	10:A:44:A:N6	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:36:U:H2'	10:A:37:A:O4'	2.19	0.43
10:A:56:C:C2	41:a:2112:G:C5	3.07	0.43
11:AA:845:LEU:HD21	11:AA:912:ASP:H	1.84	0.43
14:AE:244:VAL:HA	14:AE:269:TYR:OH	2.19	0.43
16:AG:233:ARG:HB2	16:AG:327:LEU:CD2	2.42	0.43
17:C:12:ARG:HD3	17:C:16:GLU:OE1	2.18	0.43
17:C:12:ARG:NH2	22:H:268:VAL:CG2	2.71	0.43
18:D:842:U:H3'	18:D:843:U:C5'	2.48	0.43
18:D:1333:A:H2'	18:D:1334:G:O4'	2.19	0.43
22:H:280:LEU:HB2	22:H:330:VAL:O	2.18	0.43
24:J:48:LEU:HD13	24:J:48:LEU:N	2.33	0.43
24:J:61:VAL:CG2	24:J:200:ILE:HD11	2.39	0.43
25:K:153:VAL:HG23	25:K:164:ILE:HD13	2.00	0.43
39:Y:20:SER:CB	39:Y:21:PRO:HD3	2.39	0.43
39:Y:102:ARG:H	39:Y:102:ARG:HG3	1.59	0.43
57:q:3:VAL:HA	57:q:36:ARG:O	2.19	0.43
8:7:14:U:P	23:I:132:ARG:HH12	2.41	0.42
9:9:72:LEU:HD22	9:9:72:LEU:O	2.19	0.42
10:A:22:G:O2'	10:A:23:C:O5'	2.36	0.42
14:AE:242:LEU:C	14:AE:242:LEU:HD23	2.44	0.42
14:AE:609:TYR:HD2	14:AE:610:ARG:NH1	2.17	0.42
14:AE:797:THR:HG22	14:AE:924:GLY:HA3	2.01	0.42
14:AE:950:ILE:HB	14:AE:1018:ALA:HB3	2.01	0.42
16:AG:226:ALA:O	16:AG:228:ARG:N	2.52	0.42
16:AG:271:ILE:H	16:AG:271:ILE:HG12	1.49	0.42
21:G:35:ARG:CG	22:H:10:GLU:OE2	2.64	0.42
22:H:152:LEU:CB	22:H:171:ARG:H	2.32	0.42
39:Y:64:ARG:HE	39:Y:64:ARG:HB2	1.51	0.42
40:Z:28:GLU:H	40:Z:28:GLU:HG3	1.58	0.42
41:a:2252:G:H2'	41:a:2253:G:H8	1.84	0.42
41:a:2602:A:H5"	41:a:2603:G:C5'	2.49	0.42
66:z:65:ILE:CD1	66:z:92:ARG:HB2	2.49	0.42
10:A:15:G:H1	10:A:20:U:H3	1.67	0.42
10:A:46:G:O2'	10:A:47:U:H5"	2.19	0.42
11:AA:590:PRO:HB2	11:AA:655:VAL:HG21	2.01	0.42
12:AB:19:GLU:C	12:AB:44:VAL:HG11	2.23	0.42
12:AB:95:GLY:HA2	14:AE:293:ARG:HH12	1.84	0.42
14:AE:388:ARG:HG2	14:AE:388:ARG:HH11	1.83	0.42
10:B:56:C:H2'	10:B:57:A:C5'	2.27	0.42
41:a:214:G:N2	41:a:216:A:N3	2.66	0.42
41:a:2511:U:O4	41:a:2575:C:N3	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:x:99:TYR:OH	64:x:111:ARG:NH1	2.52	0.42
4:3:39:ILE:HG22	4:3:40:ASN:N	2.34	0.42
10:A:18:G:O2'	10:A:60:U:N3	2.48	0.42
10:A:58:A:OP2	10:A:58:A:H8	2.02	0.42
10:A:68:C:H3'	10:A:69:C:H5"	1.96	0.42
11:AA:125:GLY:H	11:AA:495:ALA:HB1	1.84	0.42
13:AD:31:LEU:HD21	13:AD:39:LEU:HD12	2.00	0.42
14:AE:47:ARG:HA	14:AE:47:ARG:NE	2.35	0.42
14:AE:390:LEU:N	14:AE:390:LEU:HD13	2.35	0.42
14:AE:616:PRO:HA	14:AE:619:ILE:HG22	2.02	0.42
16:AG:10:GLU:C	16:AG:12:VAL:HG22	2.44	0.42
16:AG:216:ILE:HG13	16:AG:216:ILE:H	1.63	0.42
16:AG:277:ASP:HB2	16:AG:282:GLN:CB	2.49	0.42
16:AG:285:ILE:O	16:AG:288:MET:HE2	2.19	0.42
16:AG:354:ALA:O	16:AG:358:THR:HG22	2.19	0.42
10:B:22:G:O2'	10:B:23:C:O5'	2.36	0.42
17:C:44:ILE:HG21	22:H:339:ARG:HA	2.01	0.42
18:D:421:U:O2	18:D:421:U:O4'	2.37	0.42
25:K:150:PRO:O	25:K:153:VAL:HG22	2.18	0.42
39:Y:41:PHE:HA	39:Y:68:PHE:CE2	2.55	0.42
41:a:320:A:H2'	52:l:131:THR:HG21	2.01	0.42
41:a:973:A:O4'	41:a:1188:U:C6	2.72	0.42
41:a:1020:A:C2	41:a:1141:U:C2	3.07	0.42
43:c:37:ARG:HG2	43:c:48:THR:HG23	2.00	0.42
13:AD:211:ILE:HD12	13:AD:211:ILE:HA	1.92	0.42
14:AE:126:LEU:CD1	14:AE:223:LEU:HD22	2.49	0.42
14:AE:839:VAL:HG12	14:AE:864:LEU:HD12	2.02	0.42
22:H:119:GLY:CA	22:H:132:PRO:C	2.92	0.42
41:a:567:U:OP2	61:u:29:LYS:NZ	2.53	0.42
41:a:2469:A:N6	41:a:2481:G:O2'	2.51	0.42
41:a:2615:U:C2	49:i:4:GLN:HA	2.55	0.42
41:a:2756:U:C4	41:a:2759:G:O6	2.72	0.42
60:t:38:ILE:HD11	60:t:112:PHE:CZ	2.54	0.42
8:7:7:U:H6	8:7:7:U:H3'	1.83	0.42
9:9:80:THR:O	41:a:1108:U:OP1	2.38	0.42
11:AA:902:LEU:HD11	16:AG:111:LYS:NZ	2.33	0.42
14:AE:1357:ILE:HG22	14:AE:1359:ALA:H	1.83	0.42
16:AG:38:LYS:HB3	16:AG:39:TYR:H	1.55	0.42
16:AG:234:ALA:HB3	16:AG:271:ILE:HD13	2.01	0.42
16:AG:288:MET:HE3	16:AG:288:MET:C	2.45	0.42
18:D:294:U:OP1	18:D:610:U:O2'	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:622:A:C8	18:D:623:C:C6	3.08	0.42
18:D:1255:G:O2'	18:D:1258:G:N3	2.47	0.42
18:D:1323:G:H2'	18:D:1324:A:C8	2.55	0.42
41:a:1028:A:N6	41:a:1125:G:H2'	2.34	0.42
41:a:1394:U:C4	41:a:1395:A:C6	3.07	0.42
8:7:49:G:H5"	8:7:49:G:H8	1.85	0.42
9:9:52:MET:HE1	9:9:85:SER:HB2	2.00	0.42
11:AA:699:LEU:HG	11:AA:799:ASN:HD22	1.85	0.42
11:AA:1279:GLU:HG2	14:AE:1357:ILE:HD13	2.02	0.42
14:AE:24:LEU:CD1	14:AE:232:ASN:ND2	2.82	0.42
14:AE:144:TYR:CE1	14:AE:162:GLU:OE1	2.73	0.42
14:AE:1026:PRO:HB2	14:AE:1028:ILE:HG23	2.00	0.42
16:AG:10:GLU:CA	16:AG:12:VAL:HG22	2.50	0.42
16:AG:131:ARG:HG2	16:AG:186:VAL:CG1	2.48	0.42
18:D:37:U:O2	18:D:548:G:N2	2.53	0.42
18:D:791:G:N2	18:D:1497:G:O3'	2.53	0.42
20:F:67:ARG:HD3	20:F:67:ARG:H	1.85	0.42
39:Y:71:LYS:HB3	39:Y:72:THR:H	1.58	0.42
41:a:1082:U:N3	41:a:1086:A:C6	2.87	0.42
52:l:134:LEU:HB2	52:l:160:ALA:HB1	2.02	0.42
7:6:27:DG:H1'	7:6:28:DA:C5	2.55	0.42
11:AA:808:ASN:N	14:AE:633:ALA:HB2	2.21	0.42
11:AA:903:ARG:NH1	11:AA:903:ARG:CG	2.81	0.42
12:AB:136:VAL:HG21	12:AB:173:LEU:CD2	2.49	0.42
13:AC:48:LEU:HD23	13:AC:48:LEU:HA	1.86	0.42
14:AE:120:LEU:HA	14:AE:121:PRO:HA	1.84	0.42
16:AG:365:ILE:HB	16:AG:366:ASP:H	1.73	0.42
29:O:55:VAL:O	29:O:57:MET:N	2.52	0.42
31:Q:88:GLY:H	31:Q:114:THR:HG22	1.84	0.42
41:a:984:A:N3	41:a:984:A:H2'	2.35	0.42
41:a:1142:A:H2'	41:a:1142:A:N3	2.34	0.42
66:z:18:LEU:HD13	66:z:18:LEU:HA	1.95	0.42
9:9:50:VAL:HG21	39:Y:119:ALA:HB3	1.99	0.42
11:AA:22:LEU:HB3	11:AA:655:VAL:HG11	2.01	0.42
11:AA:1245:ALA:HB3	14:AE:375:GLU:HB3	2.01	0.42
12:AB:7:LYS:HG2	12:AB:74:VAL:HG13	2.00	0.42
12:AB:43:MET:SD	12:AB:108:VAL:HG12	2.59	0.42
12:AB:141:PHE:HE2	12:AB:173:LEU:HD21	1.83	0.42
14:AE:201:LEU:HD11	14:AE:220:ARG:NH1	2.31	0.42
14:AE:647:PRO:HG3	14:AE:697:MET:HB3	2.01	0.42
14:AE:1289:ASN:O	14:AE:1293:GLU:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:226:ALA:HB1	16:AG:228:ARG:NH1	2.34	0.42
16:AG:227:ALA:CB	16:AG:331:LEU:HA	2.46	0.42
16:AG:244:ARG:N	16:AG:244:ARG:HE	2.18	0.42
10:B:18:G:O2'	10:B:60:U:N3	2.48	0.42
18:D:197:A:C5	18:D:221:C:H4'	2.53	0.42
41:a:948:C:H1'	41:a:984:A:C8	2.55	0.42
41:a:2788:C:H2'	41:a:2789:C:C6	2.55	0.42
53:m:12:ARG:CG	53:m:44:VAL:HG11	2.50	0.42
59:s:32:LEU:HD23	59:s:54:ILE:HD13	2.01	0.42
60:t:113:MET:HE3	60:t:116:ILE:HD11	2.01	0.42
63:w:9:GLN:O	63:w:17:ARG:NH2	2.51	0.42
63:w:49:GLU:HB2	63:w:50:PRO:HD3	2.01	0.42
8:7:54:A:O3'	11:AA:688:GLN:NE2	2.53	0.42
9:9:71:CYS:SG	9:9:117:LEU:HB2	2.60	0.42
11:AA:478:ARG:HD2	11:AA:492:MET:HA	2.02	0.42
11:AA:616:ILE:HG13	11:AA:652:TYR:HB2	2.02	0.42
12:AB:64:PHE:HA	12:AB:65:PHE:HA	1.74	0.42
13:AD:46:ILE:HD11	13:AD:224:LEU:HD13	2.02	0.42
16:AG:434:LEU:HG	16:AG:455:THR:CA	2.50	0.42
10:B:58:A:OP2	10:B:58:A:H8	2.02	0.42
18:D:826:C:O2	28:N:16:ASN:ND2	2.52	0.42
22:H:274:TYR:HD1	22:H:335:ILE:HD12	1.84	0.42
23:I:9:GLY:HA3	33:S:89:MET:HE3	2.01	0.42
34:T:21:ASP:OD1	34:T:22:THR:N	2.49	0.42
39:Y:72:THR:OG1	39:Y:73:PRO:CD	2.62	0.42
39:Y:100:ILE:HB	39:Y:101:SER:H	1.71	0.42
41:a:493:G:H2'	41:a:494:G:O4'	2.20	0.42
41:a:1095:A:O2'	41:a:1096:A:O4'	2.33	0.42
48:h:37:ASN:HB2	48:h:62:TYR:HB2	2.01	0.42
59:s:114:LEU:HD12	59:s:114:LEU:HA	1.86	0.42
11:AA:1278:LEU:HD21	14:AE:484:MET:CE	2.50	0.42
14:AE:385:LEU:CD2	14:AE:390:LEU:HB2	2.50	0.42
16:AG:161:VAL:HB	16:AG:196:PHE:CE1	2.54	0.42
10:B:8:U:O2'	10:B:47:U:C4	2.72	0.42
22:H:33:LYS:HA	22:H:34:ASP:HA	1.60	0.42
22:H:292:CYS:SG	22:H:304:VAL:HB	2.60	0.42
40:Z:18:ASP:HB3	40:Z:22:LEU:HD12	2.01	0.42
41:a:36:G:N3	41:a:450:G:O2'	2.53	0.42
41:a:742:A:N1	41:a:755:U:O4	2.53	0.42
41:a:1019:U:N3	41:a:1142:A:N6	2.49	0.42
48:h:240:PHE:CD2	48:h:240:PHE:O	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:i:43:ILE:HG22	49:i:49:TYR:HB2	2.01	0.42
11:AA:894:GLN:NE2	11:AA:894:GLN:C	2.77	0.41
11:AA:895:LEU:HB3	11:AA:903:ARG:HD3	2.02	0.41
11:AA:896:THR:CB	11:AA:897:PRO:HD2	2.48	0.41
11:AA:1268:GLN:NE2	14:AE:352:ARG:HB2	2.34	0.41
14:AE:245:LEU:CG	14:AE:246:PRO:HD2	2.47	0.41
14:AE:279:LEU:HD13	14:AE:299:LEU:HD13	2.02	0.41
16:AG:208:LEU:HD23	16:AG:208:LEU:HA	1.78	0.41
16:AG:277:ASP:HB2	16:AG:282:GLN:CG	2.50	0.41
16:AG:434:LEU:CD1	16:AG:455:THR:CA	2.98	0.41
10:B:15:G:H1	10:B:20:U:H3	1.68	0.41
17:C:12:ARG:O	17:C:16:GLU:HG3	2.19	0.41
18:D:1061:G:H5'	30:P:61:ALA:HB2	2.02	0.41
20:F:32:VAL:HG11	31:Q:89:PRO:HG3	2.02	0.41
29:O:28:ILE:HD12	29:O:28:ILE:N	2.35	0.41
41:a:1082:U:C4	41:a:1086:A:N6	2.88	0.41
41:a:1406:U:H3	41:a:1596:A:H2	1.59	0.41
9:9:25:ALA:HA	9:9:96:PHE:HE1	1.85	0.41
9:9:61:ARG:C	9:9:65:GLU:HB2	2.45	0.41
11:AA:144:VAL:HG23	11:AA:515:MET:HB2	2.02	0.41
14:AE:137:ARG:HA	14:AE:142:GLU:HG2	2.02	0.41
14:AE:141:PHE:CD2	14:AE:297:ARG:HB2	2.54	0.41
14:AE:395:LYS:HB3	14:AE:395:LYS:HE3	1.45	0.41
14:AE:576:ARG:HD3	14:AE:593:ASN:HA	2.02	0.41
18:D:429:U:O2	18:D:430:A:C8	2.72	0.41
22:H:61:GLU:HG2	22:H:62:ILE:HG23	2.00	0.41
41:a:476:G:H4'	41:a:502:A:N1	2.35	0.41
41:a:1250:G:OP2	61:u:21:ARG:NH2	2.52	0.41
41:a:1839:G:C4	41:a:1927:A:C5	3.08	0.41
41:a:1921:G:O5'	41:a:1921:G:C8	2.70	0.41
10:A:65:C:C2'	10:A:66:C:H5'	2.49	0.41
11:AA:887:VAL:HG22	11:AA:913:VAL:HG22	1.95	0.41
14:AE:47:ARG:NE	14:AE:47:ARG:CA	2.84	0.41
14:AE:506:VAL:H	14:AE:506:VAL:HG12	1.59	0.41
14:AE:513:MET:HG3	14:AE:544:LEU:HD11	2.01	0.41
16:AG:299:ASP:HB3	16:AG:300:GLU:H	1.70	0.41
54:n:122:PHE:CZ	54:n:167:ARG:HA	2.55	0.41
12:AB:11:VAL:HG21	12:AB:103:ILE:CD1	2.46	0.41
12:AB:105:ASP:OD2	12:AB:105:ASP:N	2.52	0.41
12:AB:140:PRO:HB3	30:P:6:ILE:CD1	2.49	0.41
13:AD:79:LEU:HD11	14:AE:526:VAL:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AD:205:MET:HE1	13:AD:217:ILE:HG13	2.02	0.41
14:AE:820:ILE:HD11	14:AE:822:MET:HE2	2.02	0.41
14:AE:1321:SER:OG	14:AE:1349:GLU:OE2	2.22	0.41
16:AG:105:ILE:HD13	16:AG:105:ILE:H	1.85	0.41
16:AG:437:LEU:HD21	16:AG:456:LEU:CG	2.35	0.41
18:D:1235:U:H2'	18:D:1236:A:O4'	2.20	0.41
18:D:1526:G:P	20:F:42:THR:HG23	2.61	0.41
22:H:155:LYS:O	22:H:169:SER:CB	2.68	0.41
25:K:136:VAL:O	25:K:140:THR:HG23	2.20	0.41
41:a:126:A:OP1	53:m:45:SER:OG	2.38	0.41
41:a:2311:A:C2	54:n:85:ILE:HD11	2.55	0.41
61:u:109:LYS:HG2	61:u:126:ARG:HB2	2.01	0.41
3:2:46:ALA:O	3:2:50:LEU:HB2	2.21	0.41
6:5:116:DG:OP1	14:AE:1311:LYS:NZ	2.46	0.41
11:AA:906:PHE:CD1	11:AA:906:PHE:C	2.99	0.41
12:AB:43:MET:CE	12:AB:112:MET:HB2	2.51	0.41
13:AD:76:GLU:HB3	13:AD:80:GLU:HB3	2.01	0.41
14:AE:239:LEU:N	14:AE:239:LEU:HD23	2.36	0.41
14:AE:820:ILE:HG12	14:AE:884:SER:HB2	2.01	0.41
16:AG:26:ALA:CA	16:AG:117:LYS:HG2	2.51	0.41
16:AG:87:LEU:CD2	16:AG:93:VAL:HG21	2.49	0.41
16:AG:363:LEU:HD21	16:AG:407:ARG:C	2.45	0.41
10:B:7:G:O6	10:B:49:G:O6	2.39	0.41
10:B:26:G:C2	10:B:45:G:N2	2.89	0.41
18:D:502:A:H2'	18:D:503:C:O4'	2.20	0.41
18:D:548:G:C6	18:D:549:C:C4	3.08	0.41
18:D:972:C:O2'	30:P:57:VAL:HG21	2.19	0.41
21:G:187:VAL:HG21	21:G:199:VAL:HG23	2.02	0.41
25:K:133:PRO:HA	25:K:136:VAL:HG12	2.02	0.41
28:N:11:LEU:HD22	28:N:75:ILE:HD11	2.03	0.41
38:X:96:PRO:HG2	38:X:102:THR:HG23	1.97	0.41
39:Y:10:LEU:HD13	39:Y:10:LEU:HA	1.79	0.41
39:Y:102:ARG:HD2	39:Y:103:ALA:N	2.36	0.41
41:a:851:C:H2'	41:a:852:U:C6	2.55	0.41
41:a:1925:C:OP2	41:a:1925:C:C6	2.73	0.41
41:a:2294:G:OP1	64:x:10:ARG:HD3	2.21	0.41
50:j:175:LEU:CD1	50:j:193:VAL:HG12	2.51	0.41
52:l:149:ILE:HD11	52:l:188:MET:HE3	2.02	0.41
56:p:25:THR:HG22	56:p:34:THR:HG23	2.02	0.41
63:w:67:PHE:O	63:w:71:ARG:HG2	2.21	0.41
8:7:49:G:H8	8:7:49:G:C5'	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:56:C:OP1	41:a:2168:G:N3	2.53	0.41
12:AB:11:VAL:HG21	12:AB:103:ILE:HD13	2.02	0.41
14:AE:930:LEU:HA	14:AE:1244:GLN:HG3	2.02	0.41
16:AG:56:PHE:CD1	16:AG:56:PHE:N	2.88	0.41
16:AG:296:ILE:CD1	16:AG:307:ILE:HA	2.50	0.41
16:AG:307:ILE:HG13	16:AG:338:VAL:HG23	2.02	0.41
10:B:26:G:H1	10:B:44:A:N6	2.18	0.41
18:D:429:U:O2	18:D:430:A:N7	2.53	0.41
22:H:119:GLY:O	22:H:120:PHE:C	2.62	0.41
22:H:290:TYR:O	22:H:305:HIS:C	2.56	0.41
22:H:342:ILE:HG22	22:H:344:LEU:HD12	2.02	0.41
41:a:197:A:N6	41:a:2430:A:H2'	2.36	0.41
41:a:548:G:H3'	41:a:549:G:O4'	2.20	0.41
41:a:693:A:O2'	41:a:1353:A:N3	2.48	0.41
