



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 03:46 PM UTC

PDB ID : 5AFI / pdb_00005afi
EMDB ID : EMD-2847
Title : 2.9A Structure of E. coli ribosome-EF-TU complex by cs-corrected cryo-EM
Authors : Fischer, N.; Neumann, P.; Konevega, A.L.; Bock, L.V.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : 2015-01-22
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

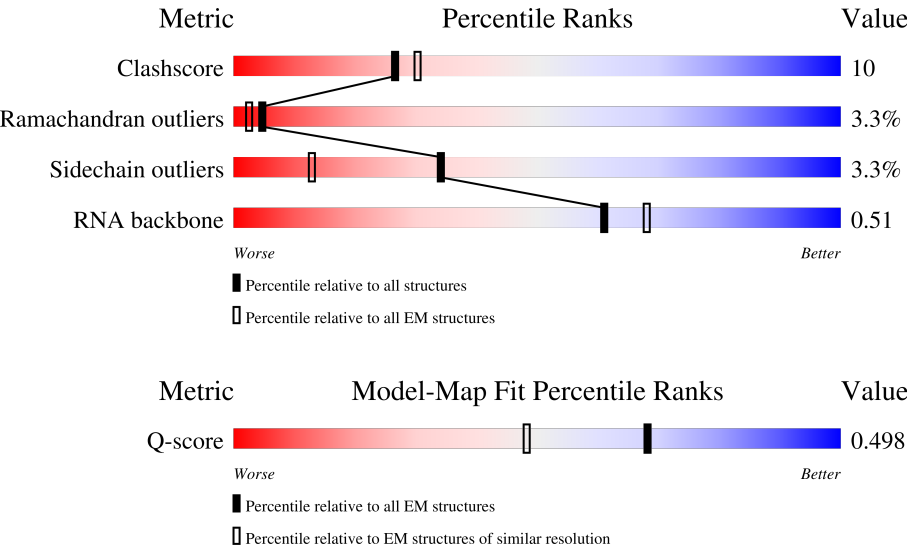
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	a	1539	8% 59% 34% 7%
2	b	240	28% 58% 30% 9%
3	c	233	8% 54% 31% 12%

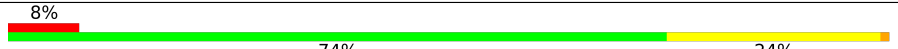
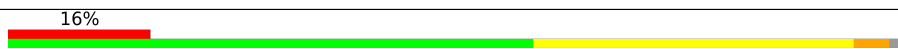
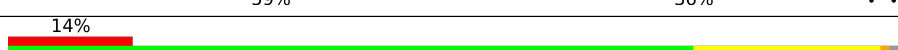
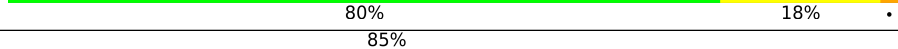
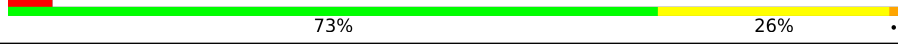
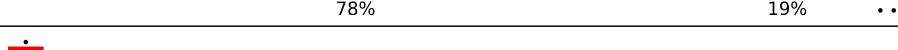
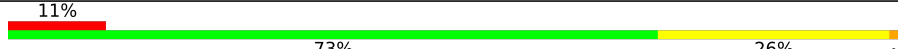
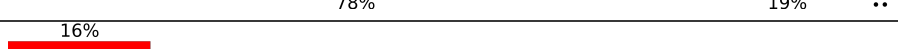
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	d	206	
5	e	167	
6	f	135	
7	g	179	
8	h	130	
9	i	130	
10	j	103	
11	k	129	
12	l	124	
13	m	118	
14	n	102	
15	o	89	
16	p	82	
17	q	84	
18	r	75	
19	s	92	
20	t	87	
21	u	71	
22	v	77	
22	w	77	
23	x	11	
24	y	77	
25	z	393	
26	A	2903	
27	B	120	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	C	273	
29	D	209	
30	E	201	
31	F	179	
32	G	177	
33	H	149	
34	I	142	
35	J	142	
36	K	123	
37	L	144	
38	M	136	
39	N	127	
40	O	117	
41	P	115	
42	Q	118	
43	R	103	
44	S	110	
45	T	100	
46	U	104	
47	V	94	
48	W	85	
49	X	78	
50	Y	63	
51	Z	59	
52	0	57	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1	55	
54	2	46	
55	3	65	
56	4	38	
57	5	165	
58	6	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	H2U	w	20	-	-	X	-
61	FME	v	105	-	-	X	-

2 Entry composition [i](#)

There are 66 unique types of molecules in this entry. The entry contains 152717 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 22 is a RNA chain called P-site fMet-tRNA^{fMet}.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0
22	w	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	11	Total	C	N	O	P	0	0
			234	105	41	77	11		

- Molecule 24 is a RNA chain called A/T-site Phe-tRNA^{Phe}.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	y	77	Total	C	N	O	P	S	0	0
			1643	740	291	534	76	2		

- Molecule 25 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	371	Total	C	N	O	S	1	0
			2881	1824	495	549	13		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2900	Total	C	N	O	P	0	0
			62276	27788	11460	20128	2900		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 34 is a protein called 50S ribosomal protein L11.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Q	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	U	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 57 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 58 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

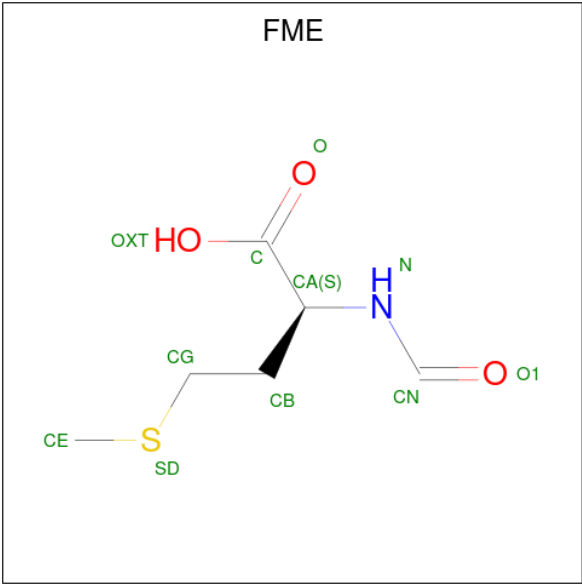
- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	a	83	Total	Mg	0
			83	83	
59	v	4	Total	Mg	0
			4	4	
59	z	1	Total	Mg	0
			1	1	
59	A	234	Total	Mg	0
			234	234	
59	B	7	Total	Mg	0
			7	7	
59	N	2	Total	Mg	0
			2	2	
59	0	1	Total	Mg	0
			1	1	
59	4	1	Total	Mg	0
			1	1	

- Molecule 60 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

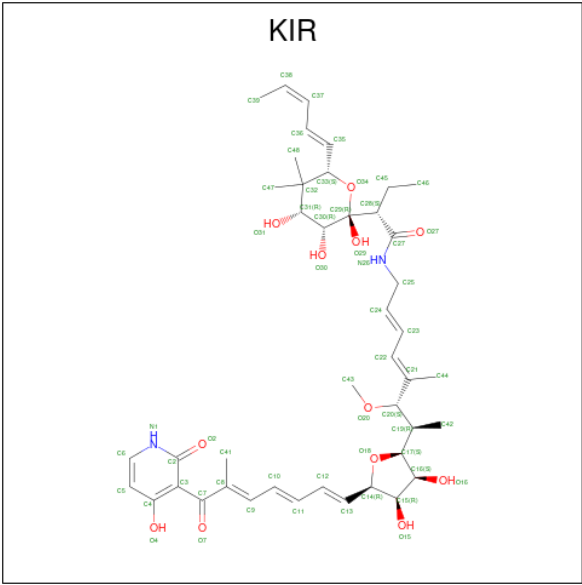
Mol	Chain	Residues	Atoms		AltConf
60	a	1	Total	Cl	0
			1	1	
60	A	1	Total	Cl	0
			1	1	

- Molecule 61 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



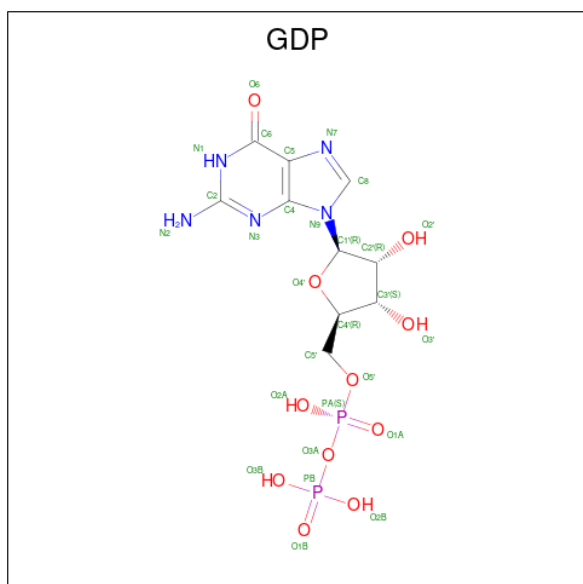
Mol	Chain	Residues	Atoms					AltConf
61	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 62 is KIRROMYCIN (CCD ID: KIR) (formula: C₄₃H₆₀N₂O₁₂).



Mol	Chain	Residues	Atoms				AltConf
62	z	1	Total	C	N	O	0
			57	43	2	12	

- Molecule 63 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 64 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
64	A	1	Total	Na	0
			1	1	
64	B	1	Total	Na	0
			1	1	

- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
65	4	1	Total	Zn	0
			1	1	
65	6	1	Total	Zn	0
			1	1	

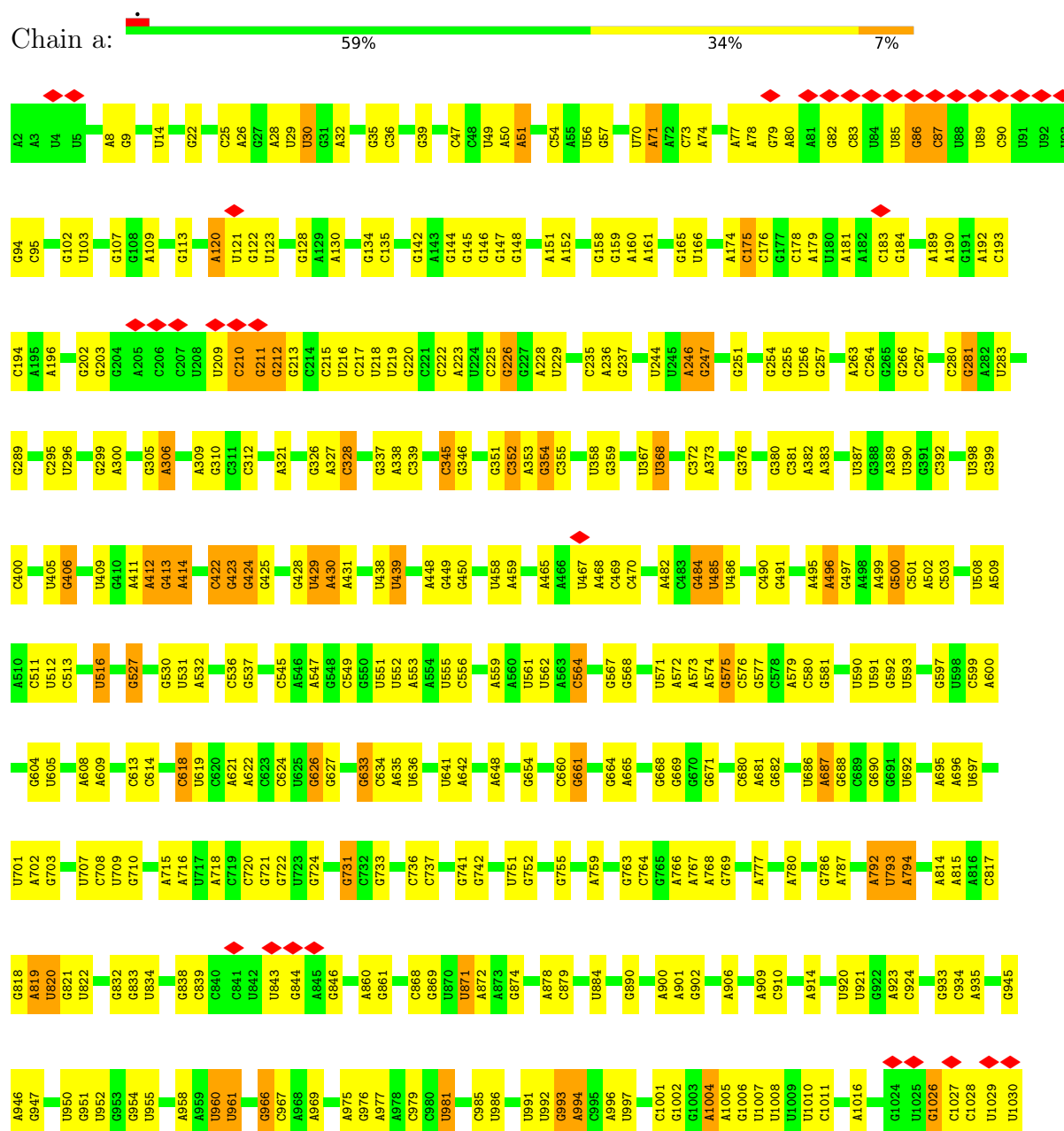
- Molecule 66 is water.

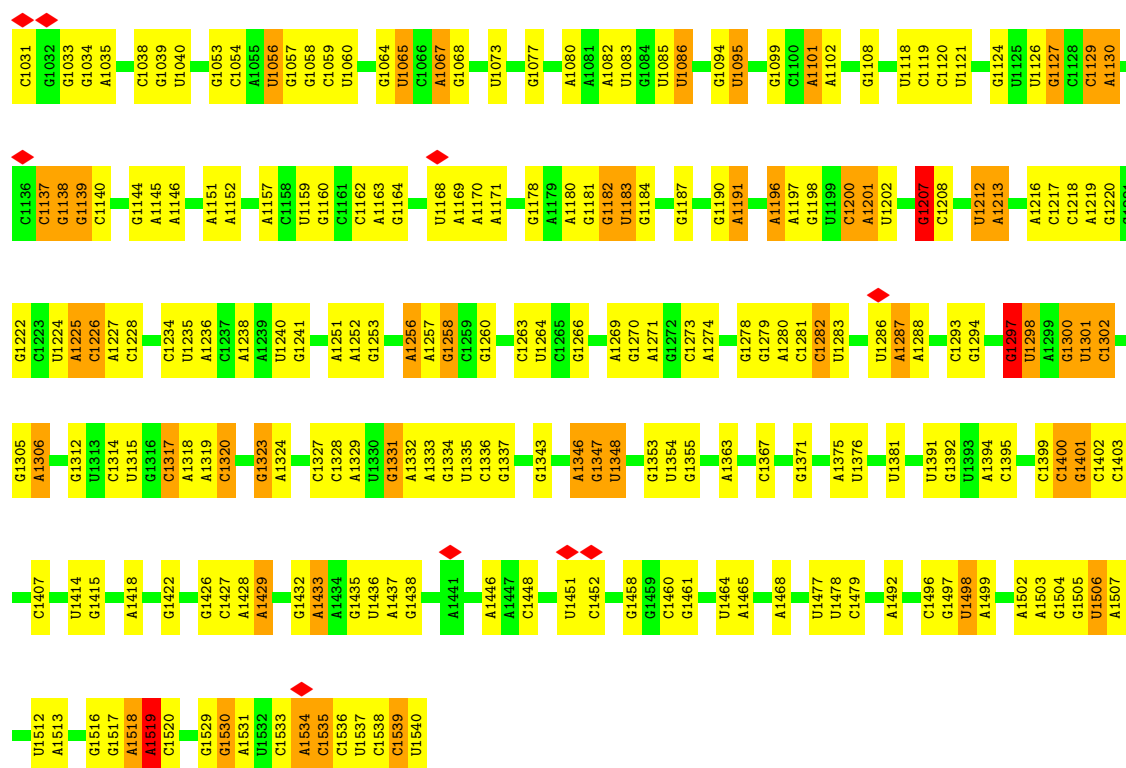
Mol	Chain	Residues	Atoms		AltConf
66	a	9	Total 9	O 9	0
66	A	9	Total 9	O 9	0
66	D	2	Total 2	O 2	0
66	K	1	Total 1	O 1	0

3 Residue-property plots

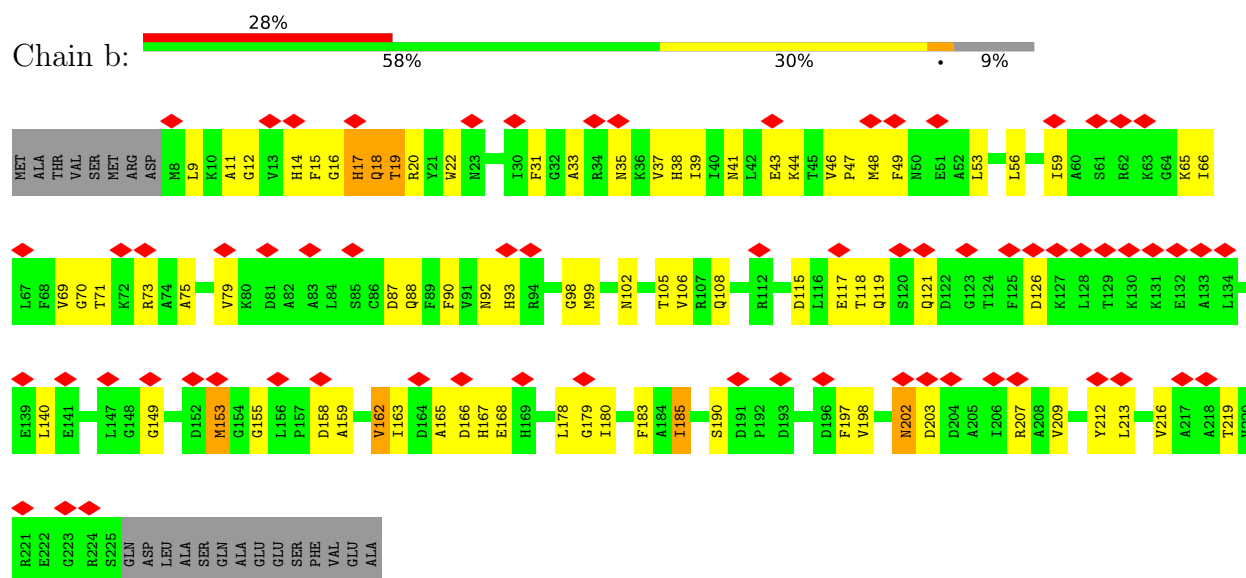
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S ribosomal RNA

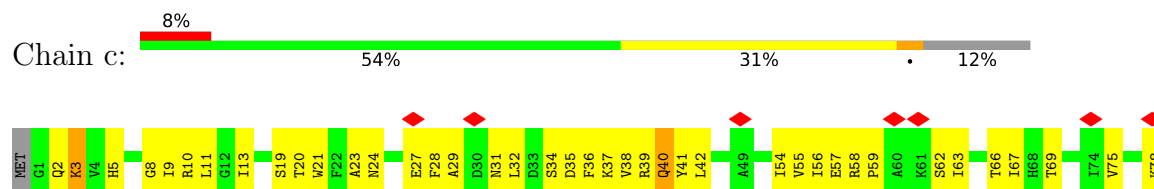


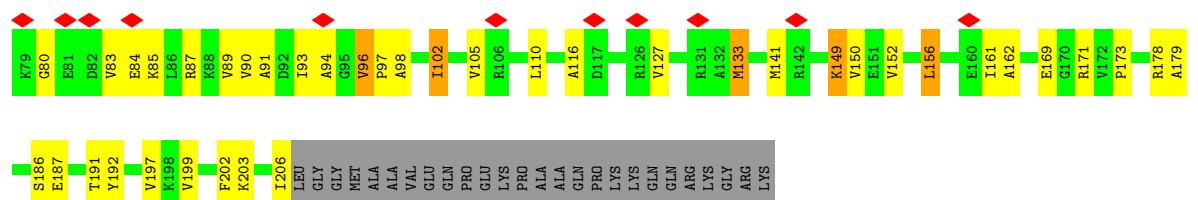


- Molecule 2: 30S ribosomal protein S2

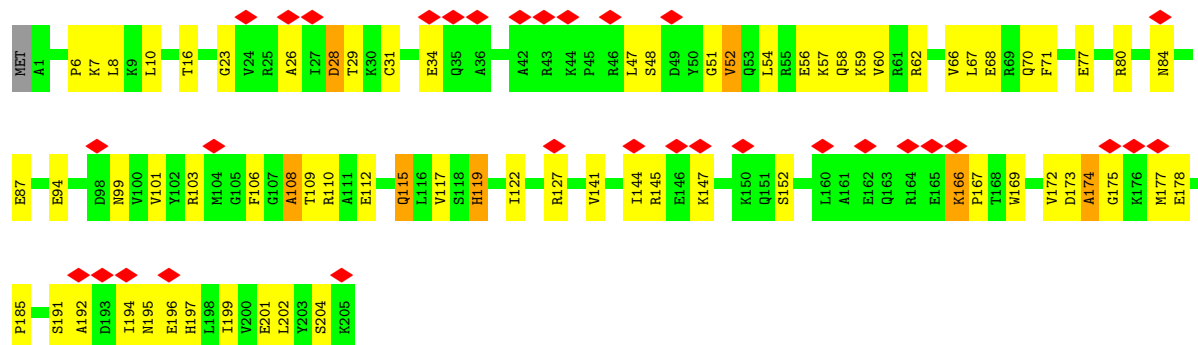


- Molecule 3: 30S ribosomal protein S3

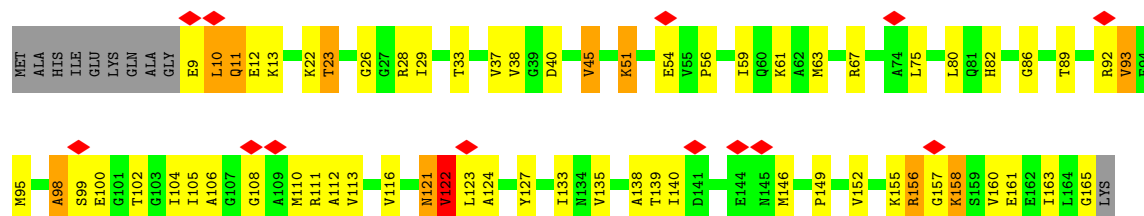




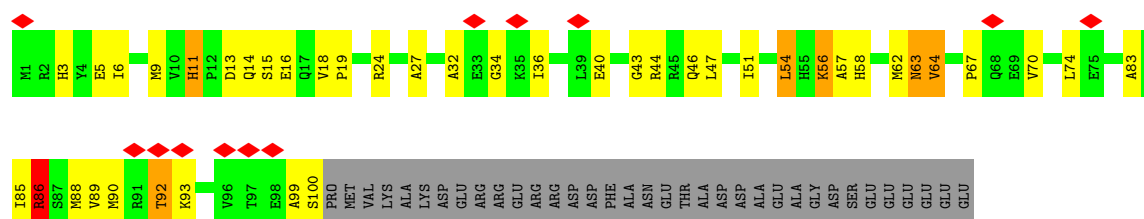
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