41:a:1548:A:H2'	41:a:1549:A:C8	2.55	0.41
41:a:1570:A:H2'	41:a:1571:A:C8	2.56	0.41
58:r:9:VAL:HG11	58:r:12:LEU:HD21	2.02	0.41
10:A:34:C:H41	27:M:83:SER:HA	1.85	0.41
11:AA:22:LEU:HD22	11:AA:603:ILE:HG21	2.02	0.41
11:AA:998:LEU:HD21	11:AA:1015:ALA:HB2	2.02	0.41
12:AB:65:PHE:HE2	12:AB:111:ILE:CD1	2.23	0.41
14:AE:136:GLU:OE1	14:AE:312:ARG:NH2	2.53	0.41
14:AE:394:ILE:O	14:AE:394:ILE:HG13	2.18	0.41
14:AE:848:VAL:HB	14:AE:858:VAL:HG22	2.02	0.41
14:AE:1350:ASN:HA	14:AE:1353:VAL:HG12	2.01	0.41
16:AG:185:SER:O	16:AG:185:SER:OG	2.37	0.41
16:AG:202:PRO:C	16:AG:204:MET:N	2.79	0.41
16:AG:254:MET:C	16:AG:256:GLY:H	2.27	0.41
18:D:218:U:H2'	18:D:219:U:O4'	2.21	0.41
18:D:580:C:H2'	18:D:581:G:O4'	2.21	0.41
18:D:1368:A:OP1	29:O:113:ARG:NH2	2.54	0.41
22:H:123:GLU:CA	22:H:128:ARG:HA	2.43	0.41
30:P:57:VAL:O	30:P:58:ASN:ND2	2.52	0.41
33:S:41:ARG:O	33:S:45:VAL:HG12	2.20	0.41
38:X:4:ILE:CG1	38:X:9:ILE:HD12	2.50	0.41
39:Y:35:MET:O	39:Y:35:MET:SD	2.79	0.41
41:a:5:A:H2'	41:a:6:A:C8	2.56	0.41
41:a:2803:G:H2'	41:a:2804:U:C5	2.55	0.41
9:9:125:ARG:NH1	9:9:125:ARG:CA	2.73	0.41
10:A:8:U:OP2	10:A:8:U:H6	2.04	0.41
14:AE:111:THR:HG23	14:AE:300:GLN:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:144:TYR:N	14:AE:144:TYR:CD1	2.88	0.41
14:AE:161:THR:CG2	14:AE:164:GLN:HB2	2.49	0.41
14:AE:1272:SER:OG	14:AE:1273:ASP:N	2.53	0.41
16:AG:152:LEU:HD11	16:AG:162:ILE:HD12	2.01	0.41
16:AG:314:LEU:HD23	16:AG:314:LEU:HA	1.85	0.41
18:D:216:U:H2'	18:D:217:C:C6	2.55	0.41
18:D:860:A:H2'	18:D:861:G:O4'	2.21	0.41
27:M:22:LEU:HD13	27:M:97:ASN:ND2	2.35	0.41
41:a:207:A:H2'	41:a:208:C:O4'	2.21	0.41
41:a:2273:A:H2'	41:a:2274:A:C8	2.55	0.41
2:1:75:PHE:CZ	2:1:104:THR:HG21	2.56	0.41
2:1:92:ARG:NE	2:1:94:ASP:OD1	2.53	0.41
9:9:50:VAL:CG1	39:Y:119:ALA:CB	2.88	0.41
9:9:73:LYS:CB	9:9:117:LEU:HD11	2.51	0.41
10:A:26:G:C2	10:A:45:G:N2	2.89	0.41
10:A:46:G:H2'	10:A:47:U:OP2	2.21	0.41
11:AA:310:ILE:HG21	11:AA:325:LEU:HB3	2.03	0.41
11:AA:524:ILE:HD12	11:AA:712:SER:HB2	2.02	0.41
11:AA:657:THR:HG21	11:AA:1188:ASP:HB2	2.03	0.41
11:AA:741:MET:HE3	11:AA:974:ARG:HH12	1.85	0.41
11:AA:936:ARG:HB2	11:AA:1042:LEU:HD12	2.03	0.41
13:AD:44:ARG:HA	13:AD:183:ILE:HD12	2.03	0.41
14:AE:1050:THR:HG23	14:AE:1057:SER:HB3	2.03	0.41
16:AG:125:MET:O	16:AG:125:MET:SD	2.79	0.41
16:AG:148:ASP:HA	16:AG:164:ARG:HD2	2.03	0.41
16:AG:204:MET:SD	16:AG:204:MET:O	2.79	0.41
16:AG:296:ILE:HD11	16:AG:307:ILE:CD1	2.50	0.41
16:AG:434:LEU:HD23	16:AG:456:LEU:CB	2.49	0.41
16:AG:437:LEU:CD2	16:AG:488:ILE:CD1	2.98	0.41
18:D:977:A:H1'	18:D:982:U:O4	2.20	0.41
18:D:977:A:O2'	18:D:979:C:OP2	2.39	0.41
18:D:1370:G:C2	18:D:1371:G:C8	3.09	0.41
24:J:100:ASN:OD1	24:J:111:ARG:NH1	2.54	0.41
39:Y:116:MET:CB	39:Y:124:MET:HG2	2.46	0.41
39:Y:122:GLU:O	39:Y:122:GLU:HG2	2.21	0.41
41:a:871:U:H2'	41:a:872:U:C6	2.56	0.41
41:a:1169:A:N3	41:a:1169:A:H5"	2.36	0.41
41:a:1182:G:H2'	41:a:1183:U:O4'	2.20	0.41
41:a:2314:A:O2'	54:n:155:THR:HG22	2.21	0.41
41:a:2602:A:H5"	41:a:2603:G:H5"	2.03	0.41
41:a:2638:G:O2'	41:a:2775:G:N2	2.42	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:h:119:GLY:O	48:h:130:LEU:HB3	2.20	0.41
52:l:48:THR:HG23	52:l:86:ALA:HB3	2.02	0.41
58:r:57:LYS:O	58:r:61:VAL:HG13	2.21	0.41
62:v:73:ILE:HG21	62:v:91:TYR:CZ	2.56	0.41
9:9:8:LYS:NZ	41:a:1046:A:N6	2.69	0.41
10:A:7:G:O6	10:A:49:G:O6	2.39	0.41
11:AA:836:LEU:HD21	11:AA:921:PRO:HD3	2.02	0.41
11:AA:1329:GLU:HA	14:AE:245:LEU:HD13	2.03	0.41
14:AE:68:TYR:O	14:AE:75:TYR:CD2	2.70	0.41
14:AE:734:ALA:O	14:AE:738:ARG:HB2	2.21	0.41
16:AG:302:LYS:HE3	16:AG:302:LYS:CA	2.51	0.41
16:AG:323:GLN:NE2	16:AG:323:GLN:C	2.79	0.41
16:AG:339:MET:SD	16:AG:347:LYS:CD	2.94	0.41
17:C:14:THR:CG2	17:C:48:ARG:HE	2.33	0.41
22:H:19:ARG:CD	22:H:73:ASP:OD1	2.65	0.41
41:a:2298:A:C5	41:a:2321:U:C4	3.09	0.41
48:h:76:ALA:HB2	48:h:96:TYR:CE1	2.55	0.41
8:7:56:G:H21	14:AE:427:PRO:HD3	1.85	0.40
9:9:72:LEU:C	9:9:72:LEU:CD2	2.94	0.40
9:9:118:ILE:CB	9:9:119:PRO:HD3	2.49	0.40
14:AE:68:TYR:CB	14:AE:75:TYR:HE2	2.34	0.40
14:AE:271:ARG:HE	14:AE:271:ARG:HB2	1.58	0.40
14:AE:596:LEU:HD23	14:AE:596:LEU:HA	1.91	0.40
16:AG:233:ARG:CB	16:AG:327:LEU:CD2	2.98	0.40
16:AG:284:VAL:HG22	16:AG:305:MET:CE	2.50	0.40
16:AG:305:MET:HE3	16:AG:305:MET:HB3	1.77	0.40
16:AG:323:GLN:HE21	16:AG:323:GLN:C	2.28	0.40
10:B:37:A:H5"	10:B:37:A:C4	2.57	0.40
10:B:65:C:C2'	10:B:66:C:H5'	2.49	0.40
18:D:110:C:O2'	35:U:25:ARG:O	2.35	0.40
18:D:798:U:H2'	18:D:799:G:O4'	2.22	0.40
18:D:1330:U:OP2	38:X:26:GLY:HA3	2.21	0.40
22:H:63:GLN:HB3	22:H:64:VAL:H	1.74	0.40
25:K:154:ALA:HA	25:K:164:ILE:HD11	2.03	0.40
38:X:16:VAL:HG13	38:X:34:LEU:CD1	2.51	0.40
38:X:16:VAL:O	38:X:20:THR:HG23	2.21	0.40
41:a:1406:U:O2'	41:a:1407:G:OP2	2.38	0.40
47:g:37:CYS:N	47:g:40:CYS:SG	2.77	0.40
61:u:74:THR:HG22	61:u:107:PHE:HB2	2.03	0.40
6:5:98:DA:H2'	6:5:99:DT:H72	2.01	0.40
8:7:20:U:H5"	8:7:20:U:H6	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:135:THR:HG22	11:AA:144:VAL:HG22	2.03	0.40
11:AA:469:VAL:HA	11:AA:472:GLU:HG2	2.02	0.40
11:AA:550:VAL:HG13	14:AE:777:HIS:CD2	2.56	0.40
11:AA:847:PRO:HB2	11:AA:1047:LEU:HD11	2.02	0.40
12:AB:64:PHE:N	12:AB:64:PHE:HD1	2.19	0.40
13:AC:42:ALA:HB1	13:AC:224:LEU:HD11	2.03	0.40
14:AE:245:LEU:HG	14:AE:246:PRO:CD	2.51	0.40
16:AG:36:LYS:HB3	16:AG:36:LYS:HE2	1.87	0.40
16:AG:218:GLU:H	16:AG:218:GLU:HG2	1.64	0.40
16:AG:448:LEU:CD2	16:AG:467:LEU:HD22	2.51	0.40
10:B:8:U:OP2	10:B:8:U:H6	2.04	0.40
18:D:915:A:C6	18:D:916:U:C4	3.09	0.40
29:O:10:GLY:HA3	29:O:78:ALA:O	2.21	0.40
33:S:16:LEU:HD13	33:S:54:ASP:HB2	2.03	0.40
34:T:43:PHE:CE2	34:T:56:LEU:HD22	2.55	0.40
37:W:50:ALA:HB1	37:W:57:HIS:HB3	2.04	0.40
56:p:52:PHE:CZ	56:p:72:LEU:HD22	2.56	0.40
66:z:66:ASN:OD1	66:z:70:ARG:NE	2.54	0.40
9:9:47:GLU:HG3	9:9:95:LEU:CD2	2.49	0.40
9:9:48:ALA:HB3	9:9:51:TYR:HD2	1.86	0.40
9:9:118:ILE:H	9:9:119:PRO:HD2	1.86	0.40
11:AA:738:GLU:HA	11:AA:741:MET:HE2	2.03	0.40
11:AA:888:THR:CB	11:AA:889:PRO:CD	2.97	0.40
11:AA:1247:SER:OG	11:AA:1248:THR:N	2.55	0.40
14:AE:450:HIS:HA	14:AE:451:PRO:HD3	1.90	0.40
14:AE:515:ARG:HG2	14:AE:516:ASP:H	1.85	0.40
16:AG:285:ILE:CA	16:AG:293:VAL:HG11	2.51	0.40
16:AG:433:ASP:O	16:AG:456:LEU:CD2	2.69	0.40
18:D:1225:A:H2'	18:D:1226:C:C5	2.56	0.40
39:Y:14:ALA:HB3	39:Y:50:LYS:HA	2.03	0.40
39:Y:116:MET:HA	39:Y:116:MET:CE	2.50	0.40
41:a:67:U:C4	41:a:74:A:C6	3.04	0.40
41:a:2641:G:OP1	59:s:78:THR:HG22	2.21	0.40
42:b:59:LEU:HD12	42:b:80:ILE:HD12	2.03	0.40
48:h:175:ARG:NH1	48:h:181:MET:HE2	2.36	0.40
48:h:232:HIS:HA	48:h:242:LYS:HE3	2.04	0.40
59:s:99:ARG:HD2	59:s:99:ARG:HA	1.93	0.40
11:AA:862:LEU:HD23	11:AA:862:LEU:C	2.46	0.40
14:AE:438:GLU:OE2	14:AE:481:ARG:NH1	2.41	0.40
16:AG:18:LEU:HD21	16:AG:125:MET:HE2	2.04	0.40
16:AG:230:PRO:HA	16:AG:269:GLU:CD	2.47	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AG:381:LEU:CA	16:AG:384:LEU:CD1	2.86	0.40
17:C:34:THR:N	17:C:38:LYS:O	2.55	0.40
18:D:1189:U:OP1	33:S:98:LYS:NZ	2.55	0.40
21:G:28:LYS:N	21:G:29:PRO:CD	2.85	0.40
22:H:29:VAL:HG23	22:H:37:LEU:HD12	2.04	0.40
41:a:526:A:O2'	41:a:2043:C:O2	2.39	0.40
41:a:1421:G:C2	41:a:1422:G:C8	3.09	0.40
41:a:2315:G:C5'	54:n:157:THR:HG23	2.52	0.40
41:a:2572:A:N7	50:j:150:GLN:NE2	2.69	0.40
43:c:36:HIS:CG	43:c:56:MET:HE3	2.57	0.40
52:l:188:MET:HE2	52:l:193:VAL:HA	2.03	0.40
54:n:171:ALA:O	54:n:174:ASP:N	2.54	0.40
10:A:71:C:H2'	10:A:72:A:C1'	2.52	0.40
11:AA:979:LEU:HD11	11:AA:1011:LEU:HD11	2.03	0.40
12:AB:129:GLU:OE1	12:AB:130:PRO:HD2	2.22	0.40
14:AE:108:ALA:HB2	14:AE:276:ASN:OD1	2.22	0.40
14:AE:109:SER:CB	14:AE:296:LYS:HG2	2.51	0.40
16:AG:77:LEU:HG	16:AG:89:LEU:HD21	2.04	0.40
16:AG:182:VAL:CG2	16:AG:204:MET:HA	2.52	0.40
16:AG:320:ARG:HD3	16:AG:320:ARG:HA	1.84	0.40
10:B:26:G:H2'	10:B:27:U:C6	2.57	0.40
10:B:46:G:H2'	10:B:47:U:OP2	2.21	0.40
18:D:152:A:N6	18:D:170:U:C2	2.89	0.40
18:D:495:A:C6	18:D:496:A:N6	2.90	0.40
18:D:890:G:O2'	18:D:906:A:N6	2.55	0.40
18:D:1473:G:H2'	18:D:1474:U:O4'	2.22	0.40
22:H:54:LYS:HE3	22:H:54:LYS:HB3	1.91	0.40
29:O:84:THR:HG21	29:O:103:PHE:CB	2.46	0.40
39:Y:52:LEU:HD21	39:Y:81:LYS:HD3	2.03	0.40
39:Y:78:LEU:CD1	39:Y:108:ILE:HG22	2.50	0.40
41:a:17:G:H2'	41:a:18:U:C6	2.56	0.40
41:a:753:A:C5	41:a:754:U:C5	3.09	0.40
41:a:1406:U:C2'	41:a:1407:G:OP2	2.69	0.40
41:a:2683:C:O2	60:t:70:ARG:NH2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	13 49
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100 100
3	2	92/100 (92%)	90 (98%)	2 (2%)	0	100 100
4	3	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	13 49
5	4	92/94 (98%)	90 (98%)	2 (2%)	0	100 100
9	9	146/165 (88%)	94 (64%)	38 (26%)	14 (10%)	0 7
11	AA	1338/1342 (100%)	1206 (90%)	128 (10%)	4 (0%)	37 73
12	AB	157/181 (87%)	129 (82%)	20 (13%)	8 (5%)	1 15
13	AC	216/329 (66%)	202 (94%)	12 (6%)	2 (1%)	14 52
13	AD	292/329 (89%)	269 (92%)	23 (8%)	0	100 100
14	AE	1329/1407 (94%)	1199 (90%)	119 (9%)	11 (1%)	16 55
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100 100
16	AG	493/495 (100%)	375 (76%)	87 (18%)	31 (6%)	1 13
17	C	64/75 (85%)	63 (98%)	1 (2%)	0	100 100
19	E	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
20	F	68/71 (96%)	68 (100%)	0	0	100 100
21	G	223/241 (92%)	210 (94%)	13 (6%)	0	100 100
22	H	255/557 (46%)	189 (74%)	54 (21%)	12 (5%)	2 16
23	I	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	25 64
24	J	203/206 (98%)	198 (98%)	5 (2%)	0	100 100
25	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	22 60
26	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	13 49
27	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	19 57
28	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	16 55
29	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	16 55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	P	97/103 (94%)	87 (90%)	8 (8%)	2 (2%)	5	30
31	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	7	37
32	R	117/124 (94%)	116 (99%)	1 (1%)	0	100	100
33	S	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
34	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
35	U	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	10	43
36	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
37	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
38	X	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	7	35
39	Y	139/142 (98%)	102 (73%)	25 (18%)	12 (9%)	0	9
40	Z	28/121 (23%)	20 (71%)	6 (21%)	2 (7%)	1	11
42	b	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
43	c	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
45	e	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
47	g	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
48	h	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	30	68
49	i	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
50	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
51	k	50/55 (91%)	50 (100%)	0	0	100	100
52	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	25	64
53	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	n	175/179 (98%)	162 (93%)	11 (6%)	2 (1%)	12	47
55	o	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
56	p	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
57	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
58	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
59	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
60	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
61	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
62	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	w	117/127 (92%)	107 (92%)	10 (8%)	0	100	100
64	x	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
65	y	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
66	z	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	52
All	All	10078/11072 (91%)	9198 (91%)	764 (8%)	116 (1%)	14	44