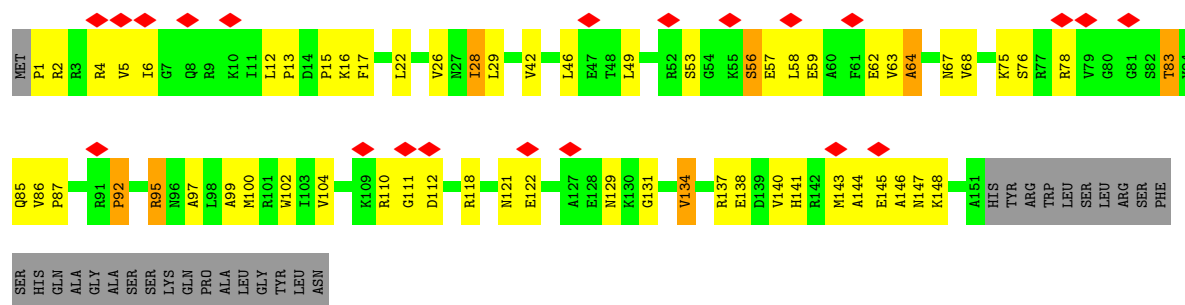


• Molecule 6: 30S ribosomal protein S6

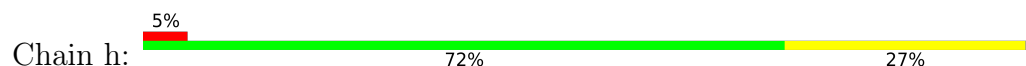


• Molecule 7: 30S ribosomal protein S7

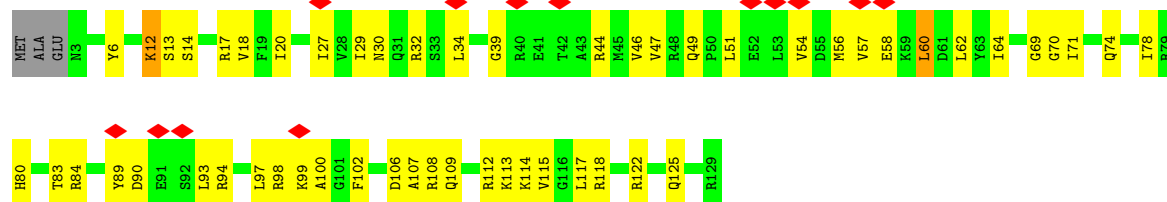




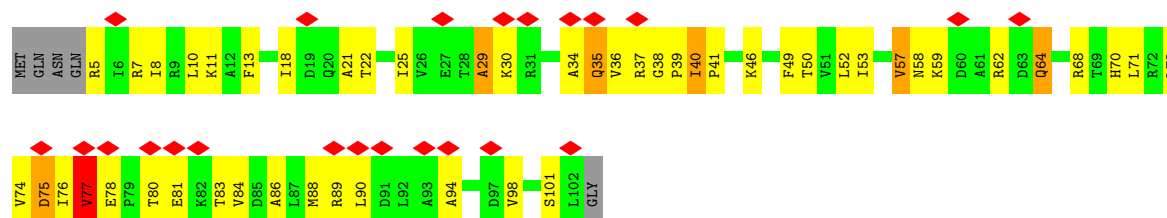
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

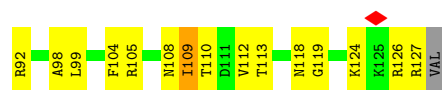


• Molecule 10: 30S ribosomal protein S10

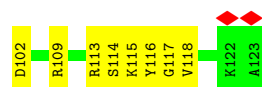
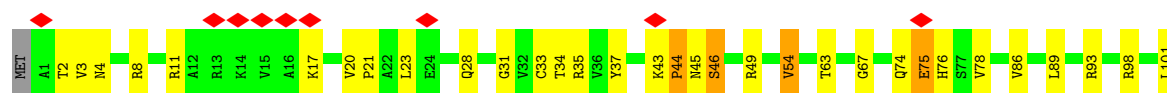


• Molecule 11: 30S ribosomal protein S11

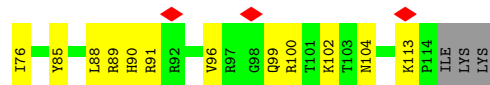




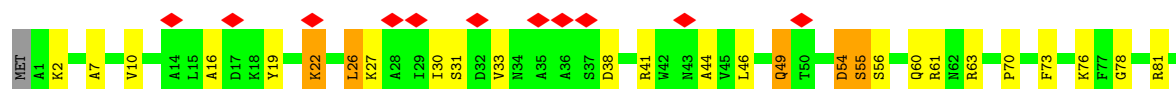
- Molecule 12: 30S ribosomal protein S12



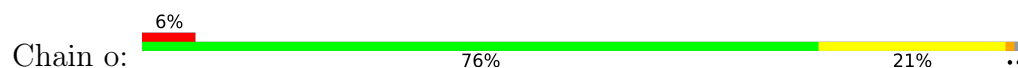
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

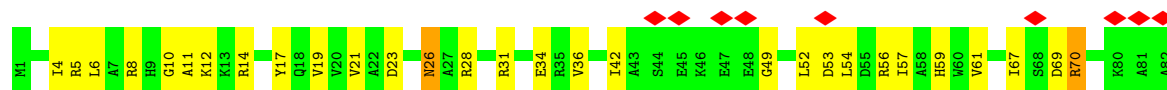


- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

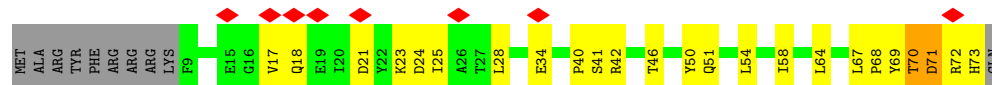




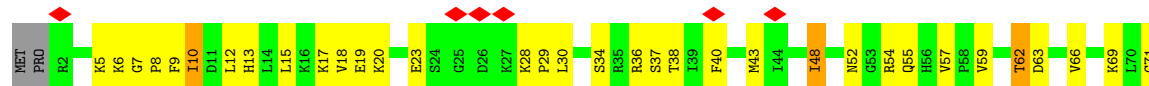
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



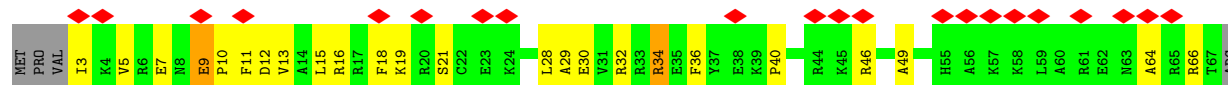
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

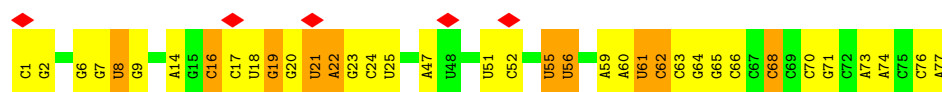


- Molecule 21: 30S ribosomal protein S21

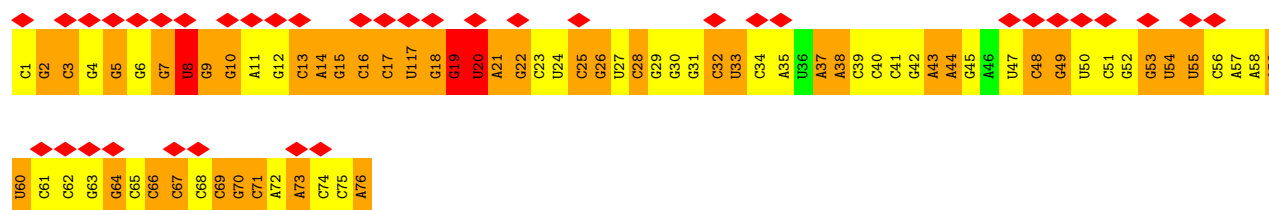


- Molecule 22: P-site fMet-tRNAfMet

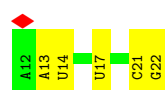




• Molecule 22: P-site fMet-tRNAfMet



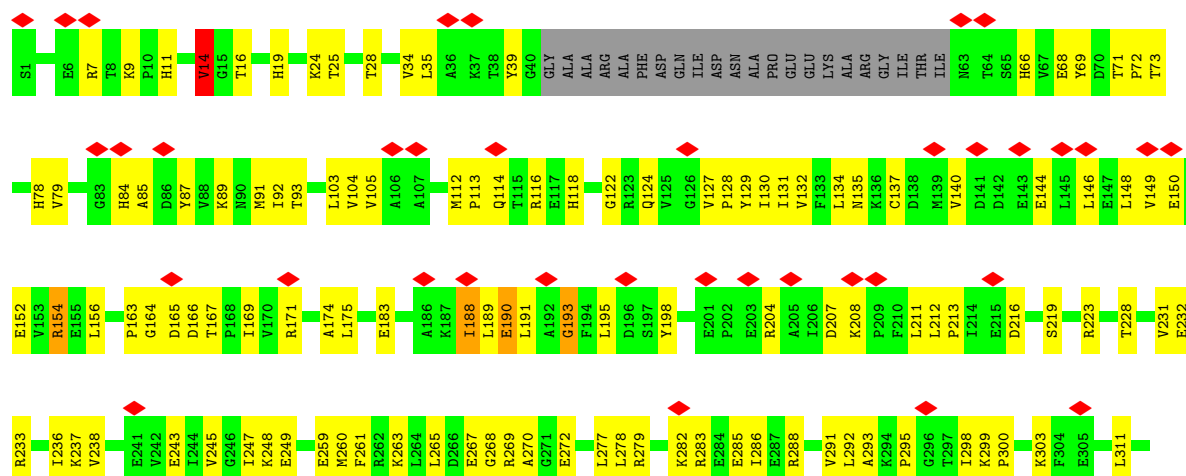
• Molecule 23: mRNA

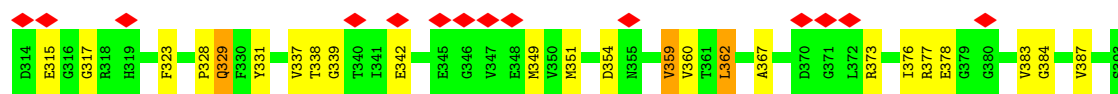


• Molecule 24: A/T-site Phe-tRNAPhe

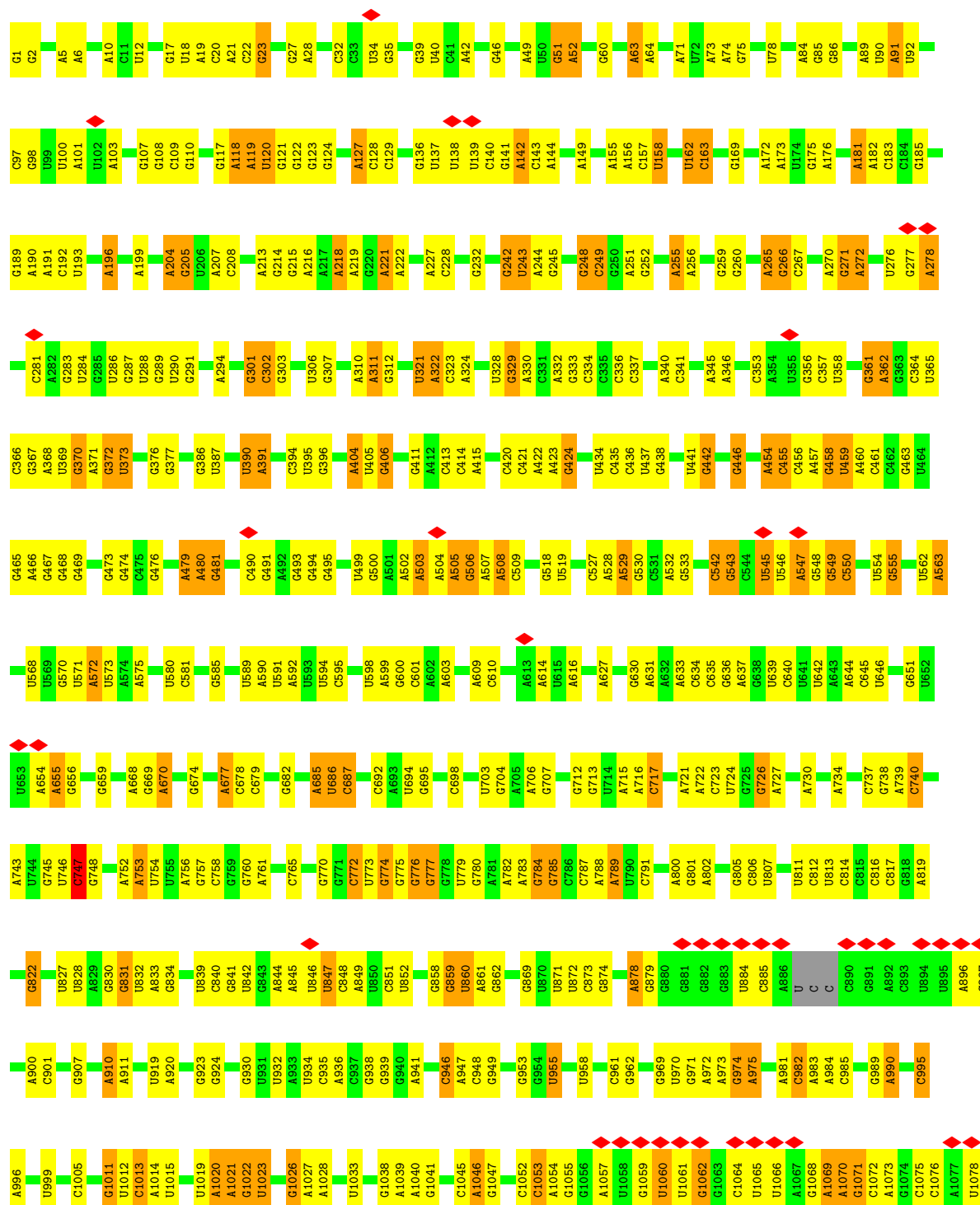


• Molecule 25: Elongation factor Tu 2

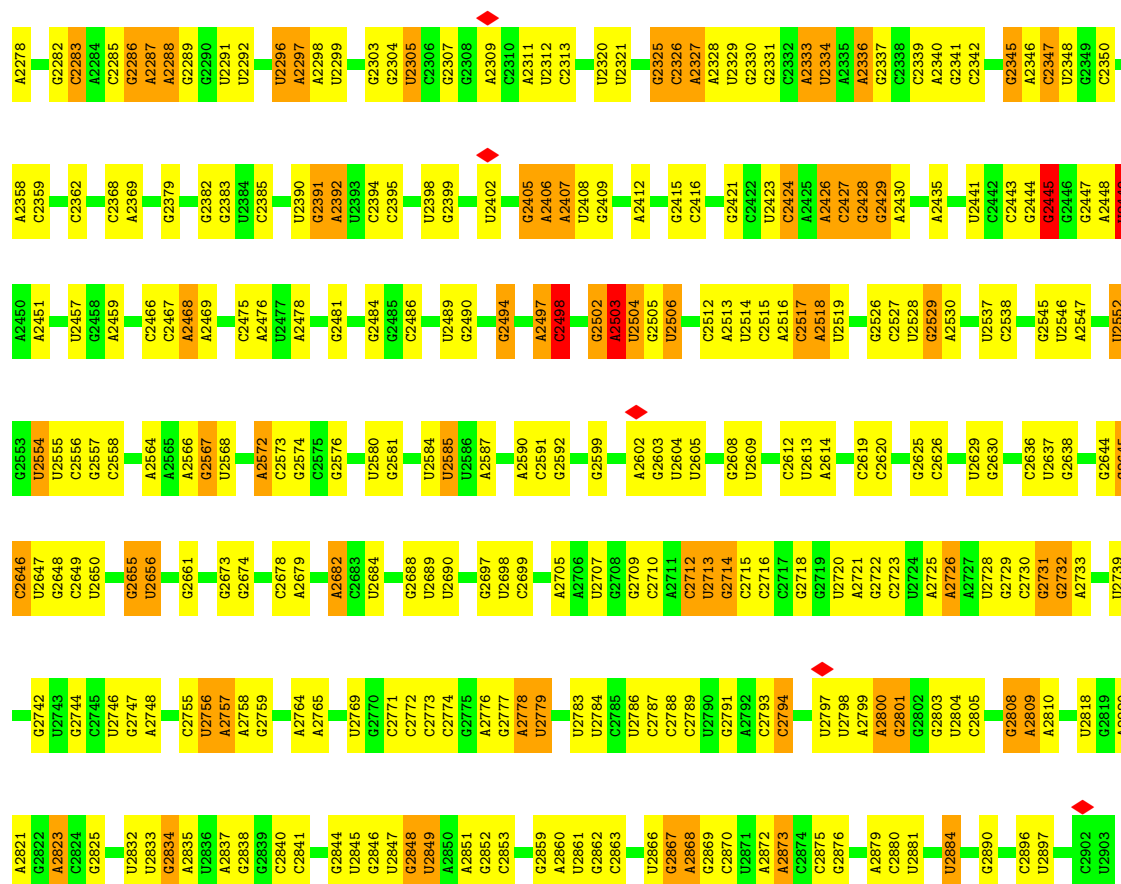




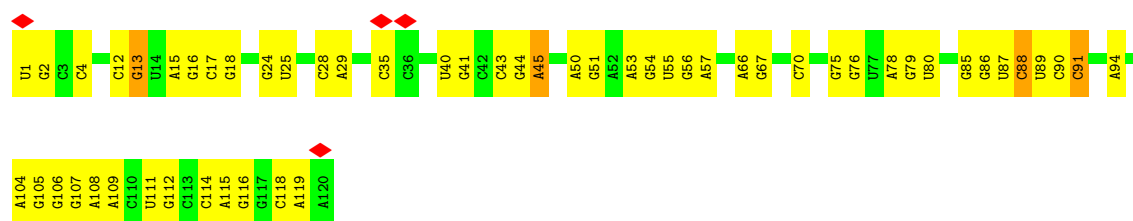
• Molecule 26: 23S ribosomal RNA



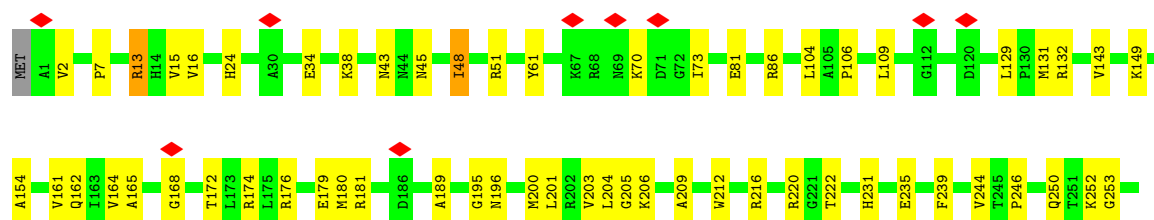
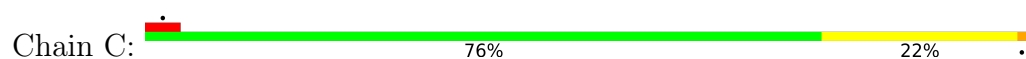


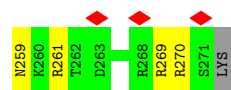


• Molecule 27: 5S ribosomal RNA

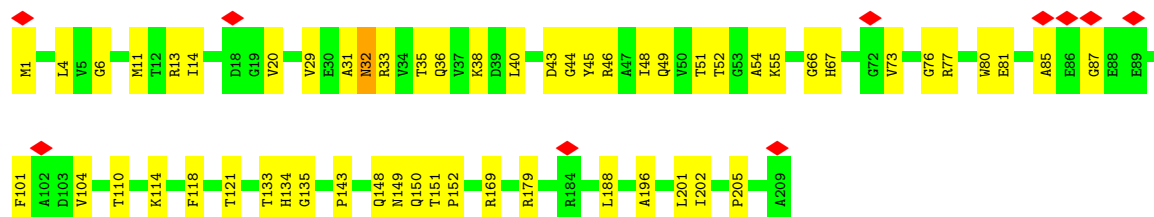
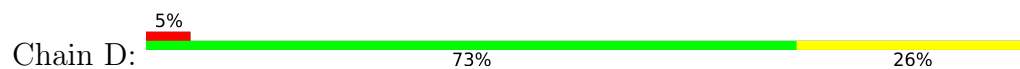


• Molecule 28: 50S ribosomal protein L2

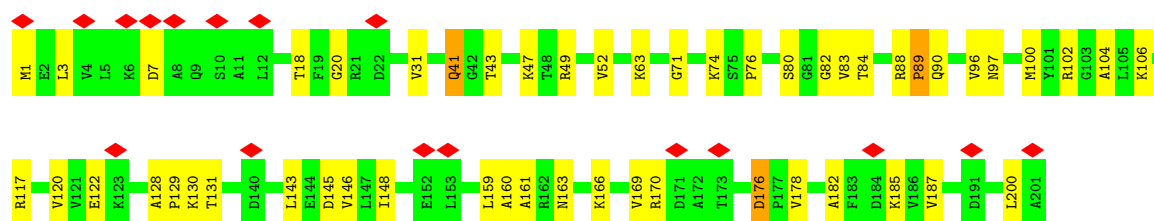
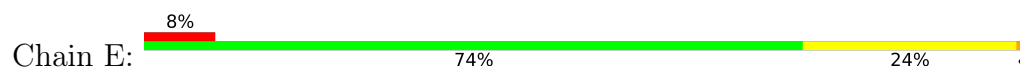




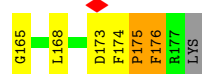
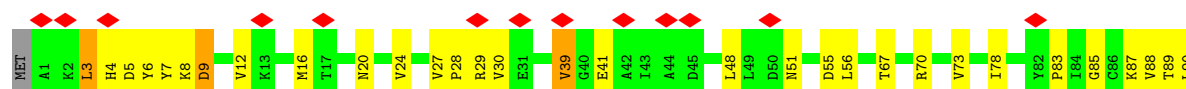
- Molecule 29: 50S ribosomal protein L3



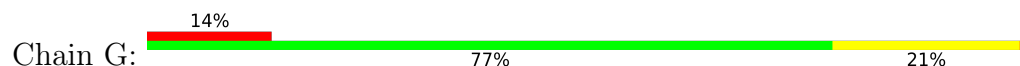
- Molecule 30: 50S ribosomal protein L4

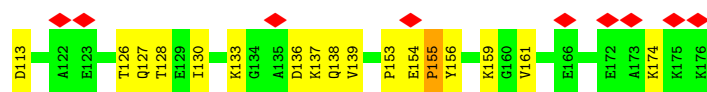


- Molecule 31: 50S ribosomal protein L5

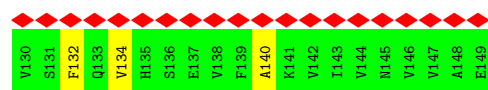
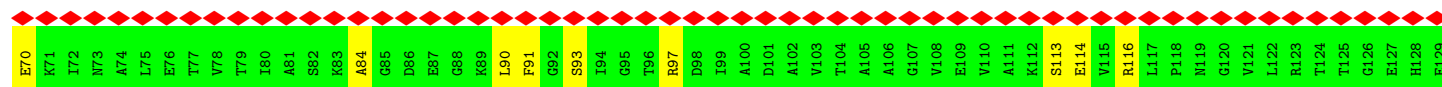
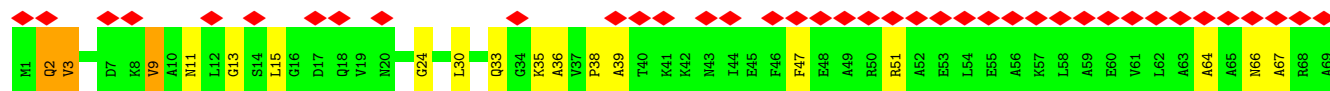
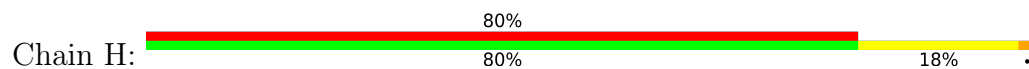


- Molecule 32: 50S ribosomal protein L6

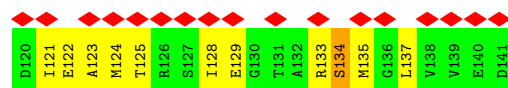
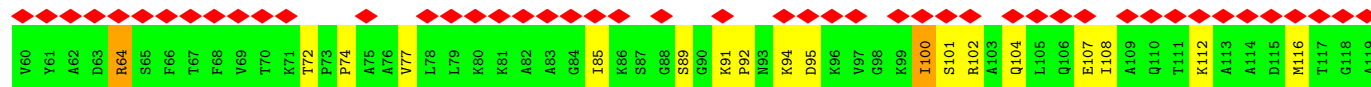
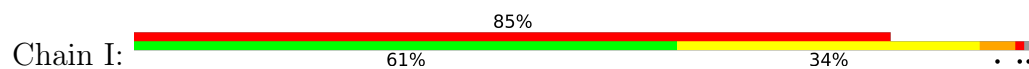