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	88	HIS
12	AB	118	VAL
12	AB	122	PRO
14	AE	291	ILE
16	AG	34	ALA
16	AG	105	ILE
16	AG	187	ARG
16	AG	227	ALA
22	H	139	ARG
22	H	153	GLU
22	H	169	SER
22	H	306	VAL
22	H	340	ARG
29	O	56	ASP
38	X	103	LYS
39	Y	48	ILE
9	9	33	VAL
9	9	119	PRO
11	AA	853	ASP
11	AA	905	ILE
11	AA	907	GLY
12	AB	124	PRO
12	AB	130	PRO
12	AB	163	SER
14	AE	175	GLU
14	AE	292	VAL
16	AG	63	LEU
16	AG	104	ARG
16	AG	242	ASP
16	AG	268	GLY
16	AG	279	ASN
16	AG	365	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	H	108	VAL
22	H	309	MET
22	H	333	LEU
23	I	80	LYS
39	Y	93	ASN
48	h	158	ALA
52	l	142	ALA
66	z	3	ARG
9	9	48	ALA
9	9	91	ALA
9	9	118	ILE
9	9	130	PRO
14	AE	51	PRO
14	AE	805	GLN
16	AG	33	THR
16	AG	102	PHE
16	AG	200	SER
16	AG	305	MET
16	AG	319	GLY
16	AG	350	ALA
16	AG	355	ALA
16	AG	396	GLU
16	AG	425	LEU
22	H	76	GLU
22	H	142	ARG
27	M	130	ASN
30	P	58	ASN
31	Q	119	ASN
38	X	105	ASN
39	Y	20	SER
39	Y	64	ARG
39	Y	106	GLN
9	9	69	PHE
9	9	73	LYS
9	9	108	VAL
9	9	129	LEU
9	9	133	GLU
12	AB	67	GLY
12	AB	141	PHE
13	AC	193	GLU
14	AE	174	ASP
14	AE	193	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	AG	48	GLN
16	AG	265	GLU
16	AG	363	LEU
16	AG	401	PRO
22	H	82	THR
30	P	90	LEU
39	Y	83	ALA
40	Z	21	GLU
54	n	40	VAL
4	3	39	ILE
14	AE	91	GLU
16	AG	224	LYS
16	AG	399	ASP
22	H	70	VAL
39	Y	22	PRO
39	Y	71	LYS
39	Y	89	SER
40	Z	7	ILE
9	9	28	ALA
13	AC	192	VAL
14	AE	49	PHE
14	AE	73	GLY
14	AE	904	ALA
16	AG	43	ILE
16	AG	70	GLN
16	AG	169	PRO
16	AG	323	GLN
16	AG	364	ASP
16	AG	382	GLU
39	Y	62	ALA
12	AB	42	VAL
26	L	96	VAL
39	Y	100	ILE
1	0	44	GLY
25	K	44	GLY
39	Y	23	VAL
11	AA	1317	PRO
31	Q	74	VAL
35	U	64	GLY
9	9	54	VAL
28	N	75	ILE
54	n	62	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	84/84 (100%)	76 (90%)	8 (10%)	7	22
2	1	93/93 (100%)	86 (92%)	7 (8%)	11	31
3	2	81/84 (96%)	77 (95%)	4 (5%)	21	42
4	3	84/85 (99%)	79 (94%)	5 (6%)	16	37
5	4	78/78 (100%)	75 (96%)	3 (4%)	28	49
9	9	112/123 (91%)	63 (56%)	49 (44%)	0	0
11	AA	1155/1157 (100%)	1130 (98%)	25 (2%)	47	65
12	AB	138/158 (87%)	108 (78%)	30 (22%)	1	5
13	AC	185/286 (65%)	184 (100%)	1 (0%)	86	89
13	AD	185/286 (65%)	185 (100%)	0	100	100
14	AE	1120/1168 (96%)	1046 (93%)	74 (7%)	14	34
15	AF	70/75 (93%)	69 (99%)	1 (1%)	62	75
16	AG	409/409 (100%)	288 (70%)	121 (30%)	0	2
17	C	57/65 (88%)	55 (96%)	2 (4%)	31	51
19	E	65/66 (98%)	61 (94%)	4 (6%)	15	36
20	F	60/61 (98%)	57 (95%)	3 (5%)	20	41
21	G	187/199 (94%)	174 (93%)	13 (7%)	12	32
22	H	137/461 (30%)	124 (90%)	13 (10%)	7	22
23	I	171/190 (90%)	163 (95%)	8 (5%)	22	44
24	J	172/173 (99%)	164 (95%)	8 (5%)	22	44
25	K	119/126 (94%)	111 (93%)	8 (7%)	13	34
26	L	91/116 (78%)	84 (92%)	7 (8%)	10	30
27	M	124/147 (84%)	113 (91%)	11 (9%)	8	25
28	N	104/105 (99%)	101 (97%)	3 (3%)	37	56
29	O	105/107 (98%)	99 (94%)	6 (6%)	17	38
30	P	86/90 (96%)	73 (85%)	13 (15%)	2	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Q	90/99 (91%)	88 (98%)	2 (2%)	47	65
32	R	101/104 (97%)	95 (94%)	6 (6%)	16	37
33	S	83/84 (99%)	79 (95%)	4 (5%)	21	43
34	T	76/77 (99%)	65 (86%)	11 (14%)	2	12
35	U	65/65 (100%)	60 (92%)	5 (8%)	10	30
36	V	74/78 (95%)	71 (96%)	3 (4%)	26	47
37	W	72/79 (91%)	66 (92%)	6 (8%)	9	27
38	X	94/96 (98%)	87 (93%)	7 (7%)	11	31
39	Y	109/110 (99%)	69 (63%)	40 (37%)	0	1
40	Z	26/85 (31%)	10 (38%)	16 (62%)	0	0
42	b	58/63 (92%)	57 (98%)	1 (2%)	56	72
43	c	67/68 (98%)	64 (96%)	3 (4%)	23	45
45	e	54/55 (98%)	51 (94%)	3 (6%)	17	38
46	f	48/49 (98%)	43 (90%)	5 (10%)	5	19
47	g	59/62 (95%)	55 (93%)	4 (7%)	13	34
48	h	216/218 (99%)	199 (92%)	17 (8%)	10	29
49	i	47/48 (98%)	41 (87%)	6 (13%)	3	14
50	j	164/164 (100%)	156 (95%)	8 (5%)	21	42
51	k	47/49 (96%)	44 (94%)	3 (6%)	14	35
52	l	165/165 (100%)	151 (92%)	14 (8%)	8	27
53	m	38/38 (100%)	36 (95%)	2 (5%)	19	40
54	n	148/150 (99%)	130 (88%)	18 (12%)	4	15
55	o	51/52 (98%)	47 (92%)	4 (8%)	10	29
56	p	136/138 (99%)	130 (96%)	6 (4%)	24	45
57	q	34/34 (100%)	31 (91%)	3 (9%)	8	25
58	r	114/114 (100%)	102 (90%)	12 (10%)	5	19
59	s	116/116 (100%)	106 (91%)	10 (9%)	8	26
60	t	104/104 (100%)	98 (94%)	6 (6%)	17	38
61	u	103/103 (100%)	96 (93%)	7 (7%)	13	34
62	v	109/109 (100%)	105 (96%)	4 (4%)	29	49
63	w	99/103 (96%)	91 (92%)	8 (8%)	9	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	x	86/87 (99%)	80 (93%)	6 (7%)	12	32
65	y	99/100 (99%)	91 (92%)	8 (8%)	9	28
66	z	89/90 (99%)	85 (96%)	4 (4%)	23	45
All	All	8313/9148 (91%)	7624 (92%)	689 (8%)	12	27