• Molecule 33: 50S ribosomal protein L9



• Molecule 34: 50S ribosomal protein L11

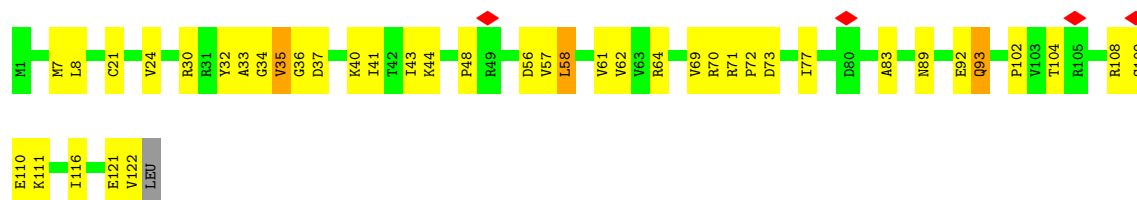


• Molecule 35: 50S ribosomal protein L13

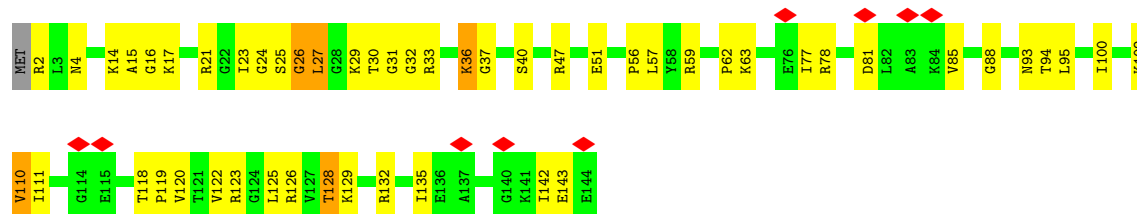


• Molecule 36: 50S ribosomal protein L14

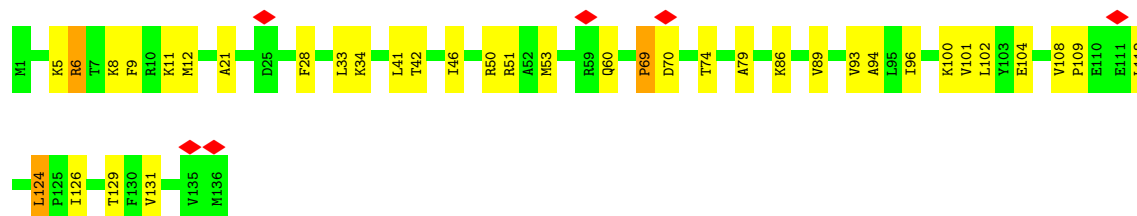




- Molecule 37: 50S ribosomal protein L15



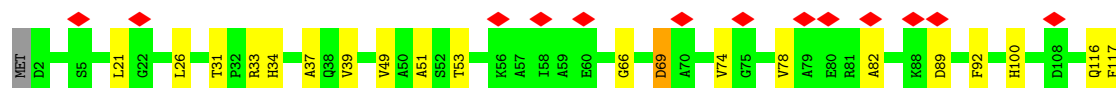
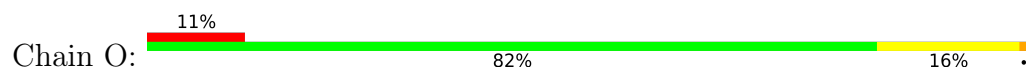
- Molecule 38: 50S ribosomal protein L16



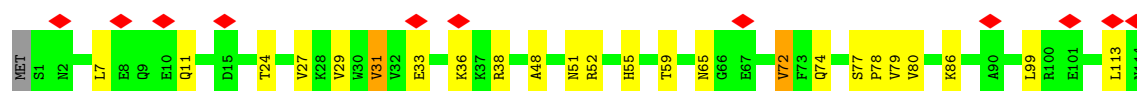
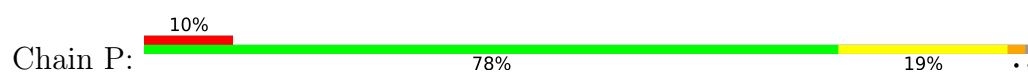
- Molecule 39: 50S ribosomal protein L17



- Molecule 40: 50S ribosomal protein L18



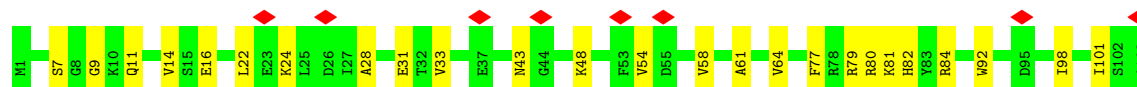
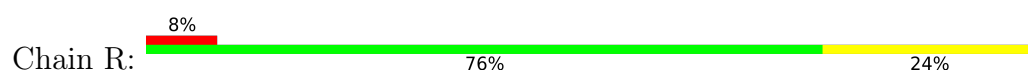
- Molecule 41: 50S ribosomal protein L19



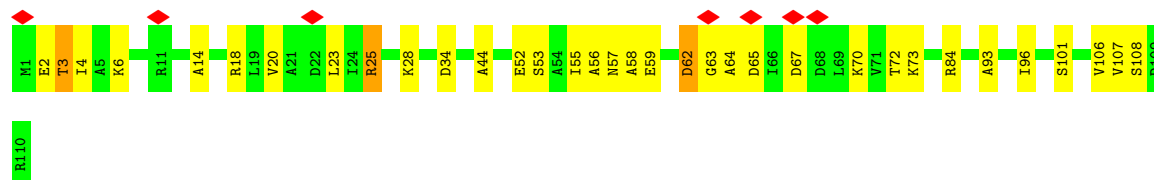
- Molecule 42: 50S ribosomal protein L20



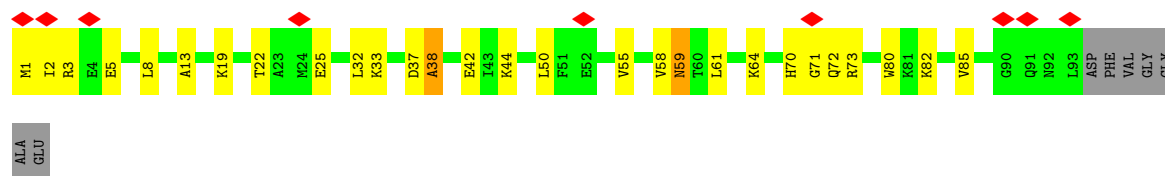
- Molecule 43: 50S ribosomal protein L21



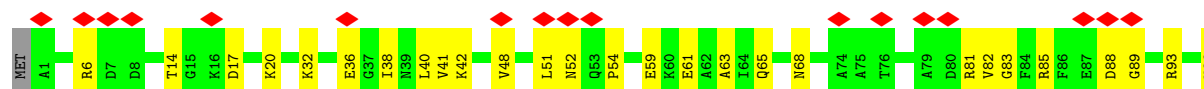
- Molecule 44: 50S ribosomal protein L22

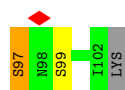


- Molecule 45: 50S ribosomal protein L23

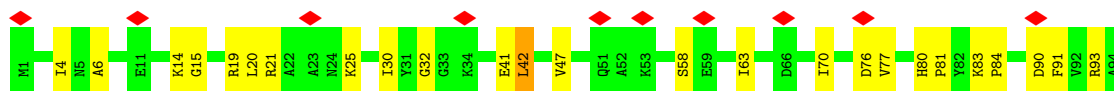
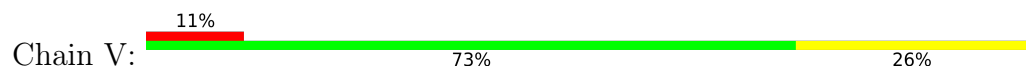


- Molecule 46: 50S ribosomal protein L24





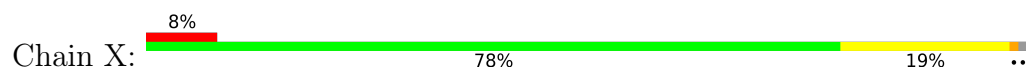
- Molecule 47: 50S ribosomal protein L25



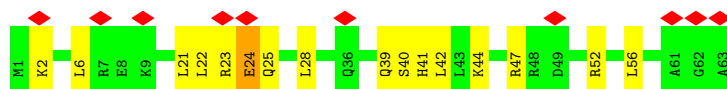
- Molecule 48: 50S ribosomal protein L27



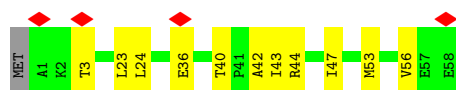
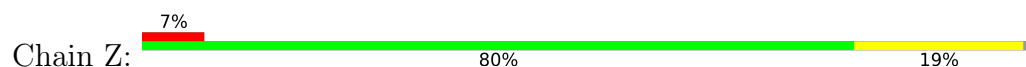
- Molecule 49: 50S ribosomal protein L28



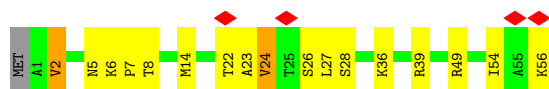
- Molecule 50: 50S ribosomal protein L29



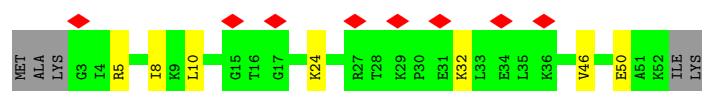
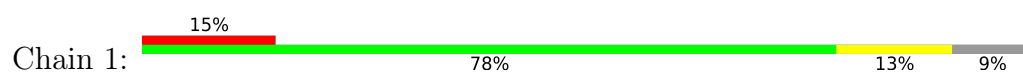
- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



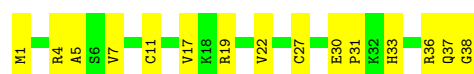
- Molecule 54: 50S ribosomal protein L34



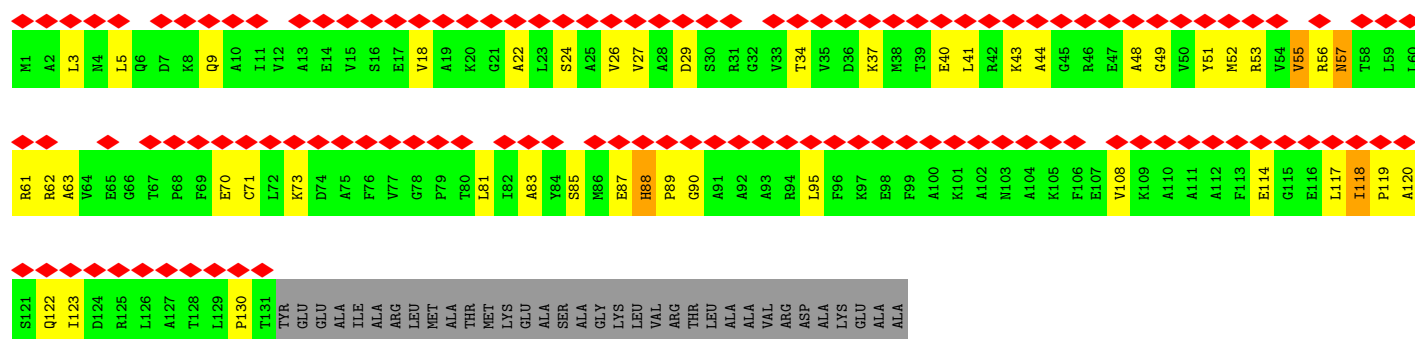
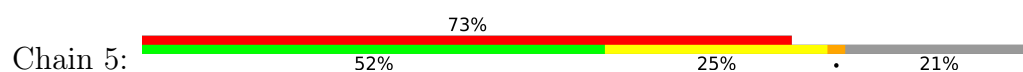
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 57: 50S ribosomal protein L10



- Molecule 58: 50S ribosomal protein L31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	417201	Depositor
Resolution determination method	Not provided	
CTF correction method	LOCAL CTF CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	192000	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	4.711	Depositor
Minimum map value	-2.426	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.214	Depositor
Recommended contour level	0.43	Depositor
Map size ($\text{\AA}$)	317.205, 317.205, 317.205	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.75525, 0.75525, 0.75525	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 7MG, ZN, MG, 2MA, FME, 1MG, UR3, OMU, 4OC, OMC, 5MC, H2U, PSU, 3TD, OMG, GDP, MA6, CL, KIR, 4SU, 6MZ, 5MU, 2MG, MIA

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	a	0.20	0/36701	0.32	2/57246 (0.0%)
2	b	0.40	0/1735	0.76	1/2338 (0.0%)
3	c	0.43	0/1651	0.76	0/2225
4	d	0.34	0/1665	0.79	0/2227
5	e	0.41	0/1154	0.80	1/1554 (0.1%)
6	f	0.46	0/835	0.85	3/1128 (0.3%)
7	g	0.50	1/1195 (0.1%)	0.85	0/1602
8	h	0.35	0/989	0.77	0/1326
9	i	0.35	0/1034	0.75	0/1375
10	j	0.51	0/796	0.88	2/1077 (0.2%)
11	k	0.37	0/885	0.85	2/1195 (0.2%)
12	l	0.36	0/969	0.80	1/1300 (0.1%)
13	m	0.50	0/892	0.85	0/1193
14	n	0.33	0/811	0.75	0/1081
15	o	0.43	0/722	0.72	0/964
16	p	0.43	0/659	0.84	0/884
17	q	0.32	0/657	0.79	0/881
18	r	0.35	0/511	0.71	0/689
19	s	0.35	0/652	0.73	0/877
20	t	0.50	0/671	0.82	1/888 (0.1%)
21	u	0.39	0/500	0.77	0/668
22	v	0.22	1/1747 (0.1%)	0.33	0/2721
22	w	0.46	0/1747	0.62	1/2721 (0.0%)
23	x	0.43	1/261 (0.4%)	0.27	0/404
24	y	0.20	1/1618 (0.1%)	0.31	0/2514
25	z	0.45	4/2935 (0.1%)	0.78	0/3970
26	A	0.23	1/69174 (0.0%)	0.34	0/107910
27	B	0.16	0/2876	0.32	0/4483
28	C	0.42	0/2121	0.82	0/2852
29	D	0.45	0/1586	0.83	1/2134 (0.0%)
30	E	0.33	0/1571	0.70	2/2113 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	F	0.39	0/1434	0.78	0/1926
32	G	0.47	0/1343	0.84	1/1816 (0.1%)
33	H	0.34	0/1122	0.73	0/1515
34	I	0.37	0/1046	0.79	2/1410 (0.1%)
35	J	0.36	0/1152	0.73	0/1551
36	K	0.36	0/947	0.72	0/1268
37	L	0.35	0/1054	0.77	1/1403 (0.1%)
38	M	0.40	0/1093	0.77	2/1460 (0.1%)
39	N	0.36	0/973	0.76	0/1301
40	O	0.42	0/902	0.74	0/1209
41	P	0.34	0/929	0.75	0/1242
42	Q	0.40	0/960	0.77	0/1278
43	R	0.43	0/829	0.82	1/1107 (0.1%)
44	S	0.37	0/864	0.83	1/1156 (0.1%)
45	T	0.35	0/744	0.79	0/994
46	U	0.47	1/787 (0.1%)	0.78	1/1051 (0.1%)
47	V	0.36	0/766	0.78	0/1025
48	W	0.39	0/582	0.83	2/769 (0.3%)
49	X	0.34	0/635	0.69	0/848
50	Y	0.43	0/510	0.73	0/677
51	Z	0.31	0/453	0.67	0/605
52	0	0.32	0/450	0.72	0/599
53	1	0.34	0/416	0.74	0/554
54	2	0.35	0/380	0.79	0/498
55	3	0.33	0/513	0.80	2/676 (0.3%)
56	4	0.33	0/303	0.77	0/397
57	5	0.37	0/1001	0.79	0/1350
58	6	0.45	0/531	0.89	0/709
All	All	0.29	10/164039 (0.0%)	0.50	30/244934 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	z	189	LEU	C-O	6.81	1.32	1.24
46	U	41	VAL	C-O	6.51	1.31	1.24
25	z	188	ILE	C-O	6.24	1.32	1.24
23	x	14	U	C1'-N1	5.80	1.57	1.48
25	z	193	GLY	N-CA	5.78	1.53	1.45
7	g	92	PRO	C-O	5.77	1.31	1.24
26	A	2552	OMU	O3'-P	5.46	1.61	1.56
22	v	8	4SU	O3'-P	5.28	1.61	1.56
24	y	8	4SU	O3'-P	5.21	1.61	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	z	154	ARG	C-O	5.00	1.30	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	w	19	G	C4'-C3'-O3'	-7.12	98.72	109.40
37	L	36	LYS	CB-CA-C	-6.12	108.51	115.79
6	f	11	HIS	CA-C-N	5.83	127.13	119.84
6	f	11	HIS	C-N-CA	5.83	127.13	119.84
48	W	69	GLY	CA-C-N	5.80	125.00	118.97
48	W	69	GLY	C-N-CA	5.80	125.00	118.97
55	3	61	LEU	CA-C-N	5.73	125.58	119.28
55	3	61	LEU	C-N-CA	5.73	125.58	119.28
6	f	90	MET	N-CA-C	5.70	115.81	108.34
43	R	64	VAL	N-CA-C	-5.69	106.92	111.81
11	k	89	GLY	CA-C-N	5.66	125.02	118.85
11	k	89	GLY	C-N-CA	5.66	125.02	118.85
46	U	51	LEU	CB-CA-C	-5.66	110.07	116.63
1	a	1297	G	P-O3'-C3'	5.42	128.34	120.20
38	M	124	LEU	CA-C-N	5.41	124.60	118.97
38	M	124	LEU	C-N-CA	5.41	124.60	118.97
20	t	69	ASN	N-CA-C	-5.27	105.67	112.68
1	a	1297	G	C2'-C3'-O3'	5.25	117.38	109.50
44	S	63	GLY	N-CA-C	5.23	120.22	113.27
29	D	66	GLY	N-CA-C	-5.17	106.44	113.37
32	G	46	ASP	CB-CA-C	-5.16	109.07	115.89
34	I	20	SER	CA-C-N	-5.16	115.06	120.38
34	I	20	SER	C-N-CA	-5.16	115.06	120.38
2	b	18	GLN	CB-CA-C	-5.14	110.67	116.63
30	E	176	ASP	CA-C-N	5.14	124.58	119.24
30	E	176	ASP	C-N-CA	5.14	124.58	119.24
12	l	101	LEU	CB-CA-C	-5.05	109.27	116.34
5	e	89	THR	CB-CA-C	-5.00	110.42	117.23
10	j	40	ILE	CA-C-N	5.00	126.09	119.84
10	j	40	ILE	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33029	0	16645	377	0
2	b	1704	0	1732	45	0
3	c	1624	0	1699	53	0
4	d	1643	0	1710	49	0
5	e	1141	0	1170	37	0
6	f	817	0	808	26	0
7	g	1181	0	1240	33	0
8	h	979	0	1034	17	0
9	i	1022	0	1070	32	0
10	j	786	0	828	38	0
11	k	869	0	878	31	0
12	l	955	0	1019	25	0
13	m	883	0	944	25	0
14	n	799	0	841	20	0
15	o	714	0	737	16	0
16	p	649	0	666	22	0
17	q	648	0	691	28	0
18	r	504	0	502	14	0
19	s	637	0	665	28	0
20	t	665	0	714	19	0
21	u	495	0	486	18	0
22	v	1644	0	839	20	0
22	w	1644	0	840	154	0
23	x	234	0	118	3	0
24	y	1643	0	850	25	0
25	z	2881	0	2894	98	0
26	A	62276	0	31346	847	0
27	B	2572	0	1302	27	0
28	C	2082	0	2157	42	0
29	D	1565	0	1616	39	0
30	E	1552	0	1619	31	0
31	F	1410	0	1447	48	0
32	G	1323	0	1374	23	0
33	H	1111	0	1148	18	0
34	I	1032	0	1088	35	0
35	J	1129	0	1162	31	0
36	K	938	0	1012	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	L	1045	0	1117	35	0
38	M	1074	0	1157	22	0
39	N	960	0	1000	26	0
40	O	892	0	923	11	0
41	P	917	0	965	17	0
42	Q	947	0	1022	22	0
43	R	816	0	839	15	0
44	S	857	0	922	22	0
45	T	738	0	807	20	0
46	U	779	0	834	17	0
47	V	753	0	780	15	0
48	W	575	0	592	9	0
49	X	625	0	655	12	0
50	Y	509	0	543	11	0
51	Z	449	0	491	7	0
52	0	444	0	461	15	0
53	1	409	0	440	4	0
54	2	377	0	418	20	0
55	3	504	0	574	16	0
56	4	302	0	341	12	0
57	5	988	0	1025	32	0
58	6	522	0	520	14	0
59	0	1	0	0	0	0
59	4	1	0	0	0	0
59	A	234	0	0	0	0
59	B	7	0	0	0	0
59	N	2	0	0	0	0
59	a	83	0	0	0	0
59	v	4	0	0	0	0
59	z	1	0	0	0	0
60	A	1	0	0	0	0
60	a	1	0	0	0	0
61	v	10	0	10	7	0
62	z	57	0	60	5	0
63	z	28	0	12	3	0
64	A	1	0	0	0	0
64	B	1	0	0	0	0
65	4	1	0	0	0	0
65	6	1	0	0	0	0
66	A	9	0	0	1	0
66	D	2	0	0	0	0
66	K	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	a	9	0	0	0	0
All	All	152717	0	103399	2498	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 10.

All (2498) 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)
22:w:18:G:H21	22:w:58:A:C5'	1.23	1.47
22:w:18:G:N2	22:w:58:A:C5'	2.03	1.21
22:w:18:G:N2	22:w:58:A:O5'	1.75	1.17
22:w:20:H2U:C5'	26:A:2112:G:H21	1.64	1.10
22:w:20:H2U:H5'	26:A:2112:G:H21	1.15	1.05
22:w:8:4SU:H5''	22:w:49:G:H5''	1.35	1.04
22:w:76:A:C2	26:A:2421:G:C6	2.53	0.97
15:o:44:GLU:HG2	15:o:45:HIS:HD2	1.30	0.97
49:X:17:ARG:HE	49:X:23:ALA:HB2	1.29	0.97
22:w:50:U:H3	22:w:64:G:H1	1.14	0.96
4:d:115:GLN:HE21	4:d:119:HIS:CE1	1.84	0.96
22:w:18:G:H21	22:w:58:A:H5'	1.30	0.94
26:A:704:G:H2'	26:A:726:G:H22	1.31	0.94
26:A:1055:G:H1	26:A:1104:C:H42	1.11	0.94
22:w:7:G:N1	22:w:66:C:N3	2.18	0.92
22:w:29:G:O6	22:w:41:C:N4	2.05	0.90
4:d:115:GLN:HE21	4:d:119:HIS:HE1	1.16	0.89
22:w:18:G:H21	22:w:58:A:C4'	1.86	0.88
1:a:1130:A:H61	1:a:1144:G:H1'	1.36	0.88
31:F:134:GLN:NE2	31:F:149:ARG:O	2.06	0.87
22:w:6:G:N2	22:w:67:C:N3	2.23	0.86
22:w:20:H2U:C5'	26:A:2112:G:N2	2.38	0.86
1:a:664:G:H22	1:a:741:G:H1	1.23	0.86
1:a:1305:G:HO2'	1:a:1306:A:H8	0.88	0.86
22:w:10:G:O6	22:w:25:C:N4	2.07	0.86
22:w:20:H2U:H5'	26:A:2112:G:N2	1.91	0.85
22:w:18:G:N2	22:w:58:A:H5'	1.83	0.85
2:b:92:ASN:OD1	2:b:93:HIS:ND1	2.10	0.84
61:v:105:FME:HE2	26:A:2585:U:O2'	1.78	0.83
26:A:585:G:N7	42:Q:5:ARG:NH1	2.26	0.83
22:w:56:C:C4	26:A:2168:G:C2	2.66	0.83
22:w:9:G:O2'	22:w:45:G:N3	2.11	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:v:59:A:O2'	22:v:61:U:OP2	1.96	0.82
22:w:7:G:O6	22:w:65:C:N4	2.12	0.82
2:b:19:THR:HG23	2:b:20:ARG:H	1.41	0.82
43:R:14:VAL:HG21	43:R:98:ILE:HG13	1.61	0.82
22:w:7:G:N2	22:w:66:C:O2	2.13	0.82
26:A:2848:G:H2'	26:A:2867:G:N2	1.95	0.82
46:U:65:GLN:HB2	46:U:68:ASN:OD1	1.80	0.82
22:w:8:4SU:O2'	22:w:21:A:N1	2.11	0.82
29:D:13:ARG:HH11	41:P:55:HIS:HA	1.44	0.82
22:w:18:G:H2'	22:w:19:G:H5'	1.60	0.82
22:w:11:A:N6	22:w:12:G:O6	2.13	0.81
1:a:1305:G:O2'	1:a:1306:A:H8	1.62	0.81
26:A:2333:A:H4'	26:A:2334:U:O5'	1.81	0.81
26:A:1060:U:H5'	26:A:1062:G:H5'	1.63	0.80
26:A:1103:A:H3'	26:A:1104:C:H5''	1.62	0.80
1:a:692:U:H5''	11:k:126:ARG:HH22	1.48	0.79
30:E:146:VAL:HG12	30:E:185:LYS:HB2	1.65	0.79
1:a:176:C:H5''	20:t:23:ARG:HH12	1.46	0.79
26:A:1041:G:H1	26:A:1114:C:H42	1.31	0.78
28:C:106:PRO:HD2	28:C:109:LEU:HD22	1.66	0.78
15:o:44:GLU:HG2	15:o:45:HIS:CD2	2.18	0.78
7:g:110:ARG:HH22	7:g:121:ASN:HB3	1.48	0.78
1:a:212:G:H2'	1:a:213:G:H8	1.48	0.78
1:a:1297:G:O2'	1:a:1298:U:OP2	2.00	0.77
10:j:59:LYS:HE2	10:j:62:ARG:HH21	1.49	0.77
25:z:329:GLN:HE21	25:z:329:GLN:N	1.81	0.77
26:A:2220:U:H4'	33:H:97:ARG:HH21	1.48	0.77
44:S:53:SER:O	44:S:57:ASN:HB2	1.83	0.77
22:w:61:C:H2'	22:w:62:C:H6	1.49	0.77
24:y:77:PHE:N	25:z:261:PHE:H	1.83	0.77
22:w:2:G:N1	22:w:70:G:O6	2.18	0.77
4:d:119:HIS:N	4:d:119:HIS:CD2	2.51	0.76
29:D:35:THR:OG1	29:D:49:GLN:HG2	1.86	0.76
35:J:80:HIS:O	35:J:82:GLY:N	2.15	0.76
5:e:156:ARG:NH1	5:e:163:ILE:HA	1.99	0.76
35:J:117:ALA:HA	35:J:120:ARG:HH21	1.49	0.76
26:A:1936:A:H2	26:A:1943:U:H3	1.31	0.76
26:A:2345:G:H4'	26:A:2346:A:H5''	1.67	0.75
24:y:58:A:O2'	24:y:60:U:OP2	2.04	0.75
26:A:2848:G:H2'	26:A:2867:G:H22	1.50	0.75
57:5:87:GLU:HG2	57:5:95:LEU:HD12	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1090:A:H61	26:A:1101:U:H3	1.35	0.75
61:v:105:FME:CE	26:A:2585:U:O2'	2.34	0.74
22:w:56:C:N4	26:A:2168:G:N2	2.34	0.74
26:A:1845:G:N2	26:A:1895:C:O2	2.14	0.74
24:y:18:G:O2'	24:y:57:G:N2	2.20	0.74
11:k:49:SER:HA	11:k:68:ARG:HH11	1.51	0.74
22:w:29:G:N1	22:w:41:C:N3	2.32	0.74
22:w:76:A:O4'	26:A:2395:C:O2	2.06	0.74
34:I:91:LYS:HG3	34:I:94:LYS:HE2	1.70	0.74
26:A:1532:A:H2	26:A:1539:U:H3	1.34	0.73
5:e:155:LYS:O	5:e:158:LYS:HE3	1.88	0.73
7:g:26:VAL:HG22	7:g:42:VAL:HG21	1.71	0.73
12:l:4:ASN:OD1	17:q:35:LYS:NZ	2.20	0.73
22:w:48:C:OP2	22:w:59:A:H5'	1.88	0.73
26:A:458:G:O2'	26:A:459:U:OP2	2.06	0.72
26:A:572:A:OP2	43:R:80:ARG:NH2	2.22	0.72
26:A:2808:G:H4'	26:A:2809:A:O5'	1.88	0.72
22:w:18:G:C2'	22:w:19:G:H5'	2.19	0.72
53:l:8:ILE:HD13	53:l:24:LYS:HE3	1.70	0.72
50:Y:6:LEU:HD13	50:Y:56:LEU:HD22	1.72	0.72
25:z:260:MET:HE1	25:z:272:GLU:HG3	1.71	0.72
44:S:73:LYS:HB2	44:S:106:VAL:HB	1.70	0.72
26:A:1022:G:H4'	26:A:1023:U:O5'	1.88	0.72
22:w:15:G:H2'	22:w:59:A:H61	1.53	0.72
11:k:84:MET:SD	11:k:110:THR:OG1	2.47	0.71
16:p:23:ASP:HB3	16:p:26:ASN:ND2	2.05	0.71
22:w:18:G:C2	22:w:58:A:H5'	2.25	0.71
41:P:33:GLU:HB2	41:P:36:LYS:HB2	1.71	0.71
11:k:124:LYS:O	21:u:34:ARG:NH1	2.22	0.71
26:A:1059:G:H22	34:I:128:ILE:HG12	1.53	0.71
22:w:55:PSU:N1	22:w:58:A:N7	2.39	0.71
24:y:77:PHE:O	25:z:261:PHE:HA	1.90	0.71
26:A:2682:A:H61	26:A:2728:U:H1'	1.55	0.71
26:A:1188:U:C2'	26:A:1189:A:H5'	2.21	0.71
1:a:1191:A:H5''	3:c:3:LYS:HE3	1.72	0.70
4:d:10:LEU:HD13	4:d:62:ARG:HD2	1.71	0.70
5:e:98:ALA:HB2	5:e:123:LEU:HG	1.73	0.70
26:A:568:U:H1'	26:A:2030:6MZ:H9C1	1.72	0.70
26:A:704:G:H1'	26:A:727:A:N6	2.05	0.70
31:F:3:LEU:HA	31:F:6:TYR:HB3	1.73	0.70
44:S:4:ILE:HG22	44:S:106:VAL:HG22	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:w:20:H2U:H51	26:A:2112:G:O2'	1.91	0.70
36:K:69:VAL:HG21	36:K:104:THR:HG21	1.72	0.70
25:z:14:VAL:O	25:z:78:HIS:HA	1.91	0.70
1:a:264:C:H4'	17:q:64:ARG:HD2	1.74	0.70
7:g:134:VAL:O	7:g:138:GLU:HG2	1.92	0.70
26:A:1213:A:N6	26:A:1236:G:H1'	2.07	0.70
20:t:24:ARG:HG2	20:t:28:ARG:HH21	1.57	0.70
22:w:18:G:O6	22:w:55:PSU:H6	1.75	0.70
2:b:53:LEU:HB3	2:b:219:THR:HG21	1.74	0.69
26:A:2644:G:C2'	26:A:2645:G:H5'	2.22	0.69
26:A:328:U:H4'	46:U:65:GLN:HE21	1.56	0.69
26:A:1341:G:N3	45:T:59:ASN:OD1	2.25	0.69
46:U:32:LYS:HB3	46:U:63:ALA:HB1	1.73	0.69
22:v:22:A:N6	22:v:47:A:H2'	2.07	0.69
22:w:14:A:H3'	22:w:15:G:C8	2.28	0.69
1:a:107:G:O6	20:t:9:ARG:HD3	1.93	0.69
12:l:109:ARG:HB2	12:l:118:VAL:HG21	1.74	0.69
47:V:20:LEU:HD11	47:V:41:GLU:HG3	1.73	0.69
2:b:183:PHE:HB3	2:b:197:PHE:HB2	1.74	0.69
5:e:93:VAL:HG11	5:e:139:THR:HG22	1.74	0.69
26:A:284:U:H3	26:A:356:G:H1	1.40	0.69
37:L:62:PRO:HB2	55:3:29:ARG:HH11	1.56	0.69
14:n:46:LEU:HG	19:s:12:LEU:HD21	1.74	0.69
22:v:64:G:H2'	22:v:65:G:C8	2.28	0.69
54:2:12:ARG:HE	54:2:44:VAL:HG21	1.58	0.69
14:n:27:LYS:O	14:n:31:SER:HB2	1.93	0.68
26:A:1046:A:H4'	57:5:61:ARG:HB3	1.75	0.68
26:A:107:G:H2'	26:A:108:G:H8	1.58	0.68
14:n:49:GLN:N	14:n:49:GLN:HE21	1.91	0.68
19:s:5:LYS:HG3	19:s:6:LYS:HG2	1.75	0.68
22:w:42:G:H5''	22:w:43:A:OP2	1.92	0.68
26:A:1565:C:O2'	26:A:1566:A:H8	1.77	0.68
28:C:196:ASN:OD1	28:C:196:ASN:O	2.11	0.68
2:b:15:PHE:HB2	2:b:39:ILE:HG23	1.76	0.68
24:y:16:H2U:H2'	24:y:17:C:H4'	1.74	0.68
9:i:34:LEU:HD11	9:i:47:VAL:HG21	1.76	0.68
14:n:54:ASP:O	14:n:56:SER:N	2.23	0.68
10:j:40:ILE:HB	10:j:73:LEU:HB2	1.76	0.68
26:A:776:G:H4'	26:A:777:G:O5'	1.94	0.68
26:A:1613:G:H4'	54:2:3:ARG:HE	1.58	0.67
26:A:2133:G:H21	26:A:2158:A:H61	1.41	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:135:VAL:O	5:e:139:THR:HG23	1.95	0.67
26:A:1011:G:O2'	26:A:1013:C:H5''	1.93	0.67
25:z:237:LYS:HG2	25:z:267:GLU:HG2	1.76	0.67
26:A:703:U:H2'	26:A:704:G:O4'	1.94	0.67
26:A:2331:G:H4'	48:W:39:THR:H	1.57	0.67
1:a:1518:MA6:H102	1:a:1519:MA6:N6	2.10	0.67
26:A:2291:U:H2'	26:A:2292:U:C6	2.29	0.67
26:A:2564:A:OP1	26:A:2648:G:H4'	1.95	0.67
36:K:40:LYS:HE3	36:K:57:VAL:HG12	1.76	0.67
26:A:189:G:H1	26:A:205:G:HO2'	1.39	0.67
26:A:655:A:H4'	26:A:656:G:H5'	1.77	0.67
12:l:78:VAL:O	12:l:102:ASP:HB2	1.95	0.67
25:z:92:ILE:HG23	62:z:401:KIR:H371	1.75	0.67
26:A:910:A:H62	38:M:12:MET:HA	1.58	0.67
4:d:117:VAL:HG22	4:d:122:ILE:HG13	1.78	0.66
22:w:56:C:H2'	22:w:57:A:H8	1.59	0.66
26:A:1478:G:H1	26:A:1513:U:H3	1.42	0.66
26:A:2339:C:H2'	26:A:2340:A:H8	1.59	0.66
1:a:951:G:OP2	13:m:100:ARG:NH2	2.28	0.66
17:q:13:SER:HB3	17:q:21:VAL:HG12	1.77	0.66
26:A:1701:A:H2'	26:A:1702:G:H5'	1.78	0.66
26:A:2759:G:H21	32:G:138:GLN:NE2	1.93	0.66
31:F:28:PRO:HB2	31:F:168:LEU:HD22	1.77	0.66
2:b:69:VAL:HB	2:b:162:VAL:HG13	1.78	0.66
47:V:21:ARG:HA	47:V:25:LYS:O	1.95	0.66
22:w:44:A:C8	22:w:44:A:OP2	2.48	0.66
26:A:545:U:H3	26:A:548:G:H1	1.41	0.66
26:A:753:A:H8	26:A:753:A:OP2	1.79	0.66
10:j:52:LEU:HD21	10:j:59:LYS:HD2	1.77	0.66
13:m:88:LEU:HD12	13:m:91:ARG:HH21	1.60	0.66
26:A:499:U:H5''	46:U:42:LYS:HE2	1.78	0.66
54:2:3:ARG:HG3	54:2:5:PHE:H	1.60	0.66
12:l:113:ARG:HB2	12:l:118:VAL:HB	1.77	0.66
26:A:5:A:H2'	26:A:6:A:C8	2.31	0.66
26:A:1999:C:H5''	26:A:2723:C:O2'	1.95	0.66
3:c:19:SER:HB3	3:c:21:TRP:HE1	1.60	0.66
21:u:36:PHE:HB3	21:u:40:PRO:HD3	1.78	0.66
26:A:1530:G:N2	26:A:1542:U:H1'	2.11	0.66
26:A:2800:A:H3'	26:A:2801:G:H5'	1.77	0.66
58:6:62:LYS:C	58:6:65:ASN:HD21	2.04	0.66
4:d:119:HIS:CD2	4:d:119:HIS:H	2.14	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:140:ILE:HG22	31:F:142:TYR:H	1.60	0.65
35:J:17:VAL:HG23	35:J:137:PRO:HB2	1.78	0.65
22:w:51:C:N3	22:w:63:G:N2	2.37	0.65
25:z:260:MET:HE2	25:z:265:LEU:HD11	1.77	0.65
28:C:165:ALA:HB3	28:C:172:THR:HB	1.76	0.65
1:a:246:A:H4'	1:a:247:G:OP1	1.96	0.65
1:a:1144:G:N2	1:a:1146:A:H62	1.94	0.65
26:A:948:C:O2	26:A:984:A:O2'	2.14	0.65
22:v:55:5MU:HN3	22:v:59:A:H62	1.42	0.65
22:w:20:H2U:H51	26:A:2112:G:H1'	1.76	0.65
26:A:503:A:H1'	26:A:506:G:OP2	1.96	0.65
26:A:2428:G:H5''	26:A:2429:G:O5'	1.96	0.65
34:I:101:SER:HB3	34:I:104:GLN:OE1	1.97	0.65
26:A:841:G:H2'	26:A:842:U:C6	2.31	0.65
26:A:218:A:H8	26:A:218:A:OP2	1.79	0.65
26:A:248:G:O5'	26:A:249:C:H5'	1.96	0.65
10:j:13:PHE:O	10:j:70:HIS:CE1	2.50	0.65
11:k:87:GLY:H	11:k:113:THR:HG22	1.62	0.65
22:w:1:C:H42	22:w:71:C:N4	1.95	0.65
14:n:19:TYR:O	14:n:22:LYS:HB3	1.97	0.65
16:p:14:ARG:HE	16:p:42:ILE:HD12	1.62	0.65
61:v:105:FME:HCN	26:A:2451:A:H2	1.61	0.65
26:A:1212:G:O2'	26:A:1236:G:N2	2.29	0.65
26:A:2786:U:H2'	26:A:2787:C:H6	1.60	0.65
13:m:24:VAL:HG23	13:m:28:ARG:HB3	1.79	0.64
1:a:203:G:H1'	1:a:465:A:H61	1.61	0.64
2:b:99:MET:HA	2:b:106:VAL:HG21	1.78	0.64
14:n:54:ASP:C	14:n:56:SER:H	2.04	0.64
10:j:35:GLN:HG2	10:j:78:GLU:HG2	1.79	0.64
25:z:150:GLU:HG2	25:z:169:ILE:HG21	1.78	0.64
26:A:5:A:H2'	26:A:6:A:H8	1.62	0.64
26:A:923:G:H2'	26:A:924:G:H8	1.63	0.64
26:A:2788:C:H2'	26:A:2789:C:C6	2.32	0.64
26:A:51:G:H4'	26:A:52:A:H5'	1.78	0.64
26:A:2131:U:O5'	26:A:2133:G:H4'	1.97	0.64
6:f:88:MET:HG2	18:r:64:LEU:HD21	1.77	0.64
35:J:117:ALA:HA	35:J:120:ARG:NH2	2.12	0.64
8:h:94:VAL:HB	8:h:99:GLY:O	1.98	0.64
26:A:1930:G:O2'	26:A:1931:U:P	2.55	0.64
2:b:98:GLY:O	2:b:102:ASN:HB3	1.97	0.64
22:w:56:C:N4	26:A:2168:G:C2	2.66	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:z:84[A]:HIS:NE2	26:A:2661:G:O2'	2.31	0.64
34:I:122:GLU:O	34:I:125:THR:HB	1.97	0.64
52:0:54:ILE:HG13	52:0:56:LYS:HB3	1.80	0.64
1:a:1178:G:N2	1:a:1181:G:OP2	2.31	0.64
11:k:23:HIS:HB3	11:k:30:ILE:HG23	1.80	0.64
28:C:48:ILE:HD11	28:C:51:ARG:HA	1.78	0.64
33:H:9:VAL:HB	33:H:13:GLY:HA3	1.78	0.64
2:b:41:ASN:HD21	2:b:43:GLU:HB2	1.63	0.64
17:q:61:ARG:NH1	17:q:73:THR:HB	2.13	0.64
19:s:9:PHE:HE2	19:s:36:ARG:HG3	1.62	0.64
26:A:704:G:H2'	26:A:726:G:N2	2.10	0.64
26:A:859:G:O2'	26:A:860:U:P	2.56	0.64
25:z:351:MET:HB2	25:z:354:ASP:OD2	1.98	0.63
37:L:93:ASN:O	37:L:95:LEU:N	2.30	0.63
12:l:45:ASN:O	12:l:46:SER:HB3	1.97	0.63
22:w:19:G:O2'	22:w:20:H2U:O4	2.14	0.63
26:A:2584:U:H3'	26:A:2585:U:H5''	1.80	0.63
22:w:5:G:N2	22:w:69:C:O2	2.31	0.63
26:A:404:A:H1'	26:A:406:G:C4	2.33	0.63
39:N:73:ASN:HA	39:N:76:VAL:HG12	1.80	0.63
22:w:76:A:H4'	26:A:2395:C:H1'	1.80	0.63
25:z:188:ILE:O	25:z:191:LEU:HB3	1.98	0.63
26:A:2097:A:H2'	26:A:2098:U:O4'	1.98	0.63
26:A:454:A:H4'	26:A:455:C:OP2	1.97	0.63
43:R:82:HIS:O	43:R:82:HIS:ND1	2.31	0.63
1:a:1086:U:H3	1:a:1099:G:H22	1.45	0.63
25:z:328:PRO:C	25:z:329:GLN:HE21	2.06	0.63
26:A:1542:U:H2'	26:A:1543:G:O4'	1.99	0.63
1:a:618:C:H1'	16:p:14:ARG:HH12	1.62	0.63
1:a:933:G:N7	7:g:2:ARG:NH2	2.42	0.63
1:a:1064:G:H1'	1:a:1190:G:N2	2.14	0.63
11:k:99:LEU:O	11:k:104:PHE:HB2	1.98	0.63
22:w:44:A:N3	22:w:44:A:H2'	2.13	0.63
26:A:370:G:O2'	26:A:424:G:OP1	2.17	0.63
26:A:1186:G:H2'	26:A:1187:G:O4'	1.99	0.63
26:A:2712:C:O2'	26:A:2713:U:H5'	1.99	0.63
3:c:110:LEU:HD13	3:c:203:LYS:HE3	1.81	0.63
26:A:1028:A:N6	26:A:1125:G:H2'	2.13	0.63
17:q:30:HIS:HD2	17:q:33:TYR:H	1.47	0.63
26:A:120:U:H5''	26:A:122:G:OP2	1.98	0.63
26:A:2537:U:H2'	26:A:2538:C:C6	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:94:A:OP1	47:V:19:ARG:HD3	1.99	0.63
9:i:94:ARG:HA	9:i:97:LEU:HB3	1.80	0.62
22:w:72:A:H4'	26:A:1852:U:H4'	1.81	0.62
25:z:342:GLU:HB3	25:z:359:VAL:HG13	1.79	0.62
26:A:242:G:HO2'	26:A:243:U:P	2.22	0.62
26:A:1055:G:H1	26:A:1104:C:N4	1.90	0.62
27:B:118:C:H2'	27:B:119:A:C8	2.34	0.62
30:E:145:ASP:HA	30:E:166:LYS:HB3	1.81	0.62
11:k:80:ASN:HB3	11:k:105:ARG:HB2	1.81	0.62
25:z:105:VAL:O	25:z:134:LEU:HA	1.99	0.62
10:j:36:VAL:HG22	10:j:38:GLY:H	1.64	0.62
26:A:1062:G:H22	34:I:134:SER:HB2	1.65	0.62
34:I:33:ASN:HB2	34:I:64:ARG:HH22	1.64	0.62
5:e:10:LEU:HD22	5:e:67:ARG:HH22	1.64	0.62
26:A:221:A:N1	26:A:265:A:O2'	2.33	0.62
26:A:1385:A:H4'	26:A:1385:A:OP1	1.98	0.62
26:A:2391:G:H2'	26:A:2424:C:H41	1.65	0.62
26:A:2394:C:H5''	37:L:63:LYS:HE3	1.81	0.62
45:T:58:VAL:HG22	45:T:85:VAL:HG13	1.80	0.62
26:A:1188:U:H2'	26:A:1189:A:H5'	1.82	0.62
26:A:1816:C:N4	28:C:34:GLU:OE2	2.33	0.62
5:e:54:GLU:HG2	5:e:56:PRO:HD2	1.82	0.62
17:q:58:VAL:HG23	17:q:77:VAL:HA	1.80	0.62