All (689) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	38	VAL
1	0	47	VAL
1	0	48	LYS
1	0	51	VAL
1	0	68	ARG
1	0	86	GLN
1	0	96	VAL
2	1	19	LEU
2	1	30	SER
2	1	41	LYS
2	1	69	LEU
2	1	97	LEU
2	1	107	VAL
2	1	110	ARG
3	2	1	MET
3	2	24	MET
3	2	37	ASP
3	2	93	LEU
4	3	52	LEU
4	3	70	VAL
4	3	72	ILE
4	3	99	ASN
4	3	101	GLU
5	4	40	ILE
5	4	69	GLU
5	4	71	LYS
9	9	1	MET
9	9	3	LEU
9	9	4	ASN
9	9	5	LEU
9	9	6	GLN
9	9	7	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	9	11	ILE
9	9	14	GLU
9	9	23	LEU
9	9	24	SER
9	9	27	VAL
9	9	31	ARG
9	9	33	VAL
9	9	34	THR
9	9	35	VAL
9	9	36	ASP
9	9	37	LYS
9	9	39	THR
9	9	42	ARG
9	9	43	LYS
9	9	52	MET
9	9	54	VAL
9	9	55	VAL
9	9	56	ARG
9	9	57	ASN
9	9	61	ARG
9	9	69	PHE
9	9	70	GLU
9	9	71	CYS
9	9	72	LEU
9	9	73	LYS
9	9	81	LEU
9	9	86	MET
9	9	94	ARG
9	9	96	PHE
9	9	98	GLU
9	9	106	PHE
9	9	107	GLU
9	9	109	LYS
9	9	113	PHE
9	9	117	LEU
9	9	122	GLN
9	9	123	ILE
9	9	125	ARG
9	9	133	GLU
9	9	134	GLU
9	9	138	ARG
9	9	142	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	9	143	MET
11	AA	145	ILE
11	AA	615	VAL
11	AA	844	LYS
11	AA	851	THR
11	AA	854	ILE
11	AA	857	VAL
11	AA	859	GLU
11	AA	862	LEU
11	AA	864	LYS
11	AA	888	THR
11	AA	890	LYS
11	AA	894	GLN
11	AA	895	LEU
11	AA	896	THR
11	AA	899	GLU
11	AA	900	LYS
11	AA	901	LEU
11	AA	902	LEU
11	AA	903	ARG
11	AA	909	LYS
11	AA	912	ASP
11	AA	913	VAL
11	AA	914	LYS
11	AA	1076	ILE
11	AA	1151	LEU
12	AB	46	THR
12	AB	64	PHE
12	AB	103	ILE
12	AB	105	ASP
12	AB	106	LYS
12	AB	107	GLU
12	AB	108	VAL
12	AB	114	ARG
12	AB	116	GLN
12	AB	117	GLN
12	AB	123	ARG
12	AB	125	LYS
12	AB	128	PHE
12	AB	132	GLU
12	AB	133	MET
12	AB	134	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	AB	135	ARG
12	AB	145	ASN
12	AB	150	GLU
12	AB	151	VAL
12	AB	153	TYR
12	AB	157	ARG
12	AB	161	SER
12	AB	162	VAL
12	AB	167	ARG
12	AB	169	THR
12	AB	171	VAL
12	AB	172	GLU
12	AB	173	LEU
12	AB	180	LYS
13	AC	232	VAL
14	AE	40	LYS
14	AE	42	GLU
14	AE	44	ILE
14	AE	46	TYR
14	AE	47	ARG
14	AE	49	PHE
14	AE	50	LYS
14	AE	52	GLU
14	AE	53	ARG
14	AE	54	ASP
14	AE	56	LEU
14	AE	60	ARG
14	AE	66	LYS
14	AE	67	ASP
14	AE	70	CYS
14	AE	74	LYS
14	AE	76	LYS
14	AE	78	LEU
14	AE	80	HIS
14	AE	81	ARG
14	AE	88	CYS
14	AE	91	GLU
14	AE	94	GLN
14	AE	95	THR
14	AE	96	LYS
14	AE	99	ARG
14	AE	100	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	AE	114	ILE
14	AE	117	LEU
14	AE	119	SER
14	AE	123	ARG
14	AE	132	LEU
14	AE	135	ILE
14	AE	142	GLU
14	AE	144	TYR
14	AE	145	VAL
14	AE	146	VAL
14	AE	147	ILE
14	AE	152	THR
14	AE	154	LEU
14	AE	157	GLN
14	AE	159	ILE
14	AE	175	GLU
14	AE	180	MET
14	AE	190	LYS
14	AE	193	ASP
14	AE	196	GLN
14	AE	210	SER
14	AE	212	THR
14	AE	216	LYS
14	AE	222	LYS
14	AE	223	LEU
14	AE	227	PHE
14	AE	233	LYS
14	AE	237	MET
14	AE	238	ILE
14	AE	239	LEU
14	AE	240	THR
14	AE	244	VAL
14	AE	271	ARG
14	AE	291	ILE
14	AE	324	LEU
14	AE	385	LEU
14	AE	386	GLU
14	AE	387	LEU
14	AE	390	LEU
14	AE	393	THR
14	AE	394	ILE
14	AE	395	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	AE	506	VAL
14	AE	514	THR
14	AE	839	VAL
14	AE	1172	LYS
14	AE	1233	ILE
15	AF	63	ILE
16	AG	5	ILE
16	AG	12	VAL
16	AG	16	LYS
16	AG	36	LYS
16	AG	37	LYS
16	AG	40	GLU
16	AG	43	ILE
16	AG	47	VAL
16	AG	49	ILE
16	AG	50	ASP
16	AG	56	PHE
16	AG	57	ASP
16	AG	61	ARG
16	AG	63	LEU
16	AG	75	ILE
16	AG	97	ILE
16	AG	103	ASP
16	AG	104	ARG
16	AG	114	ILE
16	AG	117	LYS
16	AG	123	ARG
16	AG	125	MET
16	AG	126	VAL
16	AG	131	ARG
16	AG	138	ILE
16	AG	139	THR
16	AG	144	LYS
16	AG	150	ILE
16	AG	154	LEU
16	AG	157	ASN
16	AG	162	ILE
16	AG	167	MET
16	AG	173	PHE
16	AG	174	ARG
16	AG	179	VAL
16	AG	180	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	AG	182	VAL
16	AG	187	ARG
16	AG	189	GLU
16	AG	195	LEU
16	AG	197	VAL
16	AG	199	ARG
16	AG	201	LYS
16	AG	203	GLU
16	AG	204	MET
16	AG	205	LEU
16	AG	206	ILE
16	AG	207	GLU
16	AG	210	ARG
16	AG	211	ILE
16	AG	213	VAL
16	AG	218	GLU
16	AG	219	GLU
16	AG	221	ILE
16	AG	223	ILE
16	AG	232	SER
16	AG	235	LYS
16	AG	236	ILE
16	AG	238	VAL
16	AG	239	LYS
16	AG	240	THR
16	AG	241	ASN
16	AG	243	LYS
16	AG	244	ARG
16	AG	245	ILE
16	AG	254	MET
16	AG	255	ARG
16	AG	258	ARG
16	AG	259	VAL
16	AG	260	GLN
16	AG	262	VAL
16	AG	265	GLU
16	AG	270	ARG
16	AG	271	ILE
16	AG	273	ILE
16	AG	274	VAL
16	AG	276	TRP
16	AG	278	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	AG	282	GLN
16	AG	285	ILE
16	AG	288	MET
16	AG	296	ILE
16	AG	297	VAL
16	AG	299	ASP
16	AG	300	GLU
16	AG	301	ASP
16	AG	302	LYS
16	AG	303	HIS
16	AG	305	MET
16	AG	309	VAL
16	AG	310	GLU
16	AG	313	ASN
16	AG	316	GLN
16	AG	320	ARG
16	AG	321	ASN
16	AG	323	GLN
16	AG	327	LEU
16	AG	331	LEU
16	AG	335	GLU
16	AG	336	LEU
16	AG	337	ASN
16	AG	338	VAL
16	AG	340	THR
16	AG	341	VAL
16	AG	342	ASP
16	AG	344	LEU
16	AG	356	ILE
16	AG	358	THR
16	AG	359	PHE
16	AG	361	LYS
16	AG	365	ILE
16	AG	380	THR
16	AG	387	VAL
16	AG	390	LYS
16	AG	396	GLU
16	AG	398	LEU
16	AG	399	ASP
16	AG	400	GLU
16	AG	425	LEU
16	AG	428	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	AG	429	LYS
17	C	33	ILE
17	C	74	HIS
19	E	6	SER
19	E	10	ARG
19	E	48	GLN
19	E	64	LYS
20	F	34	ARG
20	F	62	ARG
20	F	67	ARG
21	G	8	ASP
21	G	45	LYS
21	G	59	LYS
21	G	105	LYS
21	G	108	ARG
21	G	117	LEU
21	G	128	LYS
21	G	129	LEU
21	G	132	LYS
21	G	135	LEU
21	G	161	LEU
21	G	174	LYS
21	G	208	ARG
22	H	9	PHE
22	H	31	ILE
22	H	43	LYS
22	H	54	LYS
22	H	62	ILE
22	H	70	VAL
22	H	294	VAL
22	H	305	HIS
22	H	336	ASP
22	H	337	GLU
22	H	338	GLU
22	H	339	ARG
22	H	340	ARG
23	I	14	ILE
23	I	21	THR
23	I	33	LEU
23	I	75	ILE
23	I	89	LYS
23	I	175	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	I	178	LEU
23	I	200	VAL
24	J	47	ARG
24	J	48	LEU
24	J	95	GLU
24	J	104	ARG
24	J	105	MET
24	J	116	GLN
24	J	138	SER
24	J	143	VAL
25	K	10	GLU
25	K	15	LEU
25	K	60	ILE
25	K	114	VAL
25	K	115	LEU
25	K	138	ARG
25	K	141	ILE
25	K	162	GLU
26	L	7	VAL
26	L	16	GLU
26	L	24	ARG
26	L	36	ILE
26	L	38	ARG
26	L	54	LEU
26	L	86	ARG
27	M	7	ILE
27	M	17	LYS
27	M	21	GLU
27	M	23	LEU
27	M	27	VAL
27	M	50	LEU
27	M	79	ARG
27	M	91	VAL
27	M	109	ARG
27	M	130	ASN
27	M	146	GLU
28	N	96	MET
28	N	104	VAL
28	N	117	ARG
29	O	27	LYS
29	O	60	LYS
29	O	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	O	63	LEU
29	O	116	VAL
29	O	118	LEU
30	P	17	LEU
30	P	18	ILE
30	P	24	GLU
30	P	25	ILE
30	P	27	GLU
30	P	37	ARG
30	P	87	LEU
30	P	88	MET
30	P	89	ARG
30	P	90	LEU
30	P	91	ASP
30	P	92	LEU
30	P	102	LEU
31	Q	15	GLN
31	Q	107	ILE
32	R	5	ASN
32	R	12	ARG
32	R	24	LEU
32	R	62	GLU
32	R	74	LEU
32	R	102	LEU
33	S	45	VAL
33	S	46	LEU
33	S	89	MET
33	S	92	GLU
34	T	10	LYS
34	T	22	THR
34	T	39	LEU
34	T	40	GLN
34	T	64	ARG
34	T	66	LEU
34	T	67	LEU
34	T	70	LEU
34	T	73	LYS
34	T	84	ARG
34	T	85	LEU
35	U	1	MET
35	U	2	VAL
35	U	6	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	U	19	VAL
35	U	50	THR
36	V	46	VAL
36	V	75	LEU
36	V	81	LYS
37	W	21	LYS
37	W	33	THR
37	W	49	ILE
37	W	58	VAL
37	W	79	THR
37	W	81	ARG
38	X	16	VAL
38	X	25	VAL
38	X	29	ARG
38	X	59	GLU
38	X	93	ARG
38	X	101	ARG
38	X	117	LYS
39	Y	4	VAL
39	Y	10	LEU
39	Y	16	MET
39	Y	23	VAL
39	Y	27	LEU
39	Y	30	GLN
39	Y	36	GLU
39	Y	44	LYS
39	Y	45	THR
39	Y	48	ILE
39	Y	50	LYS
39	Y	52	LEU
39	Y	57	VAL
39	Y	58	ILE
39	Y	60	VAL
39	Y	61	TYR
39	Y	64	ARG
39	Y	65	SER
39	Y	67	THR
39	Y	71	LYS
39	Y	78	LEU
39	Y	80	LYS
39	Y	81	LYS
39	Y	91	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	Y	94	LYS
39	Y	95	ASP
39	Y	99	LYS
39	Y	100	ILE
39	Y	102	ARG
39	Y	104	GLN
39	Y	108	ILE
39	Y	112	LYS
39	Y	116	MET
39	Y	124	MET
39	Y	125	THR
39	Y	126	ARG
39	Y	133	ARG
39	Y	135	MET
39	Y	137	LEU
39	Y	138	VAL
40	Z	1	SER
40	Z	2	ILE
40	Z	3	THR
40	Z	4	LYS
40	Z	6	GLN
40	Z	7	ILE
40	Z	8	ILE
40	Z	14	MET
40	Z	16	VAL
40	Z	17	MET
40	Z	19	VAL
40	Z	23	ILE
40	Z	26	MET
40	Z	28	GLU
40	Z	29	LYS
40	Z	30	PHE
42	b	70	GLU
43	c	33	LEU
43	c	48	THR
43	c	71	LEU
45	e	18	LEU
45	e	58	ASN
45	e	60	LYS
46	f	3	LYS
46	f	11	ARG
46	f	25	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	f	45	ARG
46	f	55	VAL
47	g	3	LYS
47	g	16	CYS
47	g	24	ILE
47	g	47	LYS
48	h	51	THR
48	h	94	VAL
48	h	105	LEU
48	h	118	SER
48	h	125	LYS
48	h	130	LEU
48	h	141	VAL
48	h	156	ARG
48	h	183	LYS
48	h	187	ASP
48	h	195	VAL
48	h	202	LEU
48	h	203	ARG
48	h	204	VAL
48	h	205	LEU
48	h	242	LYS
48	h	271	ARG
49	i	9	THR
49	i	12	LYS
49	i	26	THR
49	i	27	SER
49	i	29	SER
49	i	40	ARG
50	j	13	ARG
50	j	18	ASP
50	j	91	THR
50	j	99	GLU
50	j	104	VAL
50	j	177	VAL
50	j	189	VAL
50	j	193	VAL
51	k	5	ILE
51	k	17	THR
51	k	24	THR
52	l	17	THR
52	l	22	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	l	40	ARG
52	l	48	THR
52	l	57	LYS
52	l	69	ARG
52	l	77	ILE
52	l	80	SER
52	l	108	ILE
52	l	109	LEU
52	l	111	GLU
52	l	122	GLU
52	l	149	ILE
52	l	179	SER
53	m	22	MET
53	m	42	LEU
54	n	6	ASP
54	n	10	ASP
54	n	26	MET
54	n	40	VAL
54	n	47	LYS
54	n	49	LEU
54	n	57	LEU
54	n	79	ILE
54	n	80	ARG
54	n	95	ARG
54	n	105	THR
54	n	117	LEU
54	n	122	PHE
54	n	123	ASP
54	n	132	VAL
54	n	140	GLU
54	n	141	ILE
54	n	163	ASP
55	o	8	ARG
55	o	30	ARG
55	o	31	HIS
55	o	55	LEU
56	p	11	VAL
56	p	85	LYS
56	p	95	ARG
56	p	125	CYS
56	p	168	VAL
56	p	171	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	q	3	VAL
57	q	26	ILE
57	q	34	LYS
58	r	1	MET
58	r	9	VAL
58	r	11	ASN
58	r	12	LEU
58	r	15	LEU
58	r	41	LYS
58	r	66	ASN
58	r	72	ILE
58	r	76	GLU
58	r	94	ILE
58	r	101	ASP
58	r	127	GLU
59	s	1	MET
59	s	30	THR
59	s	31	GLU
59	s	43	GLU
59	s	57	LEU
59	s	123	LYS
59	s	124	VAL
59	s	139	VAL
59	s	140	LEU
59	s	142	ILE
60	t	35	VAL
60	t	49	ARG
60	t	67	LYS
60	t	70	ARG
60	t	80	ASP
60	t	104	THR
61	u	5	THR
61	u	27	LEU
61	u	59	ARG
61	u	73	ILE
61	u	76	GLU
61	u	78	ARG
61	u	84	LYS
62	v	110	GLU
62	v	126	ILE
62	v	127	LYS
62	v	128	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	w	2	ARG
63	w	20	MET
63	w	24	MET
63	w	51	LEU
63	w	65	LEU
63	w	69	ARG
63	w	95	THR
63	w	116	VAL
64	x	13	ARG
64	x	31	THR
64	x	47	VAL
64	x	48	LEU
64	x	91	SER
64	x	116	GLN
65	y	8	LEU
65	y	10	GLN
65	y	27	GLU
65	y	40	LEU
65	y	81	VAL
65	y	85	SER
65	y	102	GLU
65	y	114	LEU
66	z	18	LEU
66	z	51	ARG
66	z	109	LEU
66	z	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	86	GLN
2	1	61	ASN
3	2	28	ASN
3	2	59	ASN
4	3	54	GLN
9	9	103	ASN
9	9	122	GLN
11	AA	69	GLN
11	AA	314	ASN
11	AA	330	HIS
11	AA	343	HIS
11	AA	513	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	AA	554	HIS
11	AA	688	GLN
11	AA	762	ASN
11	AA	808	ASN
11	AA	894	GLN
11	AA	965	GLN
11	AA	1237	HIS
11	AA	1268	GLN
11	AA	1313	HIS
13	AC	23	HIS
13	AD	66	HIS
13	AD	84	ASN
13	AD	117	HIS
13	AD	227	GLN
14	AE	196	GLN
14	AE	294	ASN
14	AE	424	ASN
14	AE	469	HIS
14	AE	865	HIS
14	AE	979	ASN
14	AE	1195	GLN
14	AE	1238	GLN
14	AE	1249	ASN
15	AF	7	GLN
15	AF	31	GLN
15	AF	62	GLN
16	AG	194	GLN
16	AG	260	GLN
16	AG	282	GLN
16	AG	316	GLN
16	AG	323	GLN
16	AG	324	ASN
16	AG	337	ASN
16	AG	428	ASN
19	E	55	GLN
19	E	61	GLN
21	G	18	HIS
21	G	58	ASN
21	G	94	HIS
23	I	6	HIS
23	I	123	GLN
24	J	36	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	J	40	GLN
24	J	41	HIS
25	K	97	GLN
26	L	11	HIS
26	L	63	ASN
26	L	94	HIS
27	M	97	ASN
27	M	148	ASN
29	O	81	HIS
29	O	126	GLN
30	P	58	ASN
31	Q	15	GLN
32	R	72	HIS
33	S	60	GLN
34	T	40	GLN
35	U	59	HIS
38	X	12	HIS
38	X	105	ASN
48	h	70	ASN
48	h	260	ASN
49	i	5	GLN
50	j	173	GLN
51	k	26	ASN
54	n	63	GLN
55	o	28	ASN
56	p	48	ASN
56	p	88	GLN
58	r	20	ASN
60	t	88	ASN
65	y	15	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	6 (8%)
10	B	75/76 (98%)	35 (46%)	6 (8%)
18	D	1514/1542 (98%)	291 (19%)	34 (2%)
41	a	2859/2904 (98%)	539 (18%)	0
44	d	119/120 (99%)	17 (14%)	0
8	7	30/56 (53%)	18 (60%)	4 (13%)
All	All	4672/4774 (97%)	929 (19%)	50 (1%)

All (929) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	3	G
8	7	4	U
8	7	5	U
8	7	7	U
8	7	8	U
8	7	9	U
8	7	10	U
8	7	11	U
8	7	12	U
8	7	13	U
8	7	14	U
8	7	15	U
8	7	16	U
8	7	18	U
8	7	20	U
8	7	21	U
8	7	48	G
8	7	49	G
10	A	2	G
10	A	6	G
10	A	7	G
10	A	8	U
10	A	10	G
10	A	13	C
10	A	14	A
10	A	15	G
10	A	16	C
10	A	17	C
10	A	18	G
10	A	19	G
10	A	20	U
10	A	21	A
10	A	22	G
10	A	23	C
10	A	46	G
10	A	47	U
10	A	48	C
10	A	49	G
10	A	52	G
10	A	57	A
10	A	58	A
10	A	59	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	61	C
10	A	66	C
10	A	69	C
10	A	71	C
10	A	73	A
10	B	2	G
10	B	6	G
10	B	7	G
10	B	8	U
10	B	10	G
10	B	13	C
10	B	14	A
10	B	15	G
10	B	16	C
10	B	17	C
10	B	18	G
10	B	19	G
10	B	20	U
10	B	21	A
10	B	22	G
10	B	23	C
10	B	30	G
10	B	31	G
10	B	32	C
10	B	36	U
10	B	37	A
10	B	38	A
10	B	46	G
10	B	47	U
10	B	48	C
10	B	49	G
10	B	52	G
10	B	57	A
10	B	58	A
10	B	59	A
10	B	61	C
10	B	66	C
10	B	69	C
10	B	71	C
10	B	73	A
18	D	4	U
18	D	5	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	D	9	G
18	D	22	G
18	D	29	U
18	D	32	A
18	D	39	G
18	D	41	G
18	D	47	C
18	D	48	C
18	D	50	A
18	D	51	A
18	D	52	C
18	D	54	C
18	D	69	G
18	D	70	U
18	D	71	A
18	D	72	A
18	D	74	A
18	D	76	G
18	D	82	G
18	D	83	C
18	D	84	U
18	D	87	C
18	D	90	C
18	D	94	G
18	D	95	C
18	D	96	U
18	D	108	G
18	D	120	A
18	D	122	G
18	D	128	G
18	D	131	A
18	D	141	G
18	D	144	G
18	D	148	G
18	D	149	A
18	D	160	A
18	D	164	G
18	D	173	U
18	D	181	A
18	D	182	A
18	D	197	A
18	D	198	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	D	204	G
18	D	208	U
18	D	209	U
18	D	210	C
18	D	211	G
18	D	212	G
18	D	216	U
18	D	226	G
18	D	245	U
18	D	247	G
18	D	251	G
18	D	253	A
18	D	258	G
18	D	262	A
18	D	266	G
18	D	267	C
18	D	271	C
18	D	279	A
18	D	289	G
18	D	299	G
18	D	306	A
18	D	321	A
18	D	328	C
18	D	329	A
18	D	332	G
18	D	347	G
18	D	352	C
18	D	353	A
18	D	354	G
18	D	355	C
18	D	367	U
18	D	372	C
18	D	373	A
18	D	376	G
18	D	382	A
18	D	384	G
18	D	392	C
18	D	393	A
18	D	397	A
18	D	398	U
18	D	406	G
18	D	412	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	D	413	G
18	D	414	A
18	D	421	U
18	D	422	C
18	D	424	G
18	D	429	U
18	D	446	G
18	D	451	A
18	D	457	G
18	D	458	U
18	D	460	A
18	D	463	U
18	D	464	U
18	D	467	U
18	D	468	A
18	D	469	C
18	D	478	A
18	D	479	U
18	D	481	G
18	D	484	G
18	D	485	U
18	D	486	U
18	D	505	G
18	D	509	A
18	D	511	C
18	D	518	C
18	D	519	C
18	D	526	C
18	D	531	U
18	D	532	A
18	D	533	A
18	D	542	G
18	D	547	A
18	D	559	A
18	D	562	U
18	D	568	G
18	D	572	A
18	D	573	A
18	D	576	C
18	D	577	G
18	D	579	A
18	D	596	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	D	628	G
18	D	633	G
18	D	641	U
18	D	642	A
18	D	649	A
18	D	650	G
18	D	653	U
18	D	665	A
18	D	666	G
18	D	687	A
18	D	700	G
18	D	723	U
18	D	724	G
18	D	731	G
18	D	734	G
18	D	747	A
18	D	748	G
18	D	755	G
18	D	760	G
18	D	777	A
18	D	793	U
18	D	794	A
18	D	815	A
18	D	817	C
18	D	828	U
18	D	829	G
18	D	832	G
18	D	841	C
18	D	844	G
18	D	845	A
18	D	849	G
18	D	874	G
18	D	887	G
18	D	902	G
18	D	914	A
18	D	916	U
18	D	926	G
18	D	934	C
18	D	935	A
18	D	954	G
18	D	960	U
18	D	963	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	D	969	A
18	D	972	C
18	D	975	A
18	D	976	G
18	D	991	U
18	D	992	U
18	D	993	G
18	D	996	A
18	D	999	C
18	D	1004	A
18	D	1008	U
18	D	1009	U
18	D	1017	U
18	D	1018	G
18	D	1021	A
18	D	1024	G
18	D	1026	G
18	D	1028	C
18	D	1030	U
18	D	1031	C
18	D	1037	C
18	D	1043	G
18	D	1044	A
18	D	1046	A
18	D	1065	U
18	D	1085	U
18	D	1086	U
18	D	1094	G
18	D	1095	U
18	D	1099	G
18	D	1101	A
18	D	1124	G
18	D	1133	G
18	D	1135	U
18	D	1136	C
18	D	1137	C
18	D	1139	G
18	D	1140	C
18	D	1141	C
18	D	1142	G
18	D	1143	G
18	D	1145	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	D	1146	A
18	D	1151	A
18	D	1152	A
18	D	1158	C
18	D	1159	U
18	D	1167	A
18	D	1171	A
18	D	1174	G
18	D	1175	G
18	D	1176	A
18	D	1184	G
18	D	1196	A
18	D	1197	A
18	D	1206	G
18	D	1211	U
18	D	1212	U
18	D	1213	A
18	D	1214	C
18	D	1215	G
18	D	1226	C
18	D	1227	A
18	D	1228	C
18	D	1238	A
18	D	1256	A
18	D	1257	A
18	D	1260	G
18	D	1275	A
18	D	1276	G
18	D	1278	G
18	D	1279	G
18	D	1280	A
18	D	1285	A
18	D	1286	U
18	D	1287	A
18	D	1299	A
18	D	1300	G
18	D	1302	C
18	D	1305	G
18	D	1312	G
18	D	1317	C
18	D	1320	C
18	D	1323	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	D	1329	A
18	D	1338	G
18	D	1340	A
18	D	1346	A
18	D	1347	G
18	D	1353	G
18	D	1363	A
18	D	1370	G
18	D	1378	C
18	D	1379	G
18	D	1381	U
18	D	1391	U
18	D	1396	A
18	D	1397	C
18	D	1398	A
18	D	1404	C
18	D	1419	G
18	D	1429	A
18	D	1441	A
18	D	1446	A
18	D	1447	A
18	D	1448	C
18	D	1452	C
18	D	1453	G
18	D	1475	G
18	D	1487	G
18	D	1492	A
18	D	1493	A
18	D	1494	G
18	D	1495	U
18	D	1497	G
18	D	1503	A
18	D	1506	U
18	D	1517	G
18	D	1529	G
18	D	1530	G
18	D	1534	A
41	a	10	A
41	a	15	G
41	a	34	U
41	a	35	G
41	a	46	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	58	G
41	a	60	G
41	a	63	A
41	a	71	A
41	a	74	A
41	a	75	G
41	a	83	A
41	a	84	A
41	a	85	G
41	a	93	G
41	a	96	C
41	a	102	U
41	a	103	A
41	a	110	G
41	a	114	U
41	a	118	A
41	a	119	A
41	a	120	U
41	a	122	G
41	a	131	A
41	a	136	G
41	a	139	U
41	a	140	C
41	a	141	G
41	a	145	C
41	a	163	C
41	a	165	A
41	a	181	A
41	a	196	A
41	a	199	A
41	a	200	U
41	a	215	G
41	a	216	A
41	a	222	A
41	a	225	C
41	a	248	G
41	a	249	C
41	a	261	G
41	a	264	C
41	a	265	A
41	a	266	G
41	a	267	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	271	G
41	a	272	A
41	a	275	C
41	a	276	U
41	a	278	A
41	a	285	G
41	a	311	A
41	a	324	A
41	a	329	G
41	a	330	A
41	a	353	C
41	a	359	G
41	a	361	G
41	a	362	A
41	a	371	A
41	a	372	G
41	a	373	U
41	a	375	G
41	a	383	C
41	a	386	G
41	a	396	G
41	a	405	U
41	a	411	G
41	a	412	A
41	a	420	C
41	a	424	G
41	a	435	C
41	a	451	U
41	a	456	C
41	a	457	A
41	a	477	A
41	a	481	G
41	a	491	G
41	a	501	A
41	a	503	A
41	a	504	A
41	a	505	A
41	a	509	C
41	a	522	A
41	a	529	A
41	a	532	A
41	a	543	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	546	U
41	a	547	A
41	a	548	G
41	a	549	G
41	a	551	G
41	a	563	A
41	a	569	U
41	a	573	U
41	a	575	A
41	a	588	U
41	a	603	A
41	a	609	A
41	a	613	A
41	a	614	A
41	a	615	U
41	a	616	A
41	a	618	G
41	a	620	G
41	a	621	A
41	a	627	A
41	a	637	A
41	a	645	C
41	a	647	G
41	a	654	A
41	a	664	G
41	a	668	A
41	a	685	A
41	a	686	U
41	a	710	U
41	a	717	C
41	a	730	A
41	a	738	G
41	a	757	G
41	a	764	A
41	a	765	C
41	a	775	G
41	a	776	G
41	a	782	A
41	a	784	G
41	a	785	G
41	a	800	A
41	a	802	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	805	G
41	a	812	C
41	a	819	A
41	a	827	U
41	a	828	U
41	a	845	A
41	a	846	U
41	a	858	G
41	a	859	G
41	a	869	G
41	a	878	A
41	a	881	G
41	a	883	G
41	a	884	U
41	a	885	C
41	a	888	C
41	a	891	G
41	a	892	A
41	a	893	C
41	a	895	U
41	a	896	A
41	a	897	C
41	a	899	A
41	a	907	G
41	a	910	A
41	a	914	G
41	a	915	C
41	a	931	U
41	a	941	A
41	a	945	A
41	a	946	C
41	a	953	G
41	a	961	C
41	a	974	G
41	a	983	A
41	a	984	A
41	a	985	C
41	a	995	C
41	a	996	A
41	a	999	U
41	a	1005	C
41	a	1012	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	1013	C
41	a	1022	G
41	a	1023	U
41	a	1026	G
41	a	1033	U
41	a	1041	G
41	a	1042	G
41	a	1045	C
41	a	1046	A
41	a	1047	G
41	a	1060	U
41	a	1061	U
41	a	1062	G
41	a	1063	G
41	a	1064	C
41	a	1065	U
41	a	1066	U
41	a	1067	A
41	a	1068	G
41	a	1069	A
41	a	1070	A
41	a	1071	G
41	a	1073	A
41	a	1074	G
41	a	1076	C
41	a	1079	C
41	a	1080	A
41	a	1081	U
41	a	1082	U
41	a	1083	U
41	a	1084	A
41	a	1087	G
41	a	1088	A
41	a	1090	A
41	a	1095	A
41	a	1096	A
41	a	1107	G
41	a	1110	G
41	a	1111	A
41	a	1112	G
41	a	1119	U
41	a	1122	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	1132	U
41	a	1134	A
41	a	1135	C
41	a	1142	A
41	a	1143	A
41	a	1169	A
41	a	1170	C
41	a	1173	U
41	a	1174	U
41	a	1175	A
41	a	1176	U
41	a	1177	G
41	a	1178	C
41	a	1179	G
41	a	1180	U
41	a	1186	G
41	a	1238	G
41	a	1248	G
41	a	1253	A
41	a	1256	G
41	a	1266	G
41	a	1271	G
41	a	1272	A
41	a	1273	U
41	a	1301	A
41	a	1321	A
41	a	1345	C
41	a	1352	U
41	a	1365	A
41	a	1368	G
41	a	1378	A
41	a	1379	U
41	a	1380	G
41	a	1383	A
41	a	1387	A
41	a	1395	A
41	a	1406	U
41	a	1407	G
41	a	1408	G
41	a	1411	U
41	a	1414	C
41	a	1415	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	1416	G
41	a	1417	C
41	a	1419	A
41	a	1420	A
41	a	1428	C
41	a	1452	G
41	a	1453	A
41	a	1460	U
41	a	1478	G
41	a	1482	G
41	a	1490	A
41	a	1491	G
41	a	1497	U
41	a	1503	A
41	a	1508	A
41	a	1509	A
41	a	1510	G
41	a	1515	A
41	a	1529	G
41	a	1534	U
41	a	1535	A
41	a	1536	C
41	a	1537	G
41	a	1554	U
41	a	1559	U
41	a	1566	A
41	a	1569	A
41	a	1578	U
41	a	1580	A
41	a	1581	G
41	a	1582	C
41	a	1583	A
41	a	1584	U
41	a	1589	U
41	a	1590	A
41	a	1608	A
41	a	1609	A
41	a	1610	A
41	a	1647	U
41	a	1648	U
41	a	1649	G
41	a	1651	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	1674	G
41	a	1677	A
41	a	1703	G
41	a	1714	U
41	a	1715	G
41	a	1718	G
41	a	1729	U
41	a	1730	C
41	a	1732	C
41	a	1738	G
41	a	1750	G
41	a	1755	A
41	a	1758	U
41	a	1764	C
41	a	1773	A
41	a	1791	A
41	a	1800	C
41	a	1808	A
41	a	1811	G
41	a	1816	C
41	a	1829	A
41	a	1833	C
41	a	1847	A
41	a	1848	A
41	a	1858	A
41	a	1859	U
41	a	1862	G
41	a	1864	U
41	a	1869	G
41	a	1870	C
41	a	1872	A
41	a	1873	G
41	a	1905	C
41	a	1906	G
41	a	1907	G
41	a	1913	A
41	a	1914	C
41	a	1919	A
41	a	1920	C
41	a	1922	G
41	a	1923	U
41	a	1924	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	1925	C
41	a	1926	U
41	a	1928	A
41	a	1929	G
41	a	1930	G
41	a	1936	A
41	a	1938	A
41	a	1955	U
41	a	1965	C
41	a	1967	C
41	a	1970	A
41	a	1971	U
41	a	1972	G
41	a	1987	A
41	a	1991	U
41	a	1992	G
41	a	1993	U
41	a	1997	C
41	a	2002	G
41	a	2022	U
41	a	2023	C
41	a	2027	G
41	a	2033	A
41	a	2043	C
41	a	2051	A
41	a	2052	A
41	a	2055	C
41	a	2056	G
41	a	2060	A
41	a	2061	G
41	a	2062	A
41	a	2063	C
41	a	2077	A
41	a	2097	A
41	a	2099	U
41	a	2100	G
41	a	2108	A
41	a	2110	G
41	a	2111	U
41	a	2113	U
41	a	2115	G
41	a	2116	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	2117	A
41	a	2118	U
41	a	2121	G
41	a	2122	U
41	a	2124	G
41	a	2125	G
41	a	2126	A
41	a	2127	G
41	a	2128	G
41	a	2131	U
41	a	2132	U
41	a	2133	G
41	a	2134	A
41	a	2139	U
41	a	2141	G
41	a	2146	C
41	a	2147	A
41	a	2154	A
41	a	2157	G
41	a	2158	A
41	a	2159	G
41	a	2162	G
41	a	2163	A
41	a	2164	C
41	a	2165	C
41	a	2169	A
41	a	2171	A
41	a	2172	U
41	a	2178	C
41	a	2182	U
41	a	2183	A
41	a	2185	U
41	a	2188	U
41	a	2189	U
41	a	2190	G
41	a	2191	A
41	a	2193	G
41	a	2194	U
41	a	2198	A
41	a	2204	G
41	a	2210	U
41	a	2211	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	2212	A
41	a	2213	U
41	a	2225	A
41	a	2226	C
41	a	2229	U
41	a	2238	G
41	a	2239	G
41	a	2244	U
41	a	2250	G
41	a	2268	A
41	a	2278	A
41	a	2283	C
41	a	2287	A
41	a	2297	A
41	a	2305	U
41	a	2308	G
41	a	2309	A
41	a	2315	G
41	a	2322	A
41	a	2325	G
41	a	2327	A
41	a	2333	A
41	a	2339	C
41	a	2345	G
41	a	2347	C
41	a	2350	C
41	a	2361	G
41	a	2372	U
41	a	2376	A
41	a	2383	G
41	a	2385	C
41	a	2402	U
41	a	2403	C
41	a	2406	A
41	a	2423	U
41	a	2424	C
41	a	2425	A
41	a	2426	A
41	a	2429	G
41	a	2430	A
41	a	2431	U
41	a	2434	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	2435	A
41	a	2441	U
41	a	2447	G
41	a	2448	A
41	a	2470	G
41	a	2474	U
41	a	2476	A
41	a	2478	A
41	a	2484	G
41	a	2491	U
41	a	2502	G
41	a	2506	U
41	a	2507	C
41	a	2512	C
41	a	2513	A
41	a	2518	A
41	a	2520	C
41	a	2525	G
41	a	2529	G
41	a	2535	G
41	a	2547	A
41	a	2554	U
41	a	2566	A
41	a	2567	G
41	a	2572	A
41	a	2573	C
41	a	2574	G
41	a	2585	U
41	a	2586	U
41	a	2602	A
41	a	2603	G
41	a	2609	U
41	a	2610	C
41	a	2611	C
41	a	2613	U
41	a	2629	U
41	a	2663	G
41	a	2669	G
41	a	2671	G
41	a	2689	U
41	a	2690	U
41	a	2714	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	a	2722	G
41	a	2726	A
41	a	2744	G
41	a	2748	A
41	a	2757	A
41	a	2758	A
41	a	2765	A
41	a	2777	G
41	a	2778	A
41	a	2791	G
41	a	2793	C
41	a	2796	U
41	a	2797	U
41	a	2798	U
41	a	2799	A
41	a	2801	G
41	a	2818	U
41	a	2820	A
41	a	2823	A
41	a	2825	G
41	a	2849	U
41	a	2850	A
41	a	2859	G
41	a	2861	U
41	a	2867	G
41	a	2880	C
41	a	2884	U
41	a	2885	G
41	a	2891	U
41	a	2902	C
44	d	2	G
44	d	9	G
44	d	13	G
44	d	16	G
44	d	17	C
44	d	35	C
44	d	36	C
44	d	45	A
44	d	51	G
44	d	56	G
44	d	64	G
44	d	66	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	d	88	C
44	d	89	U
44	d	90	C
44	d	99	A
44	d	109	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	4	U
8	7	7	U
8	7	10	U
8	7	47	U
10	A	6	G
10	A	7	G
10	A	9	G
10	A	22	G
10	A	60	U
10	A	70	G
10	B	6	G
10	B	7	G
10	B	9	G
10	B	22	G
10	B	37	A
10	B	60	U
18	D	7	A
18	D	70	U
18	D	121	U
18	D	181	A
18	D	183	C
18	D	197	A
18	D	209	U
18	D	305	G
18	D	328	C
18	D	428	G
18	D	496	A
18	D	517	G
18	D	531	U
18	D	532	A
18	D	562	U
18	D	641	U
18	D	722	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	D	793	U
18	D	991	U
18	D	992	U
18	D	1145	A
18	D	1196	A
18	D	1211	U
18	D	1212	U
18	D	1213	A
18	D	1214	C
18	D	1225	A
18	D	1299	A
18	D	1396	A
18	D	1432	G
18	D	1447	A
18	D	1491	G
18	D	1492	A
18	D	1493	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-43389. 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)