22:w:27:U:H4'	22:w:28:C:OP1	1.98	0.62
26:A:878:A:H3'	26:A:879:G:H8	1.64	0.62
1:a:54:C:H2'	1:a:352:C:H41	1.64	0.62
1:a:1318:A:H1'	19:s:36:ARG:HH21	1.65	0.62
6:f:15:SER:HA	6:f:18:VAL:HG23	1.82	0.62
11:k:75:GLU:C	11:k:77:GLY:H	2.08	0.62
26:A:839:U:H2'	26:A:840:C:C6	2.35	0.62
26:A:2867:G:O2'	26:A:2868:A:H8	1.82	0.62
9:i:20:ILE:HD11	9:i:60:LEU:HD13	1.81	0.62
19:s:30:LEU:HB2	19:s:48:ILE:HG22	1.81	0.62
4:d:115:GLN:NE2	4:d:119:HIS:HE1	1.93	0.61
26:A:2346:A:H3'	26:A:2347:C:C5'	2.30	0.61
48:W:33:ILE:HD11	48:W:78:ILE:HD11	1.82	0.61
57:5:53:ARG:HB3	57:5:55:VAL:HG13	1.82	0.61
8:h:28:SER:HB3	8:h:56:PRO:HB2	1.81	0.61
29:D:4:LEU:HD23	29:D:29:VAL:HG11	1.82	0.61
42:Q:70:GLN:C	42:Q:71:ASN:HD22	2.08	0.61
26:A:1026:G:H2'	26:A:1027:A:H8	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2786:U:H2'	26:A:2787:C:C6	2.35	0.61
26:A:1019:U:H3	26:A:1142:A:N6	1.98	0.61
1:a:1256:A:H1'	1:a:1258:G:C4	2.36	0.61
26:A:242:G:O2'	26:A:243:U:P	2.59	0.61
39:N:28:LEU:HD23	39:N:48:VAL:HG21	1.82	0.61
20:t:27:MET:HE1	20:t:66:ILE:HD11	1.83	0.61
41:P:59:THR:HG22	41:P:72:VAL:HG12	1.82	0.61
57:5:73:LYS:HB3	57:5:117:LEU:HD11	1.81	0.61
26:A:704:G:H1'	26:A:727:A:H61	1.64	0.61
26:A:2267:A:H5''	26:A:2268:A:H5'	1.83	0.61
26:A:2517:C:O3'	26:A:2518:A:H3'	2.00	0.61
38:M:21:ALA:HB1	38:M:100:LYS:HD3	1.83	0.61
25:z:116:ARG:HG2	25:z:156:LEU:HD21	1.82	0.61
26:A:1019:U:H2'	26:A:1020:A:H8	1.66	0.61
26:A:2655:G:O2'	26:A:2656:U:P	2.59	0.61
1:a:1064:G:H4'	1:a:1065:U:OP1	2.01	0.60
1:a:1225:A:H1'	19:s:77:ARG:HD2	1.83	0.60
8:h:86:LYS:HD2	8:h:90:GLU:HG2	1.83	0.60
1:a:113:G:H1'	1:a:354:G:H5'	1.82	0.60
10:j:7:ARG:HB3	10:j:101:SER:HB2	1.84	0.60
22:w:15:G:N2	22:w:21:A:N3	2.49	0.60
47:V:76:ASP:HB3	47:V:90:ASP:HB2	1.83	0.60
1:a:1305:G:O2'	1:a:1306:A:O5'	2.18	0.60
21:u:16:ARG:HH21	21:u:19:LYS:HE2	1.66	0.60
22:w:72:A:H4'	26:A:1852:U:C5'	2.30	0.60
22:w:76:A:O2'	26:A:2394:C:N3	2.29	0.60
26:A:1081:U:H4'	34:I:123:ALA:HB1	1.81	0.60
50:Y:24:GLU:O	50:Y:28:LEU:HB2	2.01	0.60
1:a:1432:G:H1'	1:a:1468:A:N6	2.16	0.60
26:A:1490:A:H62	28:C:73:ILE:HG23	1.67	0.60
1:a:399:G:H2'	1:a:400:C:C6	2.37	0.60
26:A:1086:A:N3	26:A:1086:A:H2'	2.17	0.60
29:D:54:ALA:HA	29:D:76:GLY:HA2	1.83	0.60
44:S:59:GLU:HA	44:S:64:ALA:HA	1.83	0.60
1:a:78:A:H2'	1:a:79:G:O4'	2.01	0.60
2:b:115:ASP:O	2:b:119:GLN:HG2	2.02	0.60
4:d:144:ILE:HD13	4:d:177:MET:HB3	1.83	0.60
7:g:67:ASN:HB3	7:g:129:ASN:HB3	1.81	0.60
26:A:2104:C:H2'	26:A:2105:U:C6	2.36	0.60
28:C:164:VAL:HG21	28:C:180:MET:HE1	1.83	0.60
47:V:4:ILE:HD13	47:V:47:VAL:HG22	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:173:ASP:C	4:d:175:GLY:H	2.10	0.60
7:g:87:PRO:HG3	7:g:148:LYS:HA	1.84	0.60
9:i:98:ARG:C	9:i:100:ALA:H	2.10	0.60
26:A:144:A:H4'	45:T:2:ILE:HD11	1.83	0.60
56:4:36:ARG:HG2	56:4:37:GLN:H	1.66	0.60
14:n:16:ALA:HA	14:n:55:SER:HA	1.82	0.60
1:a:222:C:H2'	1:a:223:A:H8	1.67	0.59
1:a:1399:C:H4'	1:a:1400:C:O5'	2.02	0.59
8:h:88:LYS:HE2	8:h:119:GLY:HA2	1.84	0.59
26:A:2271:G:H5'	48:W:16:ARG:HD3	1.84	0.59
2:b:70:GLY:HA3	2:b:79:VAL:HG21	1.85	0.59
20:t:80:ALA:O	20:t:84:LYS:HB2	2.01	0.59
26:A:100:U:H4'	26:A:101:A:O4'	2.01	0.59
26:A:2074:U:H2'	26:A:2075:U:C6	2.36	0.59
26:A:2427:C:H5'	26:A:2429:G:H5'	1.84	0.59
1:a:151:A:H2'	1:a:152:A:O4'	2.01	0.59
61:v:105:FME:O	26:A:2585:U:O2	2.20	0.59
3:c:19:SER:HB3	3:c:21:TRP:NE1	2.18	0.59
5:e:23:THR:HA	5:e:28:ARG:HA	1.85	0.59
12:l:98:ARG:HB2	12:l:116:TYR:HA	1.84	0.59
26:A:476:G:N1	26:A:479:A:OP2	2.36	0.59
30:E:1:MET:HE3	30:E:20:GLY:HA3	1.83	0.59
26:A:546:U:H2'	26:A:547:A:H4'	1.84	0.59
26:A:2557:G:H2'	26:A:2558:C:C6	2.38	0.59
4:d:119:HIS:N	4:d:119:HIS:HD2	2.00	0.59
15:o:87:ARG:HD3	15:o:88:ARG:H	1.67	0.59
26:A:434:U:O2'	26:A:436:C:N4	2.36	0.59
26:A:437:U:H2'	26:A:438:G:H8	1.67	0.59
26:A:1779:U:H5	26:A:1784:A:N7	2.01	0.59
26:A:2115:G:H4'	26:A:2166:U:O2	2.03	0.59
26:A:2238:G:H2'	26:A:2238:G:N3	2.17	0.59
1:a:345:C:OP1	41:P:38:ARG:NH2	2.35	0.59
1:a:1329:A:H5''	13:m:25:GLY:H	1.66	0.59
6:f:14:GLN:OE1	6:f:83:ALA:HA	2.02	0.59
22:w:117:U:O5'	22:w:117:U:H6	1.86	0.59
26:A:633:A:H2'	26:A:634:C:H5'	1.85	0.59
26:A:2267:A:H5''	26:A:2268:A:C5'	2.33	0.59
36:K:109:SER:O	36:K:111:LYS:N	2.35	0.59
22:w:18:G:H2'	22:w:19:G:C5'	2.32	0.59
26:A:271:G:H4'	26:A:272:A:OP1	2.03	0.59
26:A:639:U:H2'	26:A:640:C:C6	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1386:C:H2'	26:A:1387:A:C8	2.38	0.59
34:I:102:ARG:HA	34:I:129:GLU:OE2	2.03	0.59
29:D:121:THR:HG21	29:D:143:PRO:HB3	1.85	0.58
1:a:390:U:H4'	16:p:28:ARG:HH22	1.69	0.58
4:d:60:VAL:HG21	4:d:199:ILE:HD11	1.85	0.58
7:g:1:PRO:HG2	7:g:4:ARG:HB2	1.85	0.58
9:i:80:HIS:HE1	9:i:84:ARG:HH11	1.51	0.58
13:m:7:ASN:ND2	13:m:17:ALA:O	2.32	0.58
26:A:283:G:H1	26:A:357:C:H42	1.51	0.58
26:A:372:G:O2'	26:A:373:U:P	2.60	0.58
28:C:203:VAL:O	28:C:205:GLY:N	2.36	0.58
37:L:78:ARG:HB2	37:L:81:ASP:OD1	2.03	0.58
10:j:13:PHE:O	10:j:70:HIS:HE1	1.85	0.58
25:z:163:PRO:HB2	25:z:167:THR:HG23	1.85	0.58
26:A:847:U:O2	26:A:934:U:H1'	2.03	0.58
39:N:58:ASP:OD1	39:N:63:ARG:NH2	2.33	0.58
22:w:19:G:H2'	22:w:19:G:OP2	2.04	0.58
26:A:302:C:H2'	26:A:303:G:H8	1.69	0.58
45:T:13:ALA:HB3	45:T:33:LYS:HD3	1.85	0.58
1:a:1306:A:N6	1:a:1331:G:H1'	2.18	0.58
1:a:1464:U:H2'	1:a:1465:A:H8	1.69	0.58
26:A:770:G:H5''	54:2:10:LEU:HD23	1.86	0.58
22:w:1:C:H42	22:w:71:C:H42	1.49	0.58
28:C:244:VAL:HG12	28:C:250:GLN:HA	1.86	0.58
30:E:88:ARG:O	30:E:90:GLN:N	2.37	0.58
1:a:1129:C:H2'	1:a:1139:G:N7	2.19	0.58
26:A:2233:U:H2'	26:A:2234:G:C8	2.38	0.58
1:a:409:U:OP1	4:d:23:GLY:HA3	2.04	0.58
5:e:86:GLY:O	5:e:138:ALA:HB1	2.03	0.58
13:m:7:ASN:HB2	13:m:21:ILE:HG12	1.86	0.58
25:z:103:LEU:HD23	25:z:132:VAL:HG22	1.85	0.58
26:A:302:C:H2'	26:A:303:G:C8	2.39	0.58
26:A:2326:C:O2'	26:A:2327:A:OP1	2.20	0.58
26:A:2427:C:H5''	26:A:2428:G:OP1	2.03	0.58
39:N:69:ARG:O	39:N:71:ARG:N	2.28	0.58
22:w:13:C:H2'	22:w:14:A:C8	2.38	0.58
25:z:311:LEU:HB3	25:z:315:GLU:HB2	1.85	0.58
26:A:84:A:H4'	26:A:85:G:O5'	2.03	0.58
1:a:414:A:OP2	1:a:428:G:N2	2.29	0.58
3:c:179:ALA:HB1	3:c:202:PHE:HE1	1.68	0.58
19:s:30:LEU:H	19:s:48:ILE:HA	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:265:A:H4'	26:A:266:G:OP1	2.03	0.58
26:A:1956:U:H2'	26:A:1957:C:H5'	1.86	0.58
26:A:2305:U:H5''	31:F:130:GLY:HA3	1.85	0.58
26:A:2776:A:H4'	26:A:2777:G:O5'	2.04	0.58
1:a:327:A:O2'	1:a:328:C:H4'	2.04	0.57
3:c:84:GLU:HG3	3:c:87:ARG:HH22	1.68	0.57
7:g:144:ALA:O	7:g:146:ALA:N	2.36	0.57
17:q:18:LYS:HG2	17:q:46:HIS:HE1	1.68	0.57
25:z:219:SER:HB2	25:z:283:ARG:HD3	1.86	0.57
26:A:2591:C:H2'	26:A:2592:G:C8	2.39	0.57
30:E:117:ARG:HH12	37:L:2:ARG:HG2	1.68	0.57
1:a:1130:A:N6	1:a:1144:G:H1'	2.14	0.57
1:a:1207:2MG:H8	1:a:1207:2MG:H5''	1.69	0.57
25:z:212:LEU:HD12	25:z:231:VAL:HG22	1.84	0.57
26:A:479:A:H4'	26:A:480:A:OP1	2.03	0.57
26:A:686:U:O2'	54:2:5:PHE:HA	2.05	0.57
30:E:88:ARG:HD3	30:E:89:PRO:HD2	1.86	0.57
39:N:45:ARG:HG2	39:N:95:THR:HG21	1.86	0.57
44:S:3:THR:HG21	44:S:58:ALA:HB2	1.87	0.57
22:w:18:G:C2'	22:w:19:G:C5'	2.82	0.57
25:z:339:GLY:HA2	25:z:362:LEU:HA	1.86	0.57
26:A:1055:G:O2'	26:A:1084:A:N6	2.36	0.57
31:F:141:ASP:HB2	31:F:144:LYS:HD3	1.85	0.57
36:K:121:GLU:HG2	36:K:122:VAL:HG23	1.86	0.57
37:L:132:ARG:HG3	37:L:142:ILE:HD12	1.86	0.57
49:X:17:ARG:NE	49:X:23:ALA:HB2	2.11	0.57
1:a:690:G:O6	11:k:52:ARG:NH2	2.38	0.57
5:e:149:PRO:HA	5:e:152:VAL:HG22	1.87	0.57
26:A:172:A:H2'	26:A:173:A:C8	2.40	0.57
26:A:466:A:OP1	54:2:34:ARG:NH1	2.37	0.57
26:A:2391:G:H2'	26:A:2424:C:N4	2.20	0.57
31:F:134:GLN:CD	31:F:134:GLN:H	2.12	0.57
41:P:29:VAL:HG22	41:P:80:VAL:HA	1.85	0.57
1:a:244:U:O4	1:a:906:A:H1'	2.05	0.57
6:f:32:ALA:HB2	6:f:70:VAL:HG11	1.86	0.57
9:i:18:VAL:HG22	9:i:64:ILE:HG23	1.86	0.57
26:A:2339:C:H2'	26:A:2340:A:C8	2.39	0.57
1:a:792:A:H4'	1:a:793:U:O5'	2.05	0.57
1:a:1297:G:HO2'	1:a:1298:U:P	2.28	0.57
4:d:101:VAL:HG13	4:d:106:PHE:HB2	1.86	0.57
7:g:137:ARG:NH1	7:g:141:HIS:HE1	2.02	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:42:GLU:HG2	8:h:100:ILE:HG12	1.85	0.57
10:j:57:VAL:HG22	10:j:58:ASN:H	1.69	0.57
22:v:22:A:H61	22:v:47:A:H2'	1.68	0.57
26:A:495:G:H1'	44:S:57:ASN:OD1	2.04	0.57
26:A:2285:C:OP2	53:1:5:ARG:NH1	2.37	0.57
26:A:2554:U:H2'	26:A:2555:U:C6	2.39	0.57
30:E:148:ILE:O	30:E:169:VAL:HA	2.04	0.57
1:a:1200:C:H5''	1:a:1201:A:H3'	1.87	0.57
19:s:15:LEU:O	19:s:19:GLU:HG2	2.05	0.57
20:t:26:MET:HE1	20:t:56:ILE:HG12	1.86	0.57
26:A:1614:A:N1	44:S:93:ALA:HB2	2.20	0.57
30:E:3:LEU:HD13	30:E:120:VAL:HG21	1.85	0.57
55:3:30:HIS:ND1	55:3:31:ILE:HG13	2.18	0.57
1:a:599:C:H2'	1:a:600:A:H8	1.68	0.57
19:s:10:ILE:HG12	19:s:40:PHE:HE2	1.70	0.57
26:A:2328:A:H2'	26:A:2329:U:C6	2.39	0.57
26:A:2867:G:O2'	26:A:2868:A:C8	2.57	0.57
54:2:24:THR:HG23	54:2:27:GLY:H	1.70	0.57
57:5:56:ARG:HD3	57:5:81:LEU:HD21	1.87	0.57
1:a:310:G:H5''	16:p:31:ARG:HB2	1.86	0.57
2:b:153:MET:HG2	2:b:155:GLY:H	1.69	0.57
22:w:76:A:H1'	26:A:2395:C:C2	2.39	0.57
26:A:859:G:O2'	26:A:860:U:OP2	2.23	0.57
26:A:1019:U:H2'	26:A:1020:A:C8	2.40	0.57
41:P:31:VAL:HG13	41:P:38:ARG:HB3	1.86	0.57
54:2:12:ARG:NE	54:2:44:VAL:HG21	2.19	0.57
7:g:68:VAL:HG23	7:g:99:ALA:HB1	1.87	0.57
21:u:28:LEU:C	21:u:30:GLU:H	2.12	0.57
26:A:861:A:H2'	26:A:862:G:O4'	2.05	0.57
1:a:1038:C:H2'	1:a:1039:G:C8	2.40	0.56
5:e:80:LEU:HD13	5:e:122:VAL:HG11	1.87	0.56
11:k:17:ASP:HA	11:k:78:ILE:HG23	1.87	0.56
24:y:3:C:H42	24:y:70:G:H1	1.53	0.56
25:z:19:HIS:CD2	25:z:114:GLN:HB2	2.40	0.56
32:G:41:GLU:HA	32:G:54:ARG:HH21	1.69	0.56
34:I:135:MET:HB2	34:I:137:LEU:HG	1.85	0.56
36:K:40:LYS:NZ	36:K:89:ASN:OD1	2.38	0.56
57:5:34:THR:O	57:5:37:LYS:HB3	2.05	0.56
2:b:16:GLY:O	2:b:17:HIS:HB2	2.05	0.56
3:c:63:ILE:O	3:c:98:ALA:HA	2.06	0.56
4:d:103:ARG:HH12	4:d:110:ARG:HH12	1.51	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:394:C:H2'	26:A:395:U:O4'	2.05	0.56
47:V:42:LEU:HD13	47:V:47:VAL:HG21	1.86	0.56
57:5:27:VAL:HG13	57:5:83:ALA:HB3	1.87	0.56
1:a:1464:U:H2'	1:a:1465:A:C8	2.40	0.56
13:m:2:ARG:HD3	31:F:109:ARG:HH22	1.69	0.56
25:z:208:LYS:HD2	25:z:233:ARG:HH21	1.70	0.56
31:F:116:LEU:HB2	31:F:175:PRO:HB2	1.87	0.56
34:I:74:PRO:HG2	34:I:77:VAL:HG22	1.87	0.56
35:J:102:GLU:HG3	35:J:119:PHE:HZ	1.69	0.56
50:Y:2:LYS:HB3	50:Y:52:ARG:HD3	1.87	0.56
2:b:202:ASN:ND2	2:b:203:ASP:H	2.04	0.56
26:A:289:G:H2'	26:A:290:U:O4'	2.04	0.56
26:A:2518:A:H2'	26:A:2518:A:N3	2.20	0.56
1:a:1256:A:H1'	1:a:1258:G:C5	2.41	0.56
1:a:1346:A:H1'	1:a:1348:U:C2	2.40	0.56
5:e:92:ARG:HB2	5:e:127:TYR:HB2	1.87	0.56
22:w:76:A:O2'	26:A:2394:C:C2	2.58	0.56
26:A:630:G:N2	26:A:633:A:OP2	2.34	0.56
26:A:704:G:C2'	26:A:726:G:H22	2.14	0.56
26:A:1111:A:O2'	26:A:1112:G:OP1	2.22	0.56
26:A:1869:G:H1'	26:A:1872:A:N6	2.20	0.56
37:L:14:LYS:O	37:L:16:GLY:N	2.39	0.56
1:a:1059:C:O3'	14:n:85:ARG:NH2	2.39	0.56
13:m:33:LEU:HD23	13:m:40:GLU:HA	1.88	0.56
20:t:14:GLU:HA	20:t:17:ARG:HG2	1.87	0.56
26:A:2283:C:OP2	26:A:2390:U:H5	1.89	0.56
15:o:44:GLU:O	15:o:46:LYS:N	2.37	0.56
26:A:1283:G:H1'	26:A:1329:U:O2	2.05	0.56
26:A:2644:G:H2'	26:A:2645:G:H5'	1.86	0.56
39:N:34:ILE:HG13	39:N:113:ILE:HG23	1.88	0.56
22:w:10:G:N1	22:w:25:C:N3	2.46	0.56
26:A:1199:U:H1'	42:Q:3:VAL:HG22	1.88	0.56
26:A:1315:C:H2'	26:A:1316:U:H6	1.71	0.56
26:A:2297:A:N1	26:A:2321:U:H5	2.03	0.56
39:N:44:LEU:HD23	39:N:113:ILE:HD13	1.87	0.56
1:a:1016:A:HO2'	1:a:1217:C:HO2'	1.52	0.56
10:j:22:THR:HG21	10:j:39:PRO:HB3	1.86	0.56
22:w:23:C:H2'	22:w:24:U:C6	2.41	0.56
22:w:37:A:H5''	22:w:38:A:OP2	2.05	0.56
25:z:140:VAL:HB	25:z:146:LEU:HD21	1.87	0.56
26:A:162:U:O2'	26:A:163:C:H5'	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:290:U:H2'	26:A:291:G:C8	2.41	0.56
35:J:36:LEU:O	35:J:51:GLY:HA3	2.05	0.56
1:a:109:A:C6	1:a:326:G:C6	2.94	0.56
1:a:1005:A:H2'	1:a:1006:G:O4'	2.06	0.56
1:a:1169:A:H2'	1:a:1170:A:C8	2.41	0.56
1:a:1422:G:H5'	36:K:48:PRO:HG3	1.88	0.56
26:A:204:A:H4'	26:A:205:G:OP1	2.06	0.56
28:C:154:ALA:HB2	28:C:161:VAL:HG23	1.88	0.56
44:S:56:ALA:HA	44:S:59:GLU:HG2	1.87	0.56
57:5:37:LYS:HG3	57:5:41:LEU:HD12	1.88	0.56
1:a:86:G:H5''	1:a:87:C:OP1	2.06	0.55
6:f:36:ILE:HD12	6:f:64:VAL:HB	1.88	0.55
26:A:1858:A:N6	26:A:1884:G:O2'	2.38	0.55
26:A:2341:G:H2'	26:A:2342:C:O4'	2.07	0.55
27:B:118:C:H2'	27:B:119:A:H8	1.70	0.55
36:K:21:CYS:HA	36:K:41:ILE:HG22	1.87	0.55
6:f:40:GLU:OE2	6:f:100:SER:HB2	2.06	0.55
26:A:1251:C:OP2	42:Q:5:ARG:HD2	2.06	0.55
26:A:2648:G:H2'	26:A:2649:C:O4'	2.06	0.55
56:4:37:GLN:HG3	56:4:38:GLY:H	1.71	0.55
1:a:1428:A:H2'	1:a:1429:A:O4'	2.06	0.55
6:f:13:ASP:OD1	6:f:14:GLN:N	2.38	0.55
20:t:67:HIS:O	20:t:67:HIS:ND1	2.39	0.55
26:A:1040:A:H2	26:A:1115:G:H22	1.54	0.55
2:b:65:LYS:HD2	2:b:153:MET:HG3	1.87	0.55
9:i:83:THR:HG21	9:i:102:PHE:HB3	1.87	0.55
26:A:468:G:H2'	26:A:469:G:H5'	1.88	0.55
26:A:1222:U:H2'	26:A:1223:G:C8	2.40	0.55
1:a:767:A:H2'	1:a:768:A:O4'	2.07	0.55
2:b:46:VAL:HA	2:b:49:PHE:CE2	2.41	0.55
4:d:195:ASN:OD1	4:d:197:HIS:HB3	2.07	0.55
5:e:37:VAL:HG11	5:e:113:VAL:HG23	1.88	0.55
22:w:18:G:N2	22:w:58:A:O4'	2.40	0.55
26:A:301:G:H4'	26:A:302:C:OP1	2.04	0.55
26:A:368:A:H2'	26:A:369:U:O4'	2.06	0.55
38:M:11:LYS:HD2	38:M:86:LYS:HG2	1.88	0.55
57:5:29:ASP:HB2	57:5:56:ARG:HH12	1.71	0.55
1:a:1318:A:H2'	1:a:1319:A:H5'	1.89	0.55