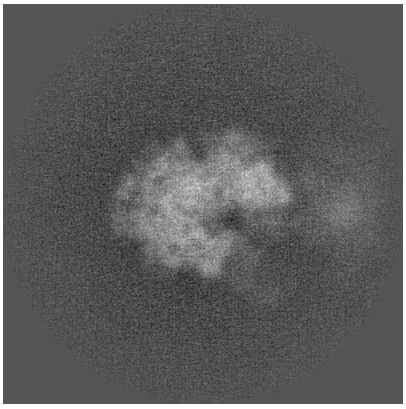
6.1.1 Primary map

X

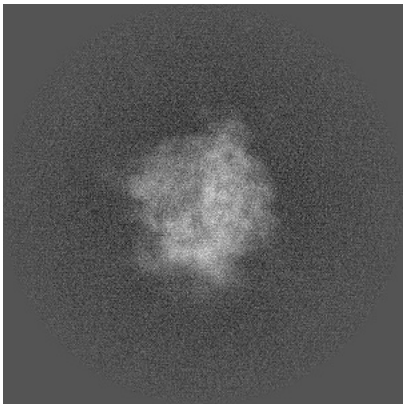
Y

Z

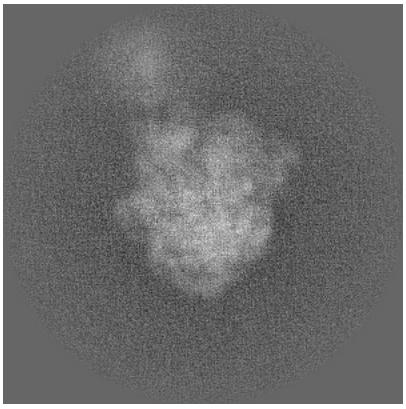
6.1.2 Raw map



X



Y

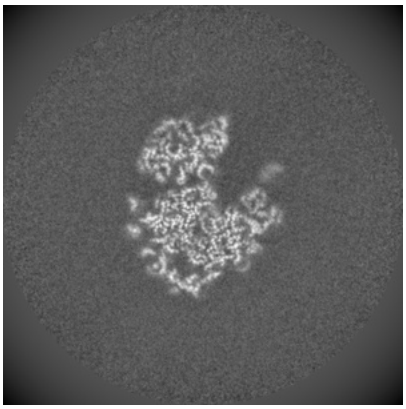


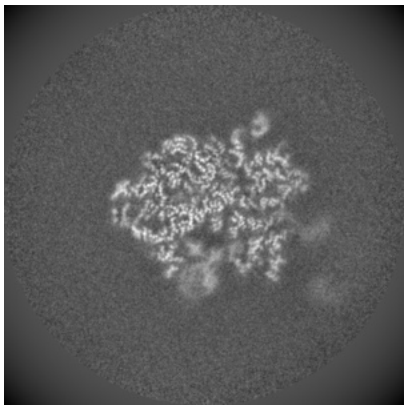
Z

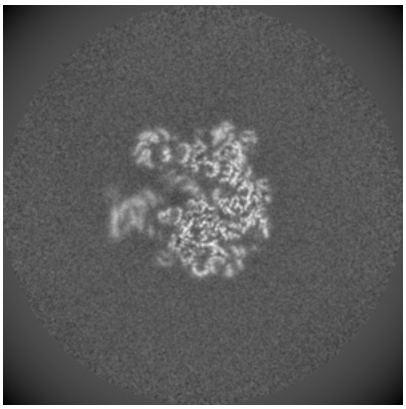
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

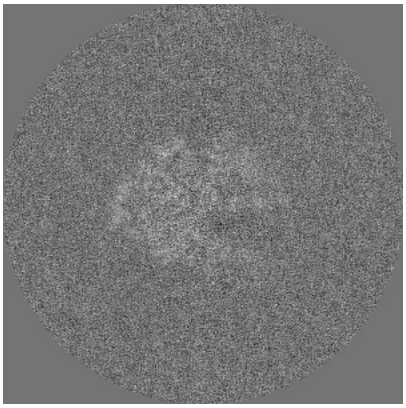
6.2.1 Primary map

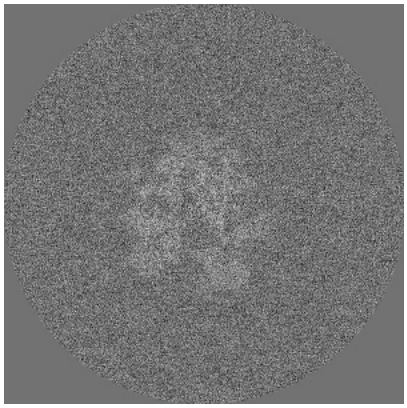

X Index: 310

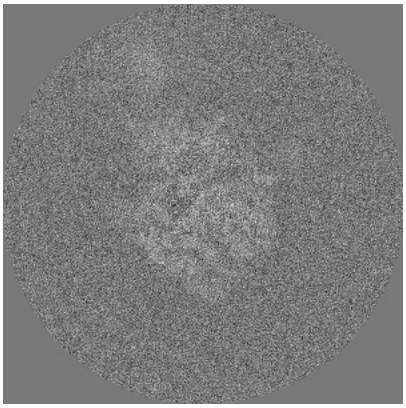

Y Index: 310


Z Index: 310

6.2.2 Raw map


X Index: 256

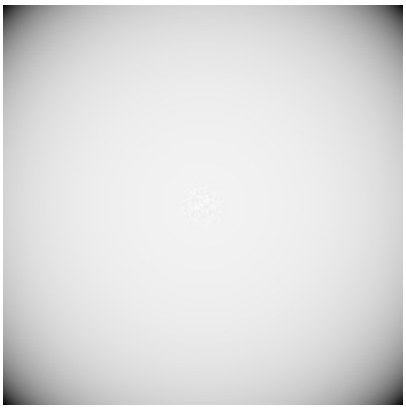

Y Index: 256


Z Index: 256

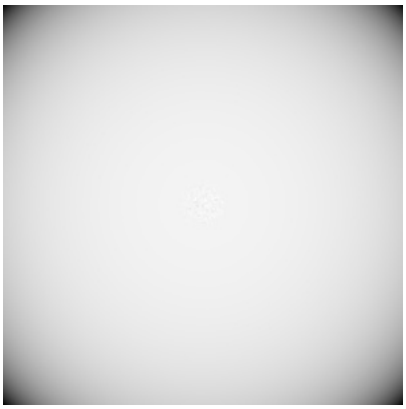
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

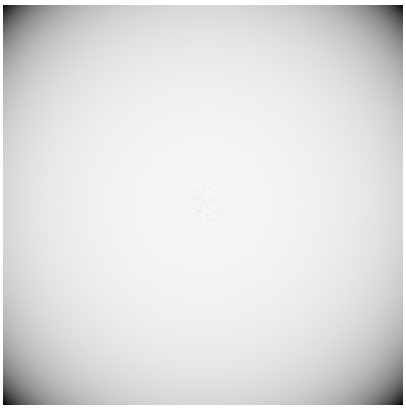
6.3.1 Primary map



X Index: 0

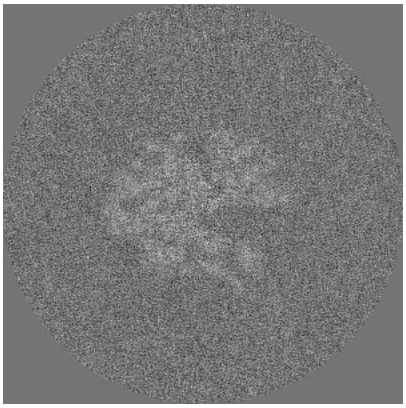


Y Index: 0

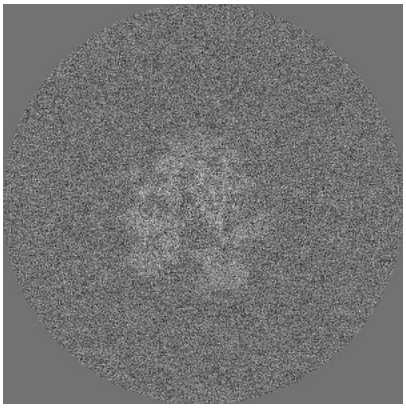


Z Index: 0

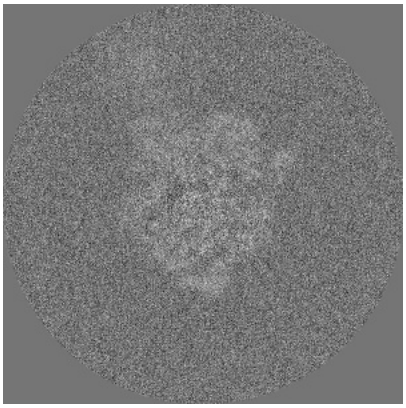
6.3.2 Raw map



X Index: 265



Y Index: 256

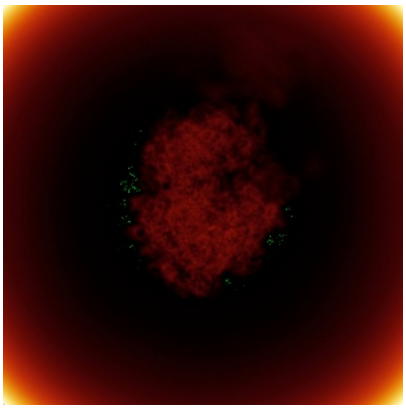


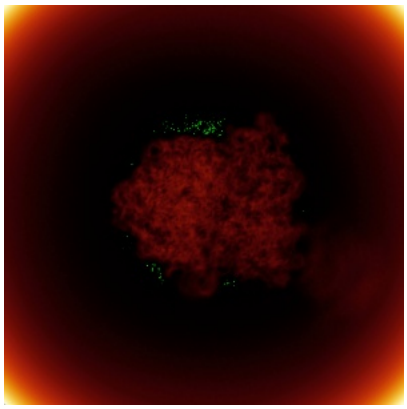
Z Index: 266

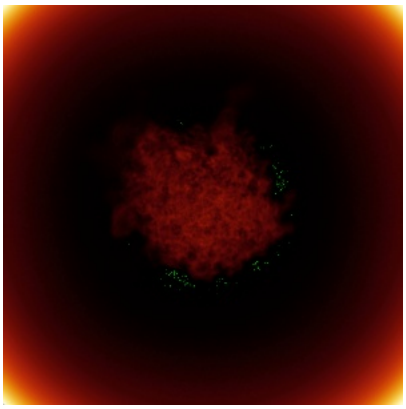
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

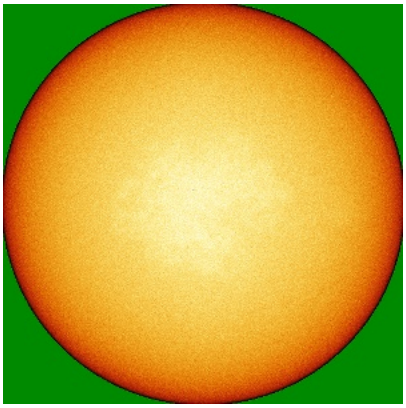
6.4.1 Primary map

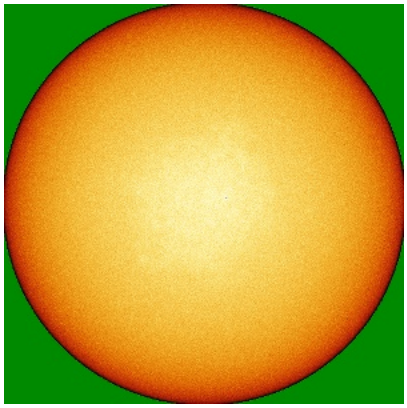

X

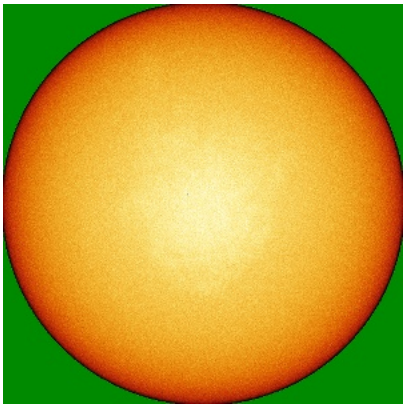

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 1e-08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X

Y

Z

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

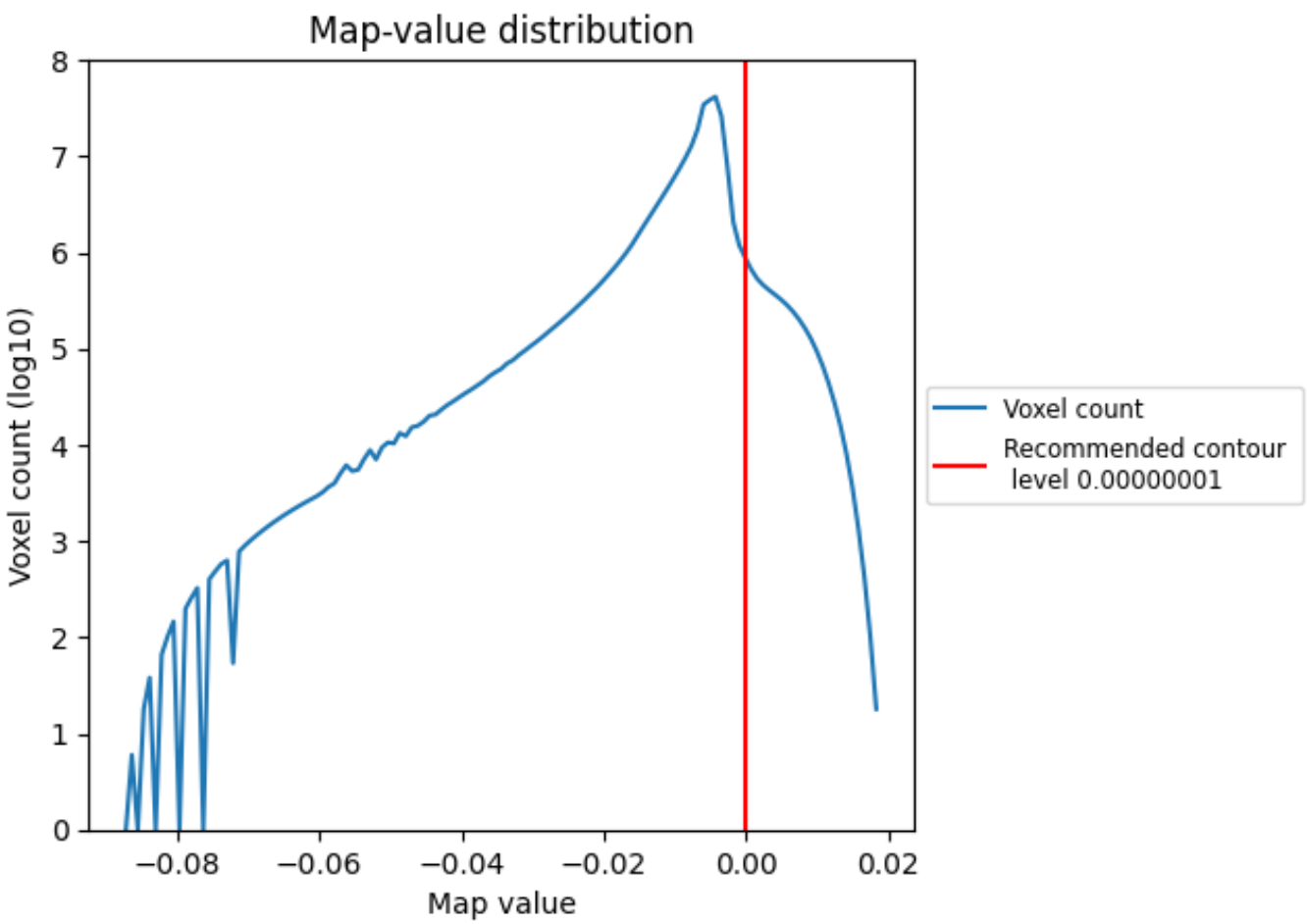
6.6 Mask visualisation (i)

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

7 Map analysis (i)

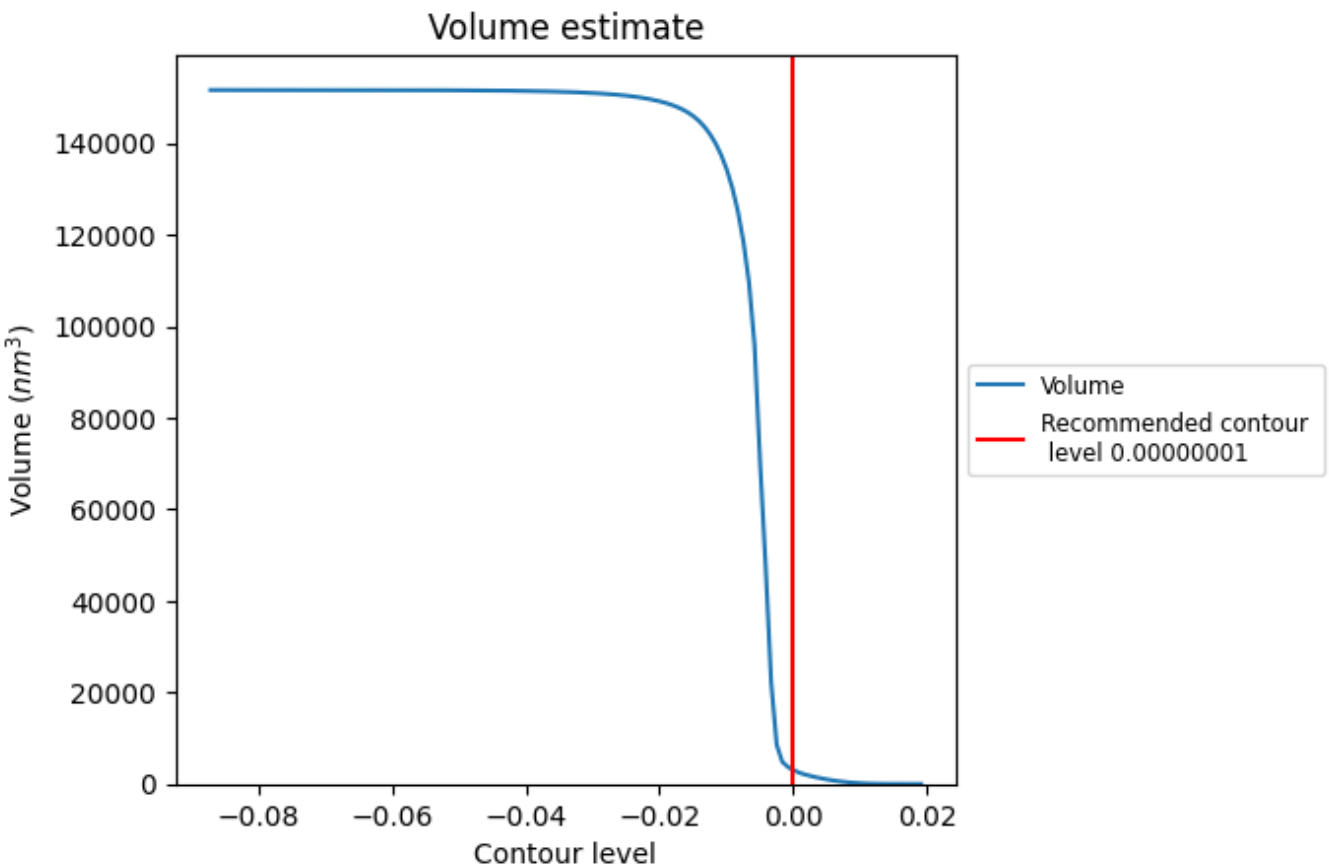
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

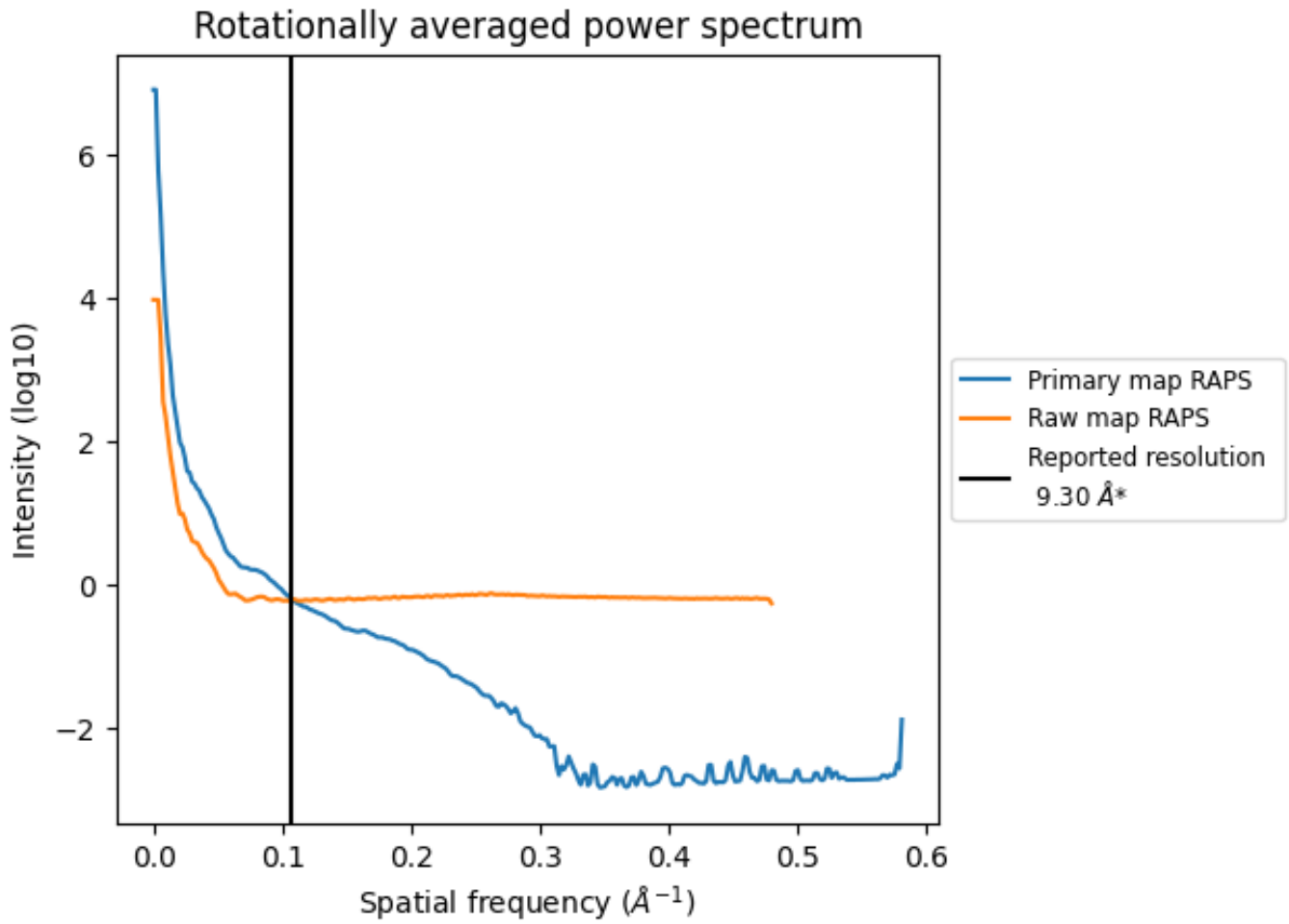
7.2 Volume estimate (i)