3:c:38:VAL:HG11	3:c:94:ALA:HB2	1.89	0.55
16:p:6:LEU:HB3	16:p:17:TYR:HB3	1.88	0.55
25:z:135:ASN:HD21	25:z:174:ALA:HB2	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:z:231:VAL:HB	25:z:270:ALA:HA	1.89	0.55
26:A:1689:A:H2'	26:A:1690:A:C8	2.41	0.55
26:A:1847:G:H21	26:A:1848:A:H62	1.54	0.55
26:A:493:G:H2'	26:A:494:G:O4'	2.07	0.55
26:A:851:C:H2'	26:A:852:U:C6	2.42	0.55
26:A:1179:G:C4	26:A:1180:U:H1'	2.42	0.55
26:A:2469:A:N6	26:A:2481:G:O2'	2.40	0.55
1:a:981:U:H4'	14:n:61:ARG:HG2	1.89	0.55
4:d:28:ASP:CG	4:d:29:THR:H	2.15	0.55
25:z:144:GLU:O	25:z:148:LEU:HB2	2.06	0.55
26:A:1396:U:H5''	26:A:1397:U:OP2	2.06	0.55
1:a:28:A:O2'	1:a:296:U:OP1	2.23	0.55
1:a:1137:C:O2'	1:a:1138:G:N2	2.40	0.55
1:a:1178:G:O2'	1:a:1180:A:N7	2.38	0.55
1:a:1512:U:H2'	1:a:1513:A:C8	2.41	0.55
3:c:20:THR:HB	3:c:57:GLU:HG2	1.88	0.55
6:f:32:ALA:HB1	6:f:67:PRO:HD2	1.87	0.55
26:A:107:G:H2'	26:A:108:G:C8	2.41	0.55
26:A:1857:G:H2'	26:A:1884:G:N2	2.21	0.55
28:C:162:GLN:OE1	28:C:174:ARG:NH2	2.40	0.55
22:w:15:G:C2'	22:w:59:A:H61	2.18	0.55
22:w:22:G:H8	22:w:22:G:OP2	1.89	0.55
26:A:2345:G:H4'	26:A:2346:A:C5'	2.36	0.55
1:a:495:A:H4'	1:a:496:A:OP1	2.07	0.54
1:a:950:U:H2'	1:a:951:G:C8	2.43	0.54
1:a:1144:G:H21	1:a:1146:A:H62	1.53	0.54
19:s:20:LYS:HA	19:s:23:GLU:HG2	1.89	0.54
20:t:23:ARG:O	20:t:26:MET:HG3	2.07	0.54
26:A:712:G:H2'	26:A:713:G:H5'	1.88	0.54
26:A:1434:A:H2'	26:A:1435:G:C8	2.42	0.54
26:A:1434:A:H2'	26:A:1435:G:H8	1.71	0.54
18:r:40:PRO:HB2	18:r:42:ARG:HG2	1.88	0.54
22:w:4:G:H5'	22:w:5:G:OP2	2.07	0.54
26:A:1330:C:O2'	26:A:1331:G:H5'	2.07	0.54
33:H:84:ALA:HA	33:H:91:PHE:H	1.73	0.54
35:J:80:HIS:C	35:J:82:GLY:H	2.13	0.54
17:q:51:GLU:H	17:q:51:GLU:CD	2.15	0.54
26:A:542:C:H3'	26:A:543:G:H5''	1.89	0.54
31:F:39:VAL:HG12	31:F:85:GLY:HA2	1.89	0.54
34:I:33:ASN:HB2	34:I:64:ARG:HH12	1.72	0.54
1:a:575:G:O2'	1:a:821:G:H5'	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:54:LEU:O	4:d:58:GLN:HG2	2.08	0.54
5:e:133:ILE:H	5:e:133:ILE:HD12	1.72	0.54
20:t:24:ARG:HG2	20:t:28:ARG:NH2	2.22	0.54
26:A:1028:A:H61	26:A:1125:G:H2'	1.71	0.54
26:A:1130:U:O2'	26:A:1131:G:OP1	2.26	0.54
26:A:1297:C:O2'	26:A:1302:A:N1	2.36	0.54
26:A:2725:A:O2'	26:A:2726:A:O5'	2.16	0.54
26:A:277:G:H1'	26:A:361:G:H1	1.71	0.54
26:A:373:U:O2'	26:A:423:A:H1'	2.07	0.54
26:A:841:G:H2'	26:A:842:U:H6	1.71	0.54
26:A:947:A:O2'	26:A:984:A:H2	1.91	0.54
26:A:969:G:H2'	26:A:970:U:C6	2.41	0.54
26:A:1405:U:H2'	26:A:1406:U:C6	2.42	0.54
26:A:1548:A:H2'	26:A:1549:A:C8	2.42	0.54
46:U:14:THR:OG1	46:U:68:ASN:ND2	2.38	0.54
1:a:210:C:H4'	1:a:211:G:C2	2.42	0.54
4:d:57:LYS:HD3	4:d:202:LEU:HD22	1.90	0.54
7:g:12:LEU:HD12	7:g:13:PRO:HD2	1.89	0.54
26:A:1794:A:H2'	26:A:1795:C:C6	2.42	0.54
1:a:144:G:H2'	1:a:145:G:O4'	2.07	0.54
22:w:18:G:N3	22:w:58:A:H5'	2.22	0.54
58:6:56:ARG:O	58:6:59:ARG:HB3	2.08	0.54
1:a:1064:G:H1'	1:a:1190:G:H21	1.73	0.54
1:a:1118:U:H2'	1:a:1119:C:H6	1.71	0.54
2:b:117:GLU:HA	2:b:140:LEU:HD11	1.88	0.54
17:q:61:ARG:HH12	17:q:73:THR:HB	1.72	0.54
19:s:52:ASN:HD21	19:s:55:GLN:HB2	1.73	0.54
20:t:61:ALA:HA	20:t:66:ILE:HB	1.90	0.54
26:A:265:A:H1'	26:A:266:G:O4'	2.08	0.54
26:A:747:5MC:CM5	26:A:2612:C:H4'	2.38	0.54
26:A:1565:C:O2'	26:A:1566:A:H2'	2.07	0.54
26:A:2576:G:H8	26:A:2581:G:O6	1.90	0.54
29:D:49:GLN:HA	29:D:80:TRP:O	2.07	0.54
57:5:88:HIS:HB2	57:5:89:PRO:HD3	1.89	0.54
57:5:114:GLU:HA	57:5:123:ILE:HB	1.90	0.54
1:a:1477:U:H2'	1:a:1478:U:C6	2.43	0.54
25:z:7:ARG:HH22	25:z:269:ARG:HB2	1.72	0.54
26:A:1021:A:N3	26:A:1022:G:H5''	2.22	0.54
26:A:1565:C:O2'	26:A:1566:A:C8	2.60	0.54
29:D:1:MET:HG2	29:D:205:PRO:HG2	1.88	0.54
38:M:74:THR:HA	38:M:89:VAL:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:5:37:LYS:O	57:5:41:LEU:HB2	2.08	0.54
2:b:33:ALA:HB3	2:b:37:VAL:O	2.08	0.53
11:k:87:GLY:N	11:k:113:THR:HG22	2.22	0.53
22:w:1:C:H2'	22:w:2:G:O4'	2.07	0.53
22:w:70:G:H5'	22:w:71:C:OP2	2.08	0.53
26:A:549:G:O2'	26:A:550:C:OP1	2.26	0.53
26:A:743:A:OP1	29:D:135:GLY:HA2	2.08	0.53
22:w:65:C:H2'	22:w:66:C:C6	2.43	0.53
26:A:468:G:N7	54:2:39:ARG:NH2	2.56	0.53
26:A:1410:G:H2'	26:A:1411:U:C6	2.43	0.53
26:A:2832:U:H1'	26:A:2834:G:C4	2.43	0.53
26:A:2852:G:H2'	26:A:2853:C:O4'	2.08	0.53
29:D:114:LYS:HE3	29:D:196:ALA:HB2	1.90	0.53
34:I:11:GLN:NE2	34:I:54:ILE:O	2.41	0.53
37:L:122:VAL:HB	37:L:142:ILE:HG23	1.89	0.53
1:a:695:A:H2'	1:a:696:A:C8	2.44	0.53
5:e:157:GLY:O	5:e:158:LYS:HB2	2.07	0.53
9:i:49:GLN:C	9:i:51:LEU:H	2.16	0.53
22:w:20:H2U:O5'	26:A:2112:G:N2	2.41	0.53
26:A:468:G:C2'	26:A:469:G:H5'	2.39	0.53
26:A:1177:G:H2'	26:A:1178:C:O4'	2.09	0.53
26:A:2884:U:H3	52:0:39:ARG:CZ	2.22	0.53
39:N:79:LEU:C	39:N:81:ASN:H	2.16	0.53
40:O:49:VAL:HG21	40:O:82:ALA:HA	1.91	0.53
57:5:57:ASN:HB2	57:5:62:ARG:HD2	1.91	0.53
1:a:1207:2MG:H2'	1:a:1208:C:O4'	2.09	0.53
6:f:5:GLU:HA	6:f:63:ASN:HA	1.90	0.53
18:r:70:THR:HG23	18:r:71:ASP:H	1.73	0.53
22:w:20:H2U:C5	26:A:2112:G:H1'	2.39	0.53
26:A:760:G:H2'	26:A:761:A:O4'	2.09	0.53
26:A:1266:G:O2'	26:A:2012:G:N1	2.38	0.53
38:M:28:PHE:HB2	38:M:104:GLU:OE1	2.08	0.53
50:Y:23:ARG:O	50:Y:25:GLN:N	2.41	0.53
1:a:82:G:N2	1:a:87:C:N3	2.56	0.53
1:a:1432:G:H1'	1:a:1468:A:H62	1.72	0.53
61:v:105:FME:CN	26:A:2506:U:O4	2.56	0.53
25:z:260:MET:HB2	25:z:265:LEU:HD11	1.91	0.53
26:A:2678:C:H2'	26:A:2679:A:O4'	2.09	0.53
26:A:2746:U:H1'	32:G:138:GLN:HE22	1.72	0.53
22:w:2:G:C6	22:w:71:C:N4	2.77	0.53
26:A:1011:G:HO2'	26:A:1013:C:H5''	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1332:G:H5''	26:A:1332:G:N3	2.24	0.53
26:A:2114:A:N6	26:A:2117:A:H62	2.05	0.53
38:M:34:LYS:HE3	38:M:131:VAL:HG11	1.91	0.53
40:O:51:ALA:HB3	40:O:78:VAL:HG22	1.91	0.53
54:2:1:MET:HE1	54:2:3:ARG:CZ	2.38	0.53
57:5:57:ASN:HD22	57:5:63:ALA:HB2	1.74	0.53
1:a:381:C:H2'	1:a:382:A:O4'	2.09	0.53
1:a:1318:A:C1'	19:s:36:ARG:HH21	2.21	0.53
2:b:166:ASP:HB2	2:b:190:SER:HA	1.89	0.53
8:h:46:GLU:O	8:h:61:THR:HB	2.08	0.53
13:m:15:VAL:HG13	13:m:33:LEU:HD22	1.91	0.53
26:A:1028:A:N3	26:A:2486:C:O2'	2.42	0.53
26:A:1203:U:H1'	37:L:4:ASN:HB3	1.90	0.53
26:A:2126:A:N1	26:A:2163:A:H1'	2.24	0.53
1:a:158:G:H2'	1:a:159:G:H8	1.74	0.53
1:a:1320:C:H4'	19:s:72:GLU:OE2	2.09	0.53
26:A:784:G:O2'	26:A:785:G:H5''	2.09	0.53
26:A:1475:G:O2'	26:A:1476:U:OP2	2.27	0.53
1:a:458:U:H2'	1:a:459:A:C8	2.43	0.53
2:b:12:GLY:HA3	2:b:207:ARG:HD3	1.91	0.53
1:a:358:U:H2'	1:a:359:G:C8	2.44	0.53
26:A:2756:U:H5''	56:4:19:ARG:HA	1.90	0.53
26:A:2879:A:H8	26:A:2881:U:O4	1.92	0.53
1:a:389:A:H3'	1:a:390:U:H6	1.73	0.52
1:a:429:U:H3	1:a:431:A:H62	1.57	0.52
8:h:10:LEU:HD12	8:h:76:ARG:HB2	1.91	0.52
12:l:43:LYS:HB3	12:l:44:PRO:HD3	1.91	0.52
26:A:390:U:H4'	26:A:391:A:O5'	2.08	0.52
26:A:844:A:H61	26:A:934:U:H3	1.56	0.52
26:A:2258:C:O2'	26:A:2426:A:H4'	2.09	0.52
26:A:2346:A:H3'	26:A:2347:C:H5'	1.91	0.52
26:A:2497:A:N3	26:A:2498:OMC:N4	2.55	0.52
44:S:14:ALA:O	44:S:18:ARG:HB2	2.08	0.52
1:a:660:C:H2'	1:a:661:G:O4'	2.09	0.52
2:b:165:ALA:HB3	2:b:190:SER:HB3	1.90	0.52
20:t:9:ARG:O	20:t:13:SER:HB3	2.08	0.52
22:w:14:A:H3'	22:w:15:G:H8	1.71	0.52
24:y:76:A:C4	25:z:259:GLU:HG3	2.44	0.52
25:z:329:GLN:HE21	25:z:329:GLN:CA	2.22	0.52
26:A:321:U:H5''	30:E:131:THR:HG23	1.91	0.52
36:K:33:ALA:HB1	36:K:37:ASP:HB2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:O:69:ASP:OD1	40:O:69:ASP:N	2.42	0.52
9:i:89:TYR:HB2	9:i:93:LEU:HD11	1.91	0.52
22:w:76:A:C4	26:A:2421:G:C2	2.98	0.52
22:w:76:A:C1'	26:A:2395:C:O2	2.57	0.52
26:A:910:A:H2'	26:A:911:A:C8	2.44	0.52
27:B:41:G:H2'	27:B:41:G:N3	2.24	0.52
1:a:715:A:H2'	1:a:716:A:C8	2.44	0.52
1:a:1157:A:N6	1:a:1178:G:H1'	2.25	0.52
2:b:65:LYS:O	2:b:158:ASP:N	2.40	0.52
2:b:178:LEU:O	2:b:180:ILE:N	2.40	0.52
11:k:82:GLU:HG3	11:k:108:ASN:OD1	2.09	0.52
13:m:90:HIS:CE1	13:m:96:VAL:HG21	2.44	0.52
19:s:18:VAL:HG11	19:s:43:MET:HG2	1.90	0.52
26:A:32:C:N4	26:A:446:G:O2'	2.43	0.52
26:A:884:U:H2'	26:A:885:C:O4'	2.09	0.52
26:A:2514:U:H2'	26:A:2515:C:C6	2.45	0.52
30:E:143:LEU:HB3	30:E:146:VAL:HG11	1.91	0.52
1:a:1039:G:H2'	1:a:1040:U:C6	2.45	0.52
7:g:62:GLU:O	7:g:64:ALA:N	2.38	0.52
22:v:64:G:H2'	22:v:65:G:H8	1.74	0.52
22:w:15:G:OP2	22:w:16:C:H5	1.93	0.52
22:w:18:G:O2'	22:w:19:G:O5'	2.28	0.52
26:A:677:A:O2'	26:A:2071:A:H5'	2.10	0.52
31:F:110:ILE:O	31:F:113:PHE:HB2	2.10	0.52
37:L:24:GLY:C	37:L:26:GLY:H	2.17	0.52
41:P:48:ALA:HB3	41:P:59:THR:OG1	2.09	0.52
1:a:958:A:C4	19:s:54:ARG:HD3	2.44	0.52
2:b:56:LEU:HD13	2:b:216:VAL:HG13	1.92	0.52
11:k:12:ARG:O	11:k:14:GLN:N	2.36	0.52
15:o:62:ARG:HH22	26:A:715:A:H4'	1.75	0.52
26:A:1701:A:C2'	26:A:1702:G:H5'	2.40	0.52
26:A:1796:U:H2'	26:A:1797:G:C8	2.44	0.52
26:A:1962:5MC:O2'	26:A:1964:G:OP2	2.28	0.52
29:D:49:GLN:NE2	29:D:67:HIS:NE2	2.52	0.52
30:E:97:ASN:HB2	30:E:100:MET:HG3	1.92	0.52
30:E:148:ILE:HB	30:E:169:VAL:HG22	1.92	0.52
47:V:30:ILE:HD11	47:V:63:ILE:HD12	1.92	0.52
47:V:76:ASP:OD1	47:V:77:VAL:N	2.41	0.52
1:a:413:G:HO2'	1:a:414:A:P	2.32	0.52
22:w:9:G:H1'	22:w:45:G:H2'	1.90	0.52
22:w:31:G:C2'	22:w:32:C:H5'	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1112:G:H2'	26:A:1113:U:C6	2.45	0.52
26:A:1682:G:C4	26:A:1757:A:H1'	2.45	0.52
26:A:2788:C:O2'	26:A:2809:A:N3	2.43	0.52
26:A:2809:A:H2'	26:A:2810:A:C8	2.45	0.52
31:F:126:ASN:OD1	31:F:156:THR:HG23	2.10	0.52
48:W:33:ILE:HG22	48:W:34:VAL:HG23	1.92	0.52
1:a:1347:G:O2'	1:a:1348:U:P	2.68	0.52
2:b:33:ALA:HB2	2:b:39:ILE:HG13	1.92	0.52
3:c:19:SER:HB2	14:n:92:GLU:O	2.10	0.52
25:z:376:ILE:O	25:z:383:VAL:HB	2.09	0.52
26:A:1930:G:HO2'	26:A:1931:U:P	2.31	0.52
26:A:2296:U:H4'	26:A:2297:A:OP1	2.08	0.52
26:A:2406:A:H5'	26:A:2407:A:OP1	2.10	0.52
27:B:104:A:H2'	27:B:105:G:O4'	2.09	0.52
38:M:41:LEU:HD22	38:M:124:LEU:HD22	1.92	0.52
45:T:70:HIS:O	45:T:72:GLN:N	2.43	0.52
52:0:54:ILE:HG23	52:0:56:LYS:H	1.74	0.52
1:a:8:A:H62	4:d:204:SER:HB2	1.74	0.52
1:a:720:C:H5''	18:r:40:PRO:HB3	1.91	0.52
1:a:1077:G:N2	1:a:1080:A:OP2	2.38	0.52
9:i:29:ILE:HA	9:i:64:ILE:O	2.10	0.52
19:s:13:HIS:O	19:s:17:LYS:HB2	2.09	0.52
24:y:65:G:H2'	24:y:66:U:C6	2.45	0.52
26:A:542:C:C3'	26:A:543:G:H5''	2.40	0.52
26:A:1088:A:H61	34:I:134:SER:HB3	1.75	0.52
40:O:89:ASP:HA	40:O:116:GLN:O	2.10	0.52
3:c:5:HIS:HB3	14:n:89:MET:HE3	1.92	0.52
7:g:78:ARG:HB3	7:g:83:THR:HG23	1.92	0.52
26:A:259:G:O2'	26:A:260:G:H5'	2.10	0.52
26:A:2391:G:O2'	26:A:2392:A:O5'	2.23	0.52
1:a:438:U:O2'	1:a:439:U:O5'	2.28	0.51
3:c:171:ARG:HG2	3:c:173:PRO:HD3	1.92	0.51
6:f:11:HIS:O	6:f:15:SER:N	2.42	0.51
22:w:18:G:C2	22:w:58:A:O4'	2.63	0.51
25:z:118:HIS:O	25:z:122:GLY:N	2.36	0.51
25:z:282:LYS:HB2	25:z:285:GLU:HG2	1.91	0.51
26:A:2230:G:H5''	49:X:29:LEU:HD12	1.92	0.51
40:O:53:THR:HG23	40:O:74:VAL:HG21	1.92	0.51
54:2:34:ARG:HH21	54:2:39:ARG:HD3	1.74	0.51
1:a:376:G:H5''	16:p:5:ARG:HB2	1.92	0.51
1:a:604:G:H2'	1:a:605:U:O4'	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:48:SER:O	4:d:51:GLY:N	2.43	0.51
26:A:192:C:OP1	66:A:3301:HOH:O	2.19	0.51
26:A:722:A:H2'	26:A:723:C:O4'	2.10	0.51
26:A:1645:G:H5''	26:A:1646:C:H5'	1.91	0.51
27:B:28:C:H2'	27:B:29:A:C8	2.45	0.51
48:W:74:LYS:H	48:W:74:LYS:HD2	1.75	0.51
14:n:26:LEU:HD23	14:n:30:ILE:HD12	1.92	0.51
26:A:1239:G:H2'	26:A:1240:U:O4'	2.10	0.51
26:A:2591:C:H2'	26:A:2592:G:H8	1.75	0.51
26:A:2808:G:HO2'	26:A:2809:A:H8	1.56	0.51
44:S:4:ILE:HD12	44:S:6:LYS:HE3	1.92	0.51
1:a:405:U:H3'	1:a:406:G:H5'	1.93	0.51
3:c:69:THR:HG21	3:c:75:VAL:HG21	1.93	0.51
4:d:47:LEU:HG	4:d:52:VAL:HG12	1.92	0.51
16:p:26:ASN:HD22	16:p:26:ASN:N	2.09	0.51
20:t:43:LYS:HD2	20:t:86:ALA:HA	1.92	0.51
26:A:413:C:H2'	26:A:414:C:C6	2.44	0.51
26:A:1509:A:H2'	26:A:1510:G:C8	2.45	0.51
26:A:2262:U:O2'	26:A:2263:C:H5'	2.10	0.51
58:6:58:ASP:O	58:6:62:LYS:HG3	2.11	0.51
1:a:82:G:H2'	1:a:83:C:O4'	2.11	0.51
2:b:105:THR:O	2:b:108:GLN:HG2	2.10	0.51
17:q:45:VAL:HG21	17:q:60:ILE:HD13	1.91	0.51
26:A:642:U:H2'	26:A:644:A:OP2	2.10	0.51
26:A:2625:G:H2'	26:A:2626:C:O4'	2.10	0.51
30:E:31:VAL:HG21	30:E:104:ALA:HB2	1.91	0.51
34:I:25:PRO:O	34:I:29:GLN:HB2	2.11	0.51
35:J:36:LEU:HD22	35:J:121:LYS:HB2	1.92	0.51
3:c:152:VAL:HG12	3:c:197:VAL:HG13	1.92	0.51
17:q:18:LYS:HG2	17:q:46:HIS:CE1	2.46	0.51
25:z:84[B]:HIS:HB2	25:z:87:TYR:HD2	1.76	0.51
26:A:2303:G:H2'	26:A:2304:G:O4'	2.10	0.51
26:A:2405:G:HO2'	26:A:2406:A:P	2.33	0.51
30:E:170:ARG:NH2	30:E:176:ASP:OD1	2.44	0.51
31:F:141:ASP:O	31:F:143:ASP:N	2.44	0.51
33:H:70:GLU:HB2	33:H:134:VAL:HG21	1.91	0.51
57:5:48:ALA:HB3	57:5:51:TYR:CE2	2.45	0.51
57:5:48:ALA:HB3	57:5:51:TYR:HE2	1.75	0.51
3:c:42:LEU:HD13	3:c:90:VAL:HG21	1.92	0.51
24:y:29:G:H2'	24:y:30:G:H8	1.75	0.51
26:A:948:C:H2'	26:A:949:G:C8	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:133:THR:HG23	29:D:134:HIS:N	2.26	0.51
31:F:39:VAL:O	31:F:41:GLU:HG2	2.11	0.51
38:M:102:LEU:HD11	38:M:126:ILE:HD11	1.91	0.51
1:a:28:A:H2'	1:a:29:U:O4'	2.11	0.51
6:f:43:GLY:HA2	6:f:58:HIS:CE1	2.46	0.51
10:j:30:LYS:O	10:j:34:ALA:HA	2.10	0.51
16:p:36:VAL:HG23	16:p:53:ASP:HB3	1.91	0.51
21:u:13:VAL:HG13	21:u:15:LEU:HG	1.92	0.51
26:A:774:G:N2	26:A:787:C:O2'	2.41	0.51
26:A:833:A:H2'	26:A:834:G:C8	2.44	0.51
26:A:2101:A:H2'	26:A:2102:G:H8	1.76	0.51
42:Q:25:GLY:O	42:Q:29:ARG:NH1	2.44	0.51