The volume at the recommended contour level is 3056 nm^3; this corresponds to an approximate mass of 2760 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 (i)

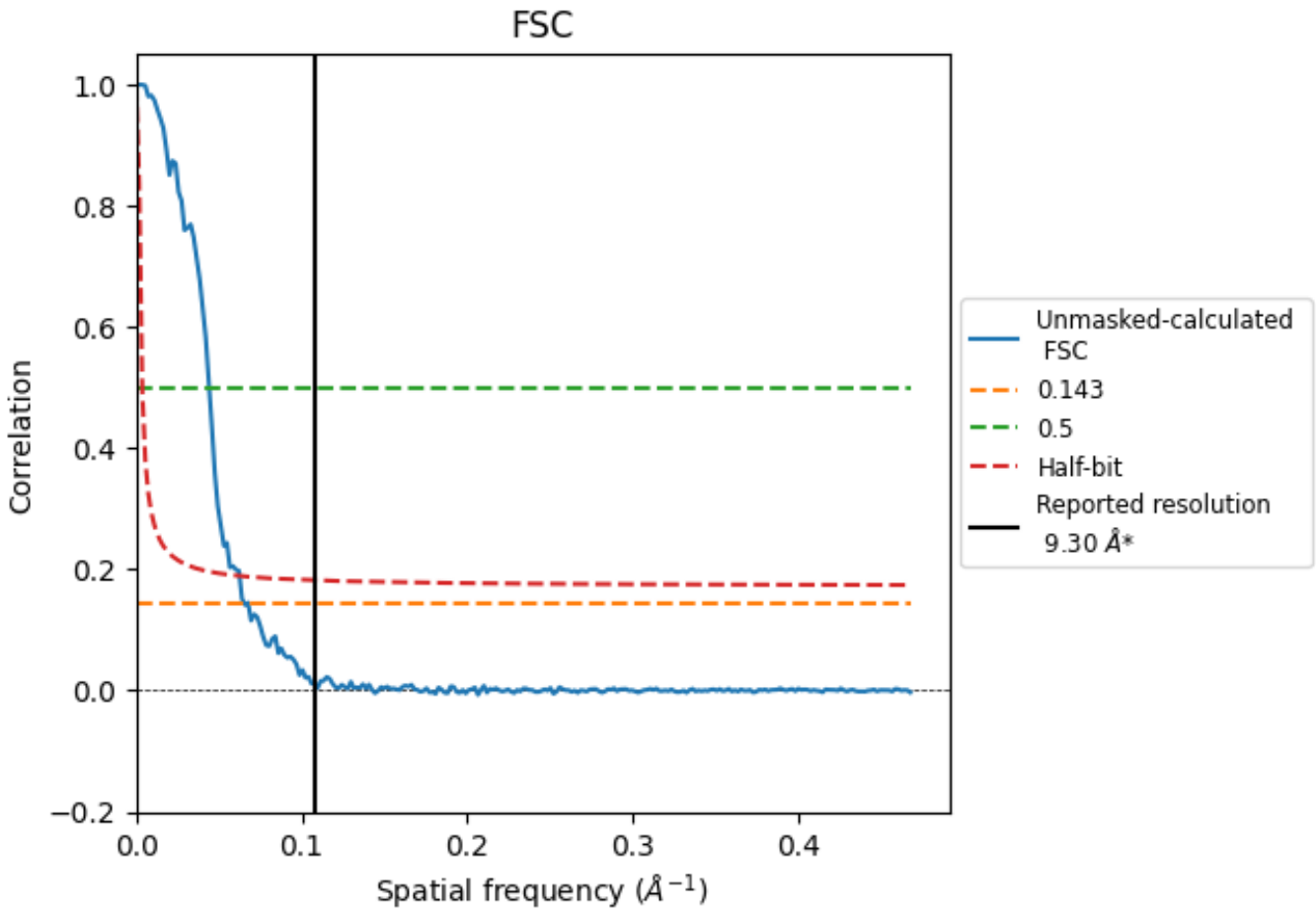


*Reported resolution corresponds to spatial frequency of 0.108 Å^{-1}

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 0.108 Å^{-1}

8.2 Resolution estimates (i)

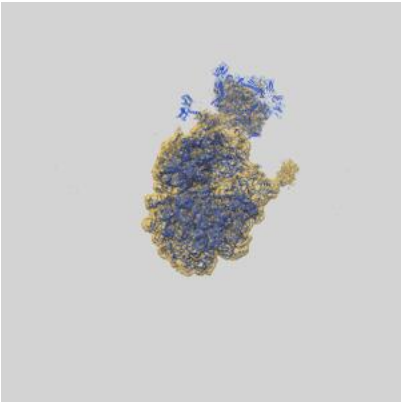
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	15.29	22.68	16.00

*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 15.29 differs from the reported value 9.3 by more than 10 %

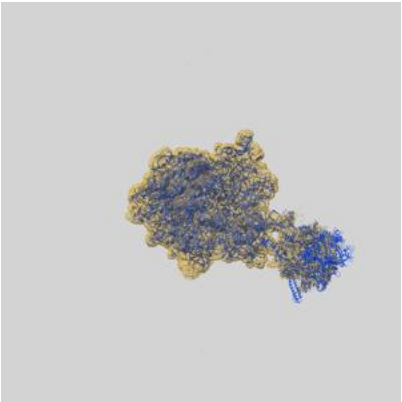
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-43389 and PDB model 8VOQ. Per-residue inclusion information can be found in section 3 on page 17.

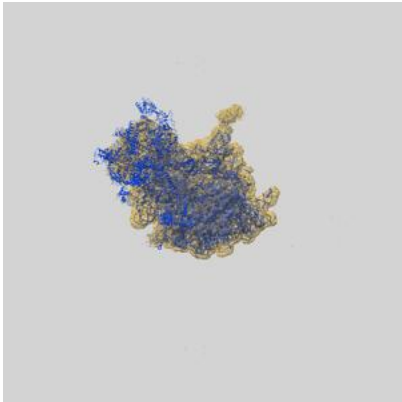
9.1 Map-model overlay (i)



X



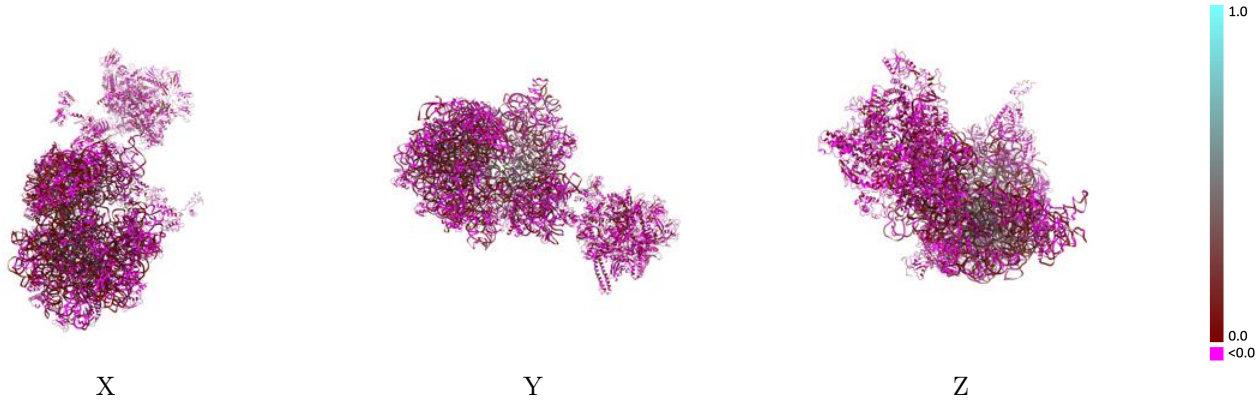
Y



Z

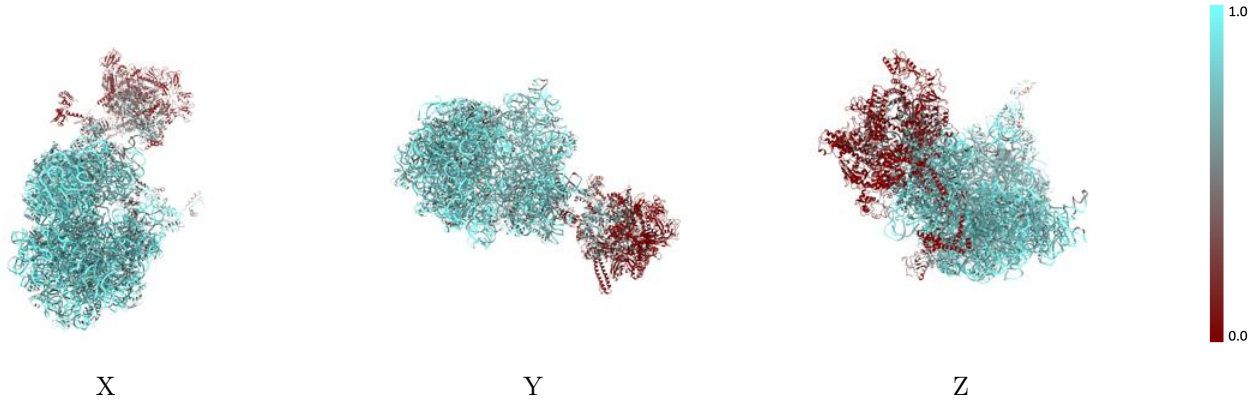
The images above show the 3D surface view of the map at the recommended contour level 1e-08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



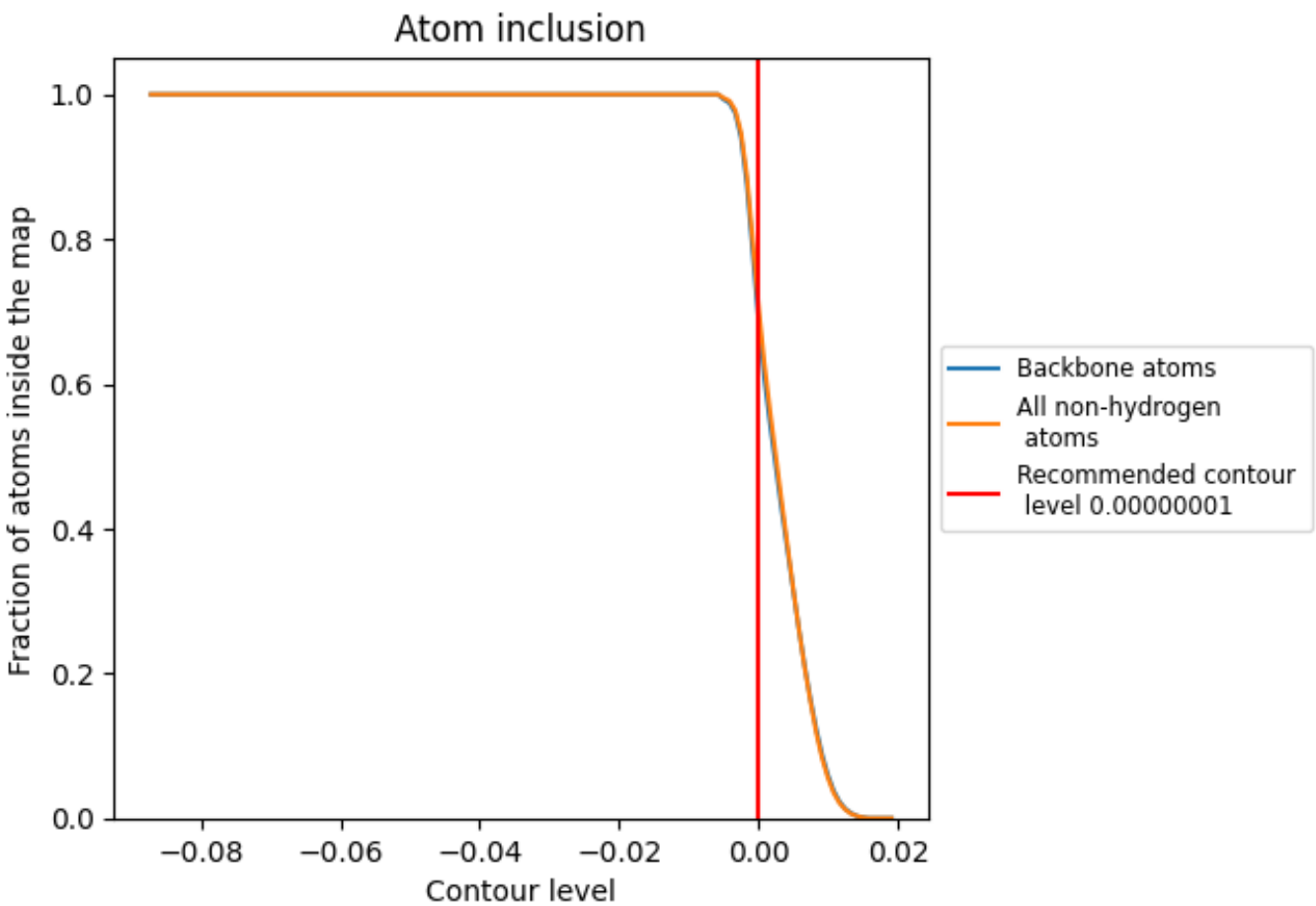
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00000001).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00000001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.0660
0	0.7800	-0.0050
1	0.7950	0.0890
2	0.7600	0.0060
3	0.7590	-0.0180
4	0.8010	0.0100
5	0.4810	0.0270
6	0.5200	0.0900
7	0.6290	0.0360
9	0.7290	0.0280
A	0.9080	0.1450
AA	0.1870	0.0120
AB	0.2910	0.0040
AC	0.0470	0.0170
AD	0.0180	0.0030
AE	0.2230	0.0270
AF	0.0850	-0.0010
AG	0.2670	0.0110
B	0.7860	0.0440
C	0.7500	-0.0300
D	0.9200	0.1110
E	0.7710	-0.0030
F	0.7620	0.0940
G	0.7050	0.0130
H	0.3570	0.0270
I	0.6560	-0.0270
J	0.7290	-0.0090
K	0.8240	0.0540
L	0.7740	-0.0170
M	0.7270	0.0190
N	0.8200	0.0620
O	0.7280	0.0080
P	0.6900	0.0230
Q	0.8080	0.0610
R	0.8480	0.1640

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S	0.7570	-0.0060
T	0.8520	0.1000
U	0.7110	-0.0450
V	0.8320	0.1160
W	0.6520	0.0040
X	0.6680	-0.0050
Y	0.7090	0.0130
Z	0.5110	0.0100
a	0.9230	0.1000
b	0.7910	-0.0090
c	0.7600	0.0530
d	0.8820	0.0440
e	0.7440	-0.0350
f	0.8210	0.0500
g	0.7360	0.0080
h	0.8060	0.0760
i	0.8180	0.0630
j	0.7800	0.0040
k	0.7560	0.0090
l	0.7680	0.0300
m	0.8870	0.1910
n	0.7520	0.0110
o	0.7560	-0.0020
p	0.7250	-0.0280
q	0.7160	-0.0490
r	0.5470	0.0070
s	0.7500	-0.0260
t	0.7680	0.0450
u	0.7750	0.0130
v	0.7970	0.0410
w	0.8170	0.0340
x	0.7600	0.0000
y	0.7160	0.0020
z	0.7810	0.0060