45:T:1:MET:HE2	45:T:3:ARG:HB2	1.93	0.51
56:4:11:CYS:HB3	56:4:33:HIS:CE1	2.46	0.51
56:4:27:CYS:SG	56:4:30:GLU:N	2.79	0.51
1:a:923:A:O2'	1:a:1399:C:OP2	2.28	0.51
12:l:21:PRO:HD2	12:l:93:ARG:HH21	1.76	0.51
15:o:34:GLN:HB3	15:o:58:MET:HE1	1.93	0.51
22:v:19:G:H1	22:v:56:PSU:H6	1.59	0.51
26:A:519:U:H5''	44:S:25:ARG:HH21	1.74	0.51
26:A:2298:A:H2'	26:A:2299:U:O4'	2.11	0.51
35:J:63:ALA:HA	35:J:69:ARG:HH22	1.75	0.51
25:z:103:LEU:HB2	25:z:130:ILE:HD11	1.93	0.51
26:A:1210:G:O6	26:A:1237:A:H2'	2.11	0.51
26:A:1815:A:H4'	26:A:1816:C:OP1	2.11	0.51
26:A:2649:C:H2'	26:A:2650:U:C6	2.46	0.51
30:E:76:PRO:HA	30:E:82:GLY:HA3	1.93	0.51
33:H:33:GLN:HB2	33:H:35:LYS:HG2	1.93	0.51
36:K:43:ILE:HD12	36:K:56:ASP:HB2	1.93	0.51
51:Z:40:THR:HG22	51:Z:43:ILE:HG12	1.92	0.51
1:a:1402:4OC:H2'	1:a:1403:C:O4'	2.11	0.50
13:m:76:ILE:HG23	13:m:90:HIS:CD2	2.46	0.50
26:A:479:A:O2'	26:A:481:G:H5''	2.11	0.50
26:A:686:U:O2'	54:2:4:THR:O	2.22	0.50
32:G:23:ILE:HD11	32:G:42:VAL:HG11	1.93	0.50
41:P:74:GLN:HB2	41:P:77:SER:HB2	1.93	0.50
46:U:36:GLU:HA	46:U:61:GLU:HG2	1.94	0.50
1:a:792:A:H1'	1:a:794:A:N7	2.26	0.50
4:d:56:GLU:OE2	4:d:59:LYS:HE2	2.11	0.50
19:s:38:THR:HG23	19:s:69:LYS:HZ3	1.77	0.50
22:w:56:C:H2'	22:w:57:A:C8	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:55:LYS:HE2	29:D:77:ARG:HA	1.92	0.50
30:E:41:GLN:OE1	30:E:43:THR:OG1	2.29	0.50
26:A:123:G:O2'	26:A:124:G:H5'	2.11	0.50
26:A:1243:C:H1'	37:L:4:ASN:O	2.11	0.50
26:A:2758:A:H2	32:G:34:ARG:HH21	1.59	0.50
39:N:56:LYS:NZ	39:N:87:PHE:O	2.44	0.50
45:T:22:THR:HA	45:T:25:GLU:HG2	1.94	0.50
1:a:909:A:H2'	1:a:910:C:O4'	2.11	0.50
1:a:1126:U:C5	10:j:73:LEU:HD11	2.46	0.50
3:c:9:ILE:HG23	3:c:10:ARG:HG3	1.92	0.50
24:y:7:A:H3'	24:y:8:4SU:H5'	1.92	0.50
24:y:76:A:H61	25:z:223:ARG:HE	1.60	0.50
25:z:213:PRO:HA	25:z:291:VAL:HG12	1.93	0.50
26:A:175:G:H2'	26:A:176:A:O4'	2.11	0.50
26:A:196:A:H5''	37:L:47:ARG:HH22	1.76	0.50
26:A:716:A:H2'	26:A:717:C:O4'	2.11	0.50
26:A:1877:A:H2'	26:A:1878:G:O4'	2.12	0.50
26:A:2515:C:H2'	26:A:2516:A:C8	2.46	0.50
26:A:2572:A:H2'	29:D:149:ASN:HD22	1.76	0.50
36:K:92:GLU:O	36:K:93:GLN:O	2.29	0.50
37:L:110:VAL:HG11	37:L:135:ILE:HD11	1.93	0.50
1:a:1137:C:H5'	1:a:1138:G:H5'	1.94	0.50
15:o:74:VAL:O	15:o:78:THR:HG23	2.11	0.50
24:y:23:A:H2'	24:y:24:G:C8	2.46	0.50
26:A:969:G:H2'	26:A:970:U:H6	1.76	0.50
26:A:1266:G:O2'	26:A:1267:U:OP2	2.30	0.50
26:A:1689:A:H2'	26:A:1690:A:H8	1.76	0.50
26:A:2224:G:H4'	26:A:2226:C:C2	2.46	0.50
26:A:2327:A:H2'	26:A:2328:A:C8	2.46	0.50
26:A:2759:G:N2	32:G:138:GLN:NE2	2.59	0.50
26:A:2845:U:H5''	41:P:51:ASN:O	2.11	0.50
36:K:24:VAL:HG13	36:K:33:ALA:HB2	1.93	0.50
58:6:44:PHE:HD1	58:6:45:THR:HG23	1.76	0.50
1:a:501:C:OP1	12:l:113:ARG:NH2	2.45	0.50
14:n:54:ASP:C	14:n:56:SER:N	2.69	0.50
26:A:301:G:OP2	46:U:81:ARG:NH1	2.41	0.50
26:A:395:U:H2'	26:A:396:G:C8	2.47	0.50
26:A:948:C:H2'	26:A:949:G:H8	1.76	0.50
26:A:1005:C:O2'	35:J:30:THR:HG21	2.11	0.50
26:A:1019:U:O2'	26:A:1020:A:H5'	2.11	0.50
26:A:2134:A:N6	26:A:2156:G:H2'	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:W:61:GLY:HA3	48:W:79:GLU:O	2.11	0.50
1:a:1375:A:H2'	1:a:1376:U:O4'	2.11	0.50
3:c:38:VAL:HG12	3:c:93:ILE:HG13	1.94	0.50
4:d:115:GLN:O	4:d:119:HIS:CD2	2.65	0.50
13:m:15:VAL:HG23	13:m:16:ILE:HD12	1.94	0.50
24:y:55:PSU:H2'	24:y:57:G:N7	2.27	0.50
27:B:111:U:O2'	27:B:112:G:H5'	2.12	0.50
1:a:599:C:H2'	1:a:600:A:C8	2.45	0.50
1:a:1534:A:H4'	1:a:1535:C:OP1	2.11	0.50
3:c:42:LEU:HD21	3:c:67:ILE:HD11	1.92	0.50
26:A:589:U:H2'	26:A:590:A:C8	2.46	0.50
26:A:1142:A:H4'	26:A:1143:A:OP1	2.10	0.50
32:G:153:PRO:HA	32:G:159:LYS:O	2.12	0.50
2:b:44:LYS:O	2:b:48:MET:HG2	2.12	0.50
4:d:84:ASN:HB3	4:d:87:GLU:OE1	2.12	0.50
11:k:83:VAL:HB	11:k:109:ILE:HG23	1.94	0.50
26:A:1106:G:H3'	26:A:1107:G:H8	1.76	0.50
39:N:103:ARG:HB2	39:N:110:MET:HE3	1.92	0.50
1:a:1314:C:H2'	1:a:1315:U:C6	2.46	0.49
25:z:299:LYS:HD2	25:z:300:PRO:HD2	1.94	0.49
31:F:3:LEU:HD11	31:F:100:GLU:HB2	1.93	0.49
36:K:102:PRO:HB3	36:K:121:GLU:HB3	1.94	0.49
1:a:1118:U:H2'	1:a:1119:C:C6	2.47	0.49
1:a:1354:U:H2'	1:a:1355:G:C8	2.46	0.49
3:c:40:GLN:NE2	3:c:41:TYR:N	2.60	0.49
4:d:59:LYS:HE3	4:d:194:ILE:HG22	1.94	0.49
12:l:35:ARG:NH1	12:l:37:TYR:HB3	2.27	0.49
26:A:39:G:H1'	30:E:43:THR:HG21	1.93	0.49
26:A:2529:G:OP2	26:A:2530:A:H5''	2.12	0.49
1:a:73:C:H2'	1:a:74:A:C8	2.48	0.49
1:a:263:A:OP1	20:t:73:ARG:NH1	2.45	0.49
1:a:448:A:H3'	1:a:449:G:H8	1.77	0.49
1:a:838:G:H2'	1:a:839:C:O4'	2.12	0.49
1:a:1414:U:H2'	1:a:1415:G:H8	1.76	0.49
10:j:52:LEU:HD23	10:j:62:ARG:HG2	1.94	0.49
26:A:580:U:H2'	26:A:581:C:C6	2.47	0.49
26:A:2020:A:H5'	52:0:8:THR:HG22	1.94	0.49
26:A:2101:A:H2'	26:A:2102:G:C8	2.47	0.49
43:R:61:ALA:HB2	43:R:98:ILE:HD13	1.94	0.49
44:S:52:GLU:HA	44:S:55:ILE:HD12	1.95	0.49
4:d:67:LEU:O	4:d:71:PHE:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:13:ASP:O	6:f:16:GLU:HB2	2.13	0.49
10:j:86:ALA:HA	10:j:90:LEU:HD12	1.95	0.49
16:p:11:ALA:HB3	16:p:14:ARG:HB2	1.94	0.49
22:w:5:G:H2'	22:w:6:G:O4'	2.12	0.49
26:A:52:A:H8	26:A:52:A:OP2	1.94	0.49
26:A:1201:U:H2'	26:A:1202:G:H8	1.77	0.49
27:B:79:G:H2'	27:B:80:U:O4'	2.13	0.49
28:C:131:MET:HE1	28:C:143:VAL:HG13	1.93	0.49
32:G:94:ARG:HD2	32:G:127:GLN:HB3	1.94	0.49
57:5:5:LEU:O	57:5:9:GLN:HB2	2.13	0.49
2:b:31:PHE:HE2	2:b:41:ASN:HB2	1.78	0.49
26:A:670:A:H8	26:A:670:A:OP2	1.95	0.49
26:A:2159:G:H2'	26:A:2160:C:O4'	2.13	0.49
31:F:133:GLU:HB3	31:F:135:ILE:HG13	1.94	0.49
52:0:24:VAL:HG22	52:0:26:SER:H	1.77	0.49
1:a:1270:G:H2'	1:a:1271:A:H8	1.78	0.49
17:q:45:VAL:HG11	17:q:60:ILE:HG12	1.94	0.49
26:A:64:A:N1	26:A:91:A:N6	2.60	0.49
26:A:721:A:H2'	26:A:722:A:C8	2.47	0.49
26:A:1378:A:O2'	26:A:1380:G:OP2	2.31	0.49
26:A:2725:A:O2'	26:A:2726:A:C8	2.66	0.49
26:A:2861:U:H2'	26:A:2862:G:H8	1.77	0.49
27:B:1:U:H2'	27:B:2:G:C8	2.47	0.49
1:a:79:G:H2'	1:a:80:A:O4'	2.12	0.49
1:a:235:C:H2'	1:a:236:A:C8	2.48	0.49
5:e:106:ALA:HB1	5:e:110:MET:HE3	1.94	0.49
8:h:77:VAL:HG12	8:h:84:ILE:HD12	1.94	0.49
12:l:31:GLY:HA3	12:l:54:VAL:HG12	1.95	0.49
12:l:49:ARG:HG3	12:l:89:LEU:HD11	1.95	0.49
25:z:34:VAL:HG21	25:z:188:ILE:HG21	1.95	0.49
26:A:473:G:O2'	26:A:474:G:H5'	2.12	0.49
26:A:873:C:H2'	26:A:874:G:H8	1.77	0.49
26:A:2291:U:H2'	26:A:2292:U:H6	1.77	0.49
26:A:2529:G:H4'	32:G:174:LYS:HE3	1.94	0.49
31:F:102:LEU:HD12	31:F:106:ALA:HB3	1.95	0.49
37:L:33:ARG:HD3	37:L:40:SER:HA	1.95	0.49
1:a:411:A:N9	1:a:413:G:H1'	2.28	0.49
1:a:618:C:O2'	16:p:14:ARG:NH1	2.46	0.49
1:a:635:A:H2'	1:a:636:U:C6	2.48	0.49
1:a:958:A:N7	19:s:54:ARG:NH1	2.60	0.49
13:m:85:TYR:O	13:m:89:ARG:HG2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:w:16:C:H5''	22:w:17:C:OP2	2.12	0.49
26:A:636:G:N7	37:L:109:LYS:HD3	2.28	0.49
26:A:1900:A:H1'	26:A:1970:A:H2'	1.95	0.49
27:B:13:G:C8	27:B:70:C:H4'	2.48	0.49
29:D:149:ASN:CG	29:D:150:GLN:H	2.20	0.49
1:a:219:U:H2'	1:a:220:G:C8	2.48	0.49
13:m:16:ILE:O	13:m:19:THR:OG1	2.27	0.49
25:z:131:ILE:HD12	25:z:195:LEU:HD23	1.95	0.49
26:A:962:G:H21	26:A:2250:G:H1	1.59	0.49
26:A:974:G:N3	26:A:974:G:H2'	2.28	0.49
31:F:134:GLN:HE22	31:F:149:ARG:N	2.11	0.49
33:H:47:PHE:HA	33:H:51:ARG:HB2	1.95	0.49
1:a:1004:A:H1'	1:a:1026:G:O6	2.13	0.49
1:a:1219:A:H2'	1:a:1220:G:C8	2.47	0.49
1:a:1498:UR3:H3U2	23:x:17:U:H4'	1.95	0.49
10:j:8:ILE:HB	10:j:74:VAL:HB	1.95	0.49
18:r:69:TYR:HB2	18:r:73:HIS:NE2	2.28	0.49
22:w:43:A:N3	22:w:43:A:H2'	2.28	0.49
22:w:56:C:C4	26:A:2168:G:N2	2.80	0.49
26:A:213:A:H2'	26:A:214:G:C8	2.48	0.49
26:A:356:G:H2'	26:A:357:C:C6	2.48	0.49
26:A:441:U:H2'	26:A:442:G:O4'	2.13	0.49
26:A:1329:U:O5'	26:A:1330:C:H5	1.95	0.49
1:a:1530:G:H2'	1:a:1531:A:C8	2.48	0.48
20:t:25:SER:O	20:t:28:ARG:HG2	2.13	0.48
22:w:76:A:C2	26:A:2421:G:O6	2.64	0.48
24:y:21:A:H5'	24:y:22:G:OP2	2.13	0.48
26:A:495:G:H5''	44:S:4:ILE:HG13	1.95	0.48
26:A:687:C:H1'	54:2:4:THR:HG22	1.95	0.48
26:A:2120:G:H2'	26:A:2121:G:C8	2.48	0.48
26:A:2698:U:H2'	26:A:2699:C:C6	2.48	0.48
1:a:1266:G:N2	1:a:1269:A:OP2	2.44	0.48
1:a:1538:C:H2'	1:a:1539:C:O4'	2.13	0.48
3:c:59:PRO:HB3	10:j:94:ALA:HB2	1.94	0.48
6:f:6:ILE:HB	6:f:62:MET:HB2	1.95	0.48
7:g:78:ARG:HD2	7:g:83:THR:HG23	1.95	0.48
10:j:46:LYS:HE2	10:j:68:ARG:HE	1.78	0.48
26:A:270:A:N1	26:A:369:U:O2'	2.40	0.48
26:A:1139:G:O2'	26:A:1140:C:H5'	2.13	0.48
26:A:2205:A:H2'	26:A:2206:C:C6	2.48	0.48
27:B:90:C:H2'	27:B:91:C:O4'	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:67:THR:O	31:F:83:PRO:HA	2.12	0.48
33:H:113:SER:O	33:H:116:ARG:NH1	2.39	0.48
46:U:88:ASP:CG	46:U:89:GLY:H	2.21	0.48
49:X:39:VAL:HG12	49:X:42:GLU:H	1.78	0.48
1:a:189:A:H2'	1:a:190:A:O4'	2.13	0.48
1:a:591:U:H3	1:a:648:A:H61	1.60	0.48
1:a:1305:G:H22	1:a:1331:G:H2'	1.78	0.48
5:e:22:LYS:HB3	5:e:29:ILE:HG23	1.95	0.48
8:h:63:LYS:HZ2	8:h:70:VAL:HG21	1.78	0.48
16:p:4:ILE:HG12	16:p:21:VAL:HG22	1.95	0.48
25:z:311:LEU:HB2	25:z:317:GLY:HA3	1.94	0.48
26:A:322:A:OP2	30:E:163:ASN:HB2	2.13	0.48
26:A:1586:A:C2	26:A:1587:G:H1'	2.48	0.48
29:D:85:ALA:C	29:D:87:GLY:H	2.22	0.48
32:G:102:ILE:O	32:G:113:ASP:HA	2.12	0.48
57:5:44:ALA:HB2	57:5:52:MET:HE2	1.95	0.48
1:a:692:U:H5''	11:k:126:ARG:NH2	2.22	0.48
1:a:871:U:H5''	1:a:872:A:OP2	2.13	0.48
1:a:1170:A:H2'	1:a:1171:A:O4'	2.13	0.48
6:f:47:LEU:HD13	6:f:51:ILE:HD12	1.95	0.48
26:A:367:G:N2	26:A:368:A:H1'	2.28	0.48
26:A:1881:C:H2'	26:A:1882:U:O4'	2.13	0.48
26:A:2516:A:O2'	26:A:2517:C:H5'	2.12	0.48
26:A:2808:G:O2'	26:A:2809:A:H8	1.97	0.48
27:B:106:G:H2'	27:B:107:G:O4'	2.13	0.48
1:a:254:G:OP1	17:q:68:LYS:O	2.32	0.48
1:a:920:U:H2'	1:a:921:U:C6	2.47	0.48
1:a:1256:A:O2'	1:a:1257:A:H5''	2.13	0.48
2:b:202:ASN:ND2	2:b:203:ASP:N	2.62	0.48
3:c:178:ARG:O	3:c:206:ILE:HA	2.12	0.48
4:d:103:ARG:NH1	4:d:110:ARG:HH12	2.10	0.48
18:r:34:GLU:HB3	21:u:18:PHE:CZ	2.48	0.48
26:A:454:A:H3'	26:A:455:C:C6	2.48	0.48
26:A:543:G:O6	26:A:550:C:N3	2.46	0.48
26:A:562:U:H2'	26:A:572:A:O4'	2.13	0.48
26:A:635:C:O2'	26:A:639:U:H5''	2.13	0.48
26:A:1900:A:O4'	26:A:1970:A:H5''	2.12	0.48
26:A:2065:C:H1'	26:A:2449:H2U:HN3	1.79	0.48
26:A:2103:C:H2'	26:A:2104:C:C6	2.48	0.48
26:A:2808:G:H2'	26:A:2890:G:O6	2.14	0.48
47:V:80:HIS:CG	47:V:81:PRO:HD2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:179:ALA:HB1	3:c:202:PHE:CE1	2.48	0.48
4:d:66:VAL:HG13	4:d:70:GLN:HE21	1.79	0.48
6:f:92:THR:OG1	6:f:93:LYS:N	2.39	0.48
10:j:49:PHE:O	10:j:64:GLN:HA	2.13	0.48
26:A:437:U:H2'	26:A:438:G:C8	2.48	0.48
26:A:2526:G:H2'	26:A:2527:C:C6	2.49	0.48
28:C:7:PRO:HB3	28:C:13:ARG:HB2	1.95	0.48
35:J:15:TRP:HB3	35:J:137:PRO:HB3	1.95	0.48
51:Z:3:THR:HB	51:Z:36:GLU:HG2	1.94	0.48
1:a:592:G:H2'	1:a:593:U:H6	1.78	0.48
1:a:996:A:H2'	1:a:997:U:C6	2.49	0.48
1:a:1354:U:H2'	1:a:1355:G:H8	1.78	0.48
3:c:91:ALA:HB2	3:c:98:ALA:HB3	1.96	0.48
3:c:96:VAL:HG22	3:c:97:PRO:HA	1.96	0.48
19:s:10:ILE:HG12	19:s:40:PHE:CE2	2.49	0.48
26:A:420:C:H2'	26:A:421:C:O4'	2.13	0.48
26:A:2405:G:O2'	26:A:2406:A:OP2	2.32	0.48
32:G:136:ASP:OD2	32:G:139:VAL:HG23	2.14	0.48
38:M:42:THR:HG22	38:M:93:VAL:HG12	1.96	0.48
44:S:28:LYS:HE3	44:S:70:LYS:NZ	2.28	0.48
1:a:766:A:H2'	1:a:767:A:O4'	2.14	0.48
1:a:1054:C:O2	1:a:1196:A:N6	2.46	0.48
4:d:173:ASP:O	4:d:175:GLY:N	2.47	0.48
9:i:49:GLN:O	9:i:51:LEU:N	2.44	0.48
10:j:37:ARG:HE	10:j:77:VAL:HG21	1.79	0.48
15:o:62:ARG:NH2	26:A:715:A:H4'	2.29	0.48
26:A:1182:G:H2'	26:A:1183:U:O4'	2.12	0.48
26:A:2172:U:OP2	26:A:2173:A:H5'	2.14	0.48
34:I:38:CYS:SG	34:I:39:LYS:N	2.87	0.48
1:a:411:A:C4	1:a:413:G:H1'	2.48	0.48
7:g:68:VAL:HG12	7:g:134:VAL:HG12	1.96	0.48
11:k:51:PHE:HE2	11:k:64:VAL:HG11	1.78	0.48
13:m:28:ARG:NH2	13:m:62:PHE:HB2	2.29	0.48
19:s:28:LYS:HE3	19:s:29:PRO:HD2	1.95	0.48
25:z:245:VAL:HG12	25:z:367:ALA:HB2	1.95	0.48
26:A:127:A:H5''	26:A:128:C:C6	2.48	0.48
26:A:692:C:H5''	28:C:38:LYS:HB3	1.96	0.48
26:A:1320:C:O2'	26:A:1321:A:H5''	2.14	0.48
26:A:1558:C:H4'	26:A:1559:U:O5'	2.13	0.48
28:C:15:VAL:HG22	28:C:205:GLY:HA3	1.96	0.48
31:F:89:THR:HG21	31:F:91:ARG:HH11	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:6:28:VAL:HG11	58:6:32:LEU:HD13	1.95	0.48
1:a:449:G:H2'	1:a:450:G:C8	2.49	0.48
1:a:946:A:H2'	1:a:947:G:C8	2.49	0.48
1:a:960:U:H4'	1:a:961:U:O5'	2.14	0.48
1:a:1301:U:O2'	1:a:1302:C:OP1	2.28	0.48
3:c:78:LYS:C	3:c:80:GLY:H	2.22	0.48
22:w:11:A:C5	22:w:12:G:N7	2.82	0.48
22:w:31:G:H2'	22:w:32:C:H5'	1.96	0.48
26:A:1019:U:H3	26:A:1142:A:H62	1.62	0.48
26:A:2071:A:H2'	26:A:2072:C:C6	2.49	0.48
26:A:2443:C:OP1	30:E:63:LYS:HD3	2.14	0.48
26:A:2720:U:H5''	41:P:52:ARG:NH2	2.28	0.48
29:D:179:ARG:HB3	29:D:188:LEU:HD12	1.95	0.48
43:R:77:PHE:HD1	43:R:84:ARG:HB3	1.79	0.48
1:a:145:G:C2	1:a:146:G:C8	3.02	0.47
1:a:299:G:H2'	1:a:300:A:C8	2.49	0.47
1:a:619:U:H4'	4:d:127:ARG:HH21	1.79	0.47
1:a:1060:U:H4'	10:j:53:ILE:HG23	1.95	0.47
1:a:1427:C:H2'	1:a:1428:A:C8	2.48	0.47
7:g:129:ASN:HA	7:g:134:VAL:HG11	1.96	0.47
25:z:103:LEU:HG	25:z:105:VAL:HG23	1.95	0.47
26:A:682:G:H5'	54:2:26:ASN:CG	2.39	0.47
26:A:831:G:H5''	37:L:37:GLY:HA2	1.95	0.47
37:L:118:THR:O	37:L:120:VAL:N	2.44	0.47
9:i:112:ARG:HH22	10:j:64:GLN:HE22	1.62	0.47
22:w:52:G:H1'	22:w:63:G:H21	1.78	0.47
22:w:76:A:N3	26:A:2421:G:N1	2.62	0.47
25:z:91:MET:HE1	25:z:118:HIS:CE1	2.49	0.47
26:A:39:G:H2'	26:A:40:U:C6	2.49	0.47
26:A:172:A:H2'	26:A:173:A:H8	1.78	0.47
26:A:322:A:H5'	26:A:340:A:H1'	1.97	0.47
26:A:528:A:C2	26:A:2042:A:H2'	2.48	0.47
26:A:1046:A:O2'	57:5:61:ARG:O	2.23	0.47
26:A:1183:U:H2'	26:A:1184:U:C6	2.49	0.47
26:A:1590:A:H2'	26:A:1591:A:H8	1.79	0.47
26:A:2051:A:H8	26:A:2051:A:OP2	1.97	0.47
26:A:2305:U:C2	31:F:150:GLY:O	2.67	0.47
26:A:2405:G:H1'	26:A:2412:A:N6	2.29	0.47
26:A:2655:G:O2'	26:A:2656:U:OP2	2.31	0.47
30:E:52:VAL:O	30:E:74:LYS:HE3	2.14	0.47
31:F:73:VAL:HG22	31:F:78:ILE:HG12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:N:69:ARG:C	39:N:71:ARG:H	2.17	0.47
57:5:41:LEU:O	57:5:44:ALA:HB3	2.15	0.47
1:a:718:A:H5'	11:k:118:ASN:OD1	2.15	0.47
1:a:900:A:H2'	1:a:901:A:C8	2.49	0.47
1:a:1120:C:H2'	1:a:1121:U:C6	2.48	0.47
1:a:1537:U:H2'	1:a:1538:C:O4'	2.14	0.47
4:d:201:GLU:OE2	5:e:111:ARG:NH2	2.48	0.47
7:g:92:PRO:HA	7:g:95:ARG:HB2	1.95	0.47
18:r:21:ASP:OD2	18:r:23:LYS:HB2	2.14	0.47
26:A:934:U:H2'	26:A:935:C:C6	2.49	0.47
31:F:165:GLY:O	31:F:168:LEU:HB3	2.14	0.47
50:Y:44:LYS:HA	50:Y:47:ARG:HH22	1.79	0.47
1:a:160:A:H2'	1:a:161:A:O4'	2.14	0.47
1:a:484:G:H4'	1:a:485:U:H5''	1.95	0.47
1:a:590:U:H2'	1:a:591:U:H6	1.79	0.47
24:y:77:PHE:CE2	25:z:66:HIS:HB2	2.49	0.47
26:A:1177:G:H2'	26:A:1178:C:C4'	2.45	0.47
26:A:1363:C:O2'	26:A:1809:A:N3	2.47	0.47
37:L:77:ILE:O	37:L:110:VAL:O	2.32	0.47
37:L:125:LEU:HB3	37:L:126:ARG:H	1.55	0.47
41:P:24:THR:O	41:P:86:LYS:HB2	2.15	0.47
43:R:28:ALA:HB3	43:R:31:GLU:HB2	1.97	0.47
55:3:26:ALA:O	55:3:27:ASN:CG	2.57	0.47
1:a:175:C:H2'	1:a:176:C:H6	1.79	0.47
1:a:1056:U:OP1	3:c:162:ALA:N	2.47	0.47
22:w:5:G:H3'	22:w:6:G:H8	1.79	0.47
22:w:7:G:O6	22:w:66:C:N4	2.37	0.47
26:A:20:C:H2'	26:A:21:A:C8	2.49	0.47
26:A:244:A:H2'	26:A:245:G:O4'	2.15	0.47
26:A:505:A:HO2'	26:A:509:C:HO2'	1.57	0.47
26:A:2178:C:H2'	26:A:2179:C:C6	2.49	0.47
26:A:2297:A:N1	26:A:2321:U:C5	2.83	0.47
26:A:2756:U:H4'	26:A:2757:A:OP1	2.15	0.47
31:F:9:ASP:OD1	31:F:9:ASP:N	2.47	0.47
35:J:75:TYR:HB3	35:J:84:ILE:HD11	1.95	0.47
37:L:122:VAL:HG21	37:L:135:ILE:HD13	1.97	0.47
42:Q:71:ASN:HD22	42:Q:71:ASN:N	2.12	0.47
1:a:1151:A:H1'	10:j:41:PRO:HB3	1.96	0.47
3:c:54:ILE:HD12	3:c:56:ILE:HD11	1.96	0.47
9:i:39:GLY:HA2	9:i:44:ARG:HB2	1.97	0.47
26:A:120:U:H4'	26:A:121:G:H5''	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1340:U:H3'	45:T:61:LEU:HD22	1.97	0.47
26:A:1454:C:H5'	39:N:63:ARG:CZ	2.45	0.47
26:A:2771:C:H2'	26:A:2772:C:C6	2.50	0.47
29:D:32:ASN:HA	29:D:51:THR:O	2.13	0.47
35:J:35:ARG:HA	35:J:40:HIS:HD2	1.79	0.47
41:P:29:VAL:HG13	41:P:79:VAL:HG22	1.96	0.47
1:a:499:A:H4'	1:a:500:G:O5'	2.15	0.47
1:a:551:U:H2'	1:a:552:U:C6	2.50	0.47
1:a:780:A:H5''	11:k:124:LYS:HE3	1.97	0.47
1:a:1226:C:N4	13:m:102:LYS:HD2	2.29	0.47
2:b:90:PHE:O	2:b:149:GLY:HA3	2.14	0.47
4:d:23:GLY:H	4:d:109:THR:HG22	1.80	0.47
5:e:9:GLU:O	5:e:40:ASP:HA	2.14	0.47
7:g:76:SER:OG	7:g:83:THR:HG22	2.15	0.47
9:i:12:LYS:HA	9:i:109:GLN:OE1	2.15	0.47
11:k:46:ALA:HA	11:k:65:ALA:HB2	1.97	0.47
11:k:75:GLU:C	11:k:77:GLY:N	2.70	0.47
15:o:88:ARG:NH2	26:A:716:A:OP2	2.48	0.47
20:t:74:HIS:O	20:t:78:LEU:HB2	2.15	0.47
26:A:108:G:H2'	26:A:109:C:O4'	2.15	0.47
26:A:121:G:H4'	26:A:149:A:H5'	1.95	0.47
26:A:181:A:H2'	26:A:182:A:C8	2.49	0.47
26:A:404:A:H1'	26:A:406:G:N9	2.30	0.47
26:A:1052:C:H2'	26:A:1053:C:C5	2.50	0.47
26:A:1430:G:H2'	26:A:1431:A:O4'	2.15	0.47
26:A:1715:G:HO2'	26:A:1716:U:H6	1.58	0.47
26:A:2014:A:H2'	26:A:2015:A:C8	2.50	0.47
26:A:2266:A:H8	26:A:2266:A:OP1	1.98	0.47
26:A:2286:G:H4'	26:A:2287:A:O5'	2.14	0.47
27:B:75:G:H2'	27:B:76:G:O4'	2.14	0.47
29:D:48:ILE:O	29:D:81:GLU:HA	2.15	0.47
31:F:39:VAL:C	31:F:41:GLU:H	2.22	0.47
36:K:34:GLY:O	36:K:36:GLY:N	2.47	0.47
45:T:80:TRP:CZ3	45:T:82:LYS:HB3	2.50	0.47
49:X:48:LEU:HB3	49:X:50:VAL:HG13	1.96	0.47
1:a:1007:U:H2'	1:a:1008:U:H6	1.80	0.47
1:a:1187:G:H5'	9:i:114:LYS:HE3	1.96	0.47
17:q:56:ASP:HB2	17:q:79:GLU:O	2.15	0.47
25:z:149:VAL:O	25:z:152:GLU:HB2	2.15	0.47
26:A:1287:A:H5'	39:N:103:ARG:HH11	1.80	0.47
26:A:1857:G:H1'	26:A:1885:A:N6	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2391:G:OP2	55:3:34:LYS:HD2	2.14	0.47
26:A:2408:U:H2'	26:A:2409:G:H8	1.80	0.47
34:I:33:ASN:HB2	34:I:64:ARG:NH2	2.29	0.47
34:I:133:ARG:HA	34:I:137:LEU:O	2.15	0.47
1:a:70:U:H5''	1:a:71:A:OP1	2.14	0.47
1:a:833:G:C6	1:a:834:U:C4	3.02	0.47
2:b:92:ASN:OD1	2:b:93:HIS:N	2.48	0.47
12:l:74:GLN:O	12:l:76:HIS:N	2.48	0.47
14:n:41:ARG:O	14:n:44:ALA:HB3	2.14	0.47
18:r:25:ILE:HA	18:r:28:LEU:HB3	1.96	0.47
18:r:50:TYR:O	18:r:54:LEU:HB2	2.15	0.47
21:u:11:PHE:O	21:u:13:VAL:N	2.48	0.47
22:w:18:G:N3	22:w:58:A:O4'	2.48	0.47
25:z:35:LEU:O	25:z:39:TYR:HB2	2.15	0.47
26:A:635:C:H2'	26:A:636:G:O4'	2.15	0.47
26:A:1636:U:H2'	26:A:1637:A:C8	2.50	0.47
26:A:1692:U:O2'	26:A:1693:U:H2'	2.15	0.47
26:A:2467:C:H2'	26:A:2468:A:O4'	2.14	0.47
26:A:2875:C:O2'	26:A:2876:G:H5'	2.14	0.47
40:O:26:LEU:HD13	40:O:39:VAL:HG22	1.97	0.47
46:U:85:ARG:NH1	46:U:99:SER:OG	2.47	0.47
1:a:950:U:H2'	1:a:951:G:H8	1.77	0.47
1:a:1367:C:H4'	10:j:50:THR:HG21	1.97	0.47
1:a:1437:A:H2'	1:a:1438:G:H8	1.79	0.47
10:j:81:GLU:HA	10:j:84:VAL:HG12	1.95	0.47
11:k:63:GLN:HG3	11:k:98:ALA:HB2	1.96	0.47
12:l:67:GLY:O	12:l:98:ARG:NH1	2.48	0.47
22:v:16:C:H4'	22:v:61:U:H1'	1.97	0.47
22:w:6:G:N1	22:w:67:C:N3	2.63	0.47
62:z:401:KIR:H101	62:z:401:KIR:H411	1.70	0.47
26:A:321:U:H4'	26:A:322:A:OP2	2.14	0.47
26:A:974:G:H1'	26:A:975:A:H8	1.80	0.47
26:A:1477:A:H2'	26:A:1478:G:O4'	2.15	0.47
26:A:1530:G:H22	26:A:1542:U:H1'	1.79	0.47
26:A:1728:C:O2'	26:A:1729:U:C6	2.68	0.47
26:A:2287:A:C2'	26:A:2288:A:O5'	2.63	0.47
26:A:2584:U:C3'	26:A:2585:U:H5''	2.44	0.47
26:A:2823:A:OP1	29:D:118:PHE:HB2	2.15	0.47
31:F:138:PRO:HB3	58:6:32:LEU:HD11	1.97	0.47
32:G:41:GLU:HB3	32:G:52:GLY:O	2.15	0.47
32:G:70:LEU:O	32:G:74:MET:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:H:64:ALA:O	33:H:67:ALA:HB3	2.15	0.47
39:N:49:GLU:HB2	39:N:50:PRO:HD3	1.96	0.47
8:h:104:SER:HB2	8:h:125:ILE:HD11	1.98	0.46
9:i:56:MET:O	9:i:58:GLU:N	2.48	0.46
12:l:34:THR:HA	12:l:75:GLU:O	2.15	0.46
22:w:1:C:N4	22:w:71:C:N4	2.63	0.46
25:z:216:ASP:HB3	25:z:228:THR:OG1	2.15	0.46
26:A:251:A:H2'	26:A:252:G:O4'	2.15	0.46
26:A:2552:OMU:H5	26:A:2556:C:H41	1.79	0.46
31:F:12:VAL:O	31:F:16:MET:HG2	2.15	0.46
42:Q:85:ALA:HB2	42:Q:115:ALA:HB2	1.97	0.46
1:a:1297:G:O2'	1:a:1298:U:P	2.72	0.46
1:a:1367:C:H5''	9:i:115:VAL:HG23	1.96	0.46
15:o:55:LEU:O	15:o:58:MET:HG2	2.16	0.46
16:p:52:LEU:HG	16:p:57:ILE:HD11	1.97	0.46
26:A:1109:C:N3	26:A:1110:G:N2	2.63	0.46
26:A:1315:C:H2'	26:A:1316:U:C6	2.50	0.46
26:A:1538:G:H2'	26:A:1539:U:C6	2.50	0.46
26:A:2777:G:H1'	26:A:2779:U:H5	1.80	0.46
27:B:50:A:H2'	27:B:51:G:O4'	2.15	0.46
46:U:96:LYS:O	46:U:97:SER:O	2.34	0.46
51:Z:40:THR:HG23	51:Z:42:ALA:H	1.80	0.46
1:a:77:A:H2'	1:a:78:A:C8	2.50	0.46
1:a:337:G:H2'	1:a:338:A:C8	2.51	0.46
1:a:575:G:HO2'	1:a:821:G:H5'	1.80	0.46
22:w:19:G:C4	22:w:57:A:C2	3.03	0.46
26:A:435:C:H2'	26:A:436:C:H5'	1.96	0.46
26:A:554:U:H2'	26:A:555:G:O4'	2.15	0.46
26:A:1038:G:H2'	26:A:1039:A:C8	2.49	0.46
26:A:1085:A:H61	57:5:34:THR:HG22	1.81	0.46
26:A:1751:U:H2'	26:A:1752:C:C6	2.51	0.46
26:A:2862:G:H2'	26:A:2863:C:C6	2.51	0.46
1:a:29:U:C2'	1:a:30:U:H5'	2.45	0.46
1:a:567:G:H2'	1:a:568:G:O4'	2.15	0.46
1:a:1222:G:H5''	19:s:77:ARG:HH11	1.81	0.46
1:a:1458:G:H5'	20:t:26:MET:HB3	1.97	0.46
4:d:94:GLU:HG2	4:d:185:PRO:HG2	1.97	0.46
5:e:13:LYS:NZ	5:e:112:ALA:HB1	2.30	0.46
5:e:156:ARG:HH11	5:e:163:ILE:HA	1.78	0.46
22:w:76:A:N1	26:A:2421:G:C5	2.84	0.46
26:A:336:C:O2'	26:A:337:C:H5'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:674:G:H5''	30:E:71:GLY:H	1.81	0.46
26:A:685:A:H5''	26:A:788:A:H62	1.80	0.46
26:A:1980:G:O2'	26:A:1982:U:OP2	2.26	0.46
26:A:2721:A:H1'	26:A:2873:A:O2'	2.16	0.46
1:a:8:A:N6	4:d:201:GLU:O	2.49	0.46
1:a:102:G:H2'	1:a:103:U:C6	2.51	0.46
1:a:193:C:H2'	1:a:194:C:H6	1.81	0.46
1:a:1054:C:H42	23:x:22:G:N2	2.14	0.46
1:a:1163:A:H2'	1:a:1164:G:C8	2.51	0.46
1:a:1335:U:H5''	1:a:1336:C:H5'	1.98	0.46
16:p:56:ARG:O	16:p:59:HIS:HB3	2.16	0.46
19:s:76:THR:OG1	19:s:77:ARG:N	2.48	0.46
26:A:1418:G:H2'	26:A:1579:A:H62	1.80	0.46
26:A:1684:G:H2'	26:A:1685:C:C6	2.51	0.46
26:A:2139:U:H2'	26:A:2140:G:C8	2.51	0.46
26:A:2645:G:H4'	26:A:2732:G:H1'	1.97	0.46
26:A:2714:G:O2'	26:A:2715:C:H5'	2.14	0.46
1:a:35:G:H2'	1:a:36:C:C6	2.51	0.46
1:a:368:U:OP2	25:z:279:ARG:HD3	2.16	0.46
1:a:592:G:H2'	1:a:593:U:C6	2.51	0.46
3:c:23:ALA:HB3	3:c:28:PHE:HD1	1.81	0.46
7:g:46:LEU:HD23	7:g:57:GLU:HB3	1.97	0.46
10:j:7:ARG:O	10:j:101:SER:HB2	2.15	0.46
10:j:37:ARG:HB2	10:j:75:ASP:HB2	1.97	0.46
22:v:51:U:H2'	22:v:52:C:H6	1.81	0.46
22:v:70:C:H2'	22:v:71:G:C8	2.50	0.46
22:w:38:A:H5''	22:w:39:C:OP2	2.15	0.46
26:A:772:C:O2'	26:A:773:U:H5'	2.16	0.46
26:A:2444:G:OP2	30:E:63:LYS:HD2	2.16	0.46
26:A:2705:A:O2'	26:A:2852:G:OP1	2.26	0.46
37:L:30:THR:O	37:L:32:GLY:N	2.48	0.46
1:a:246:A:N3	1:a:247:G:H1'	2.31	0.46
5:e:82:HIS:CE1	5:e:146:MET:HG3	2.50	0.46
10:j:5:ARG:N	10:j:77:VAL:HA	2.31	0.46
10:j:7:ARG:HD3	10:j:75:ASP:OD1	2.16	0.46
15:o:45:HIS:C	15:o:47:LYS:H	2.23	0.46
22:w:71:C:H2'	22:w:72:A:O4'	2.16	0.46
26:A:185:G:H4'	26:A:218:A:H4'	1.98	0.46
26:A:259:G:C2'	26:A:260:G:H5'	2.46	0.46
26:A:923:G:H2'	26:A:924:G:C8	2.48	0.46
26:A:1152:C:H2'	26:A:1153:C:C6	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1212:G:H1'	26:A:1237:A:N6	2.30	0.46
26:A:1343:G:H1'	26:A:1597:A:C4	2.51	0.46
26:A:2688:G:H1'	26:A:2721:A:N6	2.31	0.46
35:J:99:ARG:NH1	35:J:102:GLU:OE2	2.49	0.46
36:K:35:VAL:HG22	36:K:69:VAL:HG12	1.98	0.46
51:Z:47:ILE:HD13	51:Z:56:VAL:HG21	1.97	0.46
1:a:1512:U:H2'	1:a:1513:A:H8	1.81	0.46
21:u:19:LYS:H	21:u:19:LYS:HD2	1.81	0.46
25:z:208:LYS:HG3	25:z:233:ARG:HD2	1.98	0.46
26:A:807:U:H1'	26:A:2445:2MG:OP1	2.15	0.46
26:A:1088:A:H61	34:I:134:SER:CB	2.29	0.46
26:A:1310:G:H1'	26:A:1611:C:H5''	1.96	0.46
26:A:2515:C:H2'	26:A:2516:A:H8	1.81	0.46
32:G:126:THR:HG22	32:G:128:THR:H	1.81	0.46
1:a:1401:G:OP2	1:a:1401:G:H8	1.99	0.46
9:i:12:LYS:O	9:i:14:SER:N	2.47	0.46
15:o:45:HIS:O	15:o:47:LYS:N	2.45	0.46
26:A:1306:C:N4	26:A:1606:C:H2'	2.30	0.46
26:A:1318:U:H2'	26:A:1319:C:C6	2.51	0.46
26:A:2331:G:O2'	26:A:2336:A:N1	2.46	0.46
26:A:2629:U:O2'	26:A:2630:G:H5''	2.15	0.46
27:B:13:G:N7	27:B:70:C:H4'	2.31	0.46
31:F:4:HIS:CD2	31:F:8:LYS:HE3	2.51	0.46
31:F:129:MET:HG3	31:F:153:ILE:HB	1.98	0.46
39:N:38:LEU:HB3	39:N:39:PRO:HD3	1.97	0.46
40:O:37:ALA:HB3	40:O:78:VAL:HG21	1.98	0.46
46:U:17:ASP:HB3	46:U:20:LYS:HD2	1.98	0.46
1:a:985:C:H2'	1:a:986:U:C6	2.51	0.46
7:g:17:PHE:CE1	7:g:22:LEU:HD21	2.51	0.46
22:w:58:A:O3'	22:w:60:U:OP2	2.34	0.46
25:z:278:LEU:HD11	25:z:292:LEU:HD11	1.98	0.46
26:A:287:G:H2'	26:A:288:U:C6	2.51	0.46
26:A:1045:C:H1'	26:A:1047:G:C2	2.51	0.46
26:A:1188:U:O2'	26:A:1189:A:H5'	2.16	0.46
26:A:1715:G:O2'	26:A:1716:U:H6	1.98	0.46
26:A:1744:A:H3'	26:A:1745:A:H8	1.81	0.46
26:A:1819:A:H3'	28:C:176:ARG:HG2	1.98	0.46
26:A:1951:U:H2'	26:A:1953:A:OP2	2.15	0.46
26:A:2100:G:H1	26:A:2189:U:H3	1.64	0.46
34:I:42:ASN:HA	34:I:45:THR:HB	1.97	0.46
36:K:41:ILE:HG13	36:K:58:LEU:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:M:5:LYS:O	38:M:6:ARG:HG2	2.16	0.46
1:a:225:C:H2'	1:a:226:G:O4'	2.16	0.45
1:a:696:A:H1'	1:a:786:G:O2'	2.16	0.45
1:a:1101:A:H4'	1:a:1102:A:O5'	2.15	0.45
5:e:45:VAL:HG12	5:e:116:VAL:HG23	1.98	0.45
9:i:14:SER:HB2	9:i:69:GLY:HA3	1.97	0.45
13:m:7:ASN:ND2	13:m:20:SER:HB2	2.31	0.45
17:q:13:SER:O	17:q:20:ILE:HA	2.16	0.45
22:v:16:C:O2'	22:v:61:U:H4'	2.16	0.45
25:z:24:LYS:NZ	63:z:402:GDP:O3B	2.45	0.45
25:z:260:MET:O	25:z:263:LYS:HB2	2.15	0.45
25:z:272:GLU:N	25:z:272:GLU:OE1	2.46	0.45
25:z:303:LYS:HA	25:z:360:VAL:O	2.16	0.45
26:A:1:G:H2'	26:A:2:G:H8	1.80	0.45
26:A:871:U:H2'	26:A:872:U:C6	2.50	0.45
26:A:974:G:H1'	26:A:975:A:C8	2.52	0.45
26:A:2329:U:H2'	26:A:2330:G:C8	2.51	0.45
26:A:2742:G:OP1	56:4:36:ARG:HD3	2.16	0.45
34:I:121:ILE:HA	34:I:124:MET:HE3	1.98	0.45
58:6:58:ASP:OD1	58:6:58:ASP:N	2.49	0.45
1:a:56:U:H2'	1:a:57:G:C8	2.52	0.45
3:c:32:LEU:O	3:c:35:ASP:HB3	2.16	0.45
19:s:34:SER:OG	19:s:37:SER:HB3	2.16	0.45
22:w:49:G:C2	22:w:50:U:C2	3.03	0.45
26:A:811:U:N3	37:L:21:ARG:NH2	2.64	0.45
26:A:973:A:H5'	26:A:1188:U:H1'	1.98	0.45
26:A:2183:A:H2'	26:A:2184:A:C8	2.51	0.45
26:A:2808:G:H2'	26:A:2890:G:C6	2.51	0.45
58:6:37:CYS:SG	58:6:39:LYS:O	2.73	0.45
1:a:128:G:H5'	17:q:5:ARG:HH22	1.81	0.45
1:a:555:U:H2'	1:a:556:C:C6	2.51	0.45
1:a:590:U:H2'	1:a:591:U:C6	2.51	0.45
2:b:66:ILE:HD12	2:b:159:ALA:HB3	1.98	0.45
6:f:9:MET:HE1	6:f:51:ILE:HD13	1.98	0.45
7:g:111:GLY:HA2	7:g:118:ARG:HD3	1.98	0.45
10:j:29:ALA:HB1	10:j:83:THR:HG23	1.98	0.45
18:r:54:LEU:O	18:r:58:ILE:HG12	2.17	0.45
22:w:6:G:C2	22:w:67:C:N3	2.84	0.45
26:A:930:G:H1'	51:Z:24:LEU:HD21	1.97	0.45
26:A:1297:C:OP1	26:A:2710:C:H4'	2.16	0.45
26:A:1361:G:H2'	26:A:1362:C:C6	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1604:C:H2'	26:A:1605:C:C6	2.51	0.45
26:A:1916:A:H2'	26:A:1917:PSU:O4'	2.16	0.45
26:A:2840:C:H2'	26:A:2841:C:C6	2.52	0.45
32:G:95:ALA:HB1	32:G:130:ILE:HD11	1.97	0.45
34:I:48:ILE:HG13	34:I:49:GLU:H	1.80	0.45
37:L:95:LEU:HD22	37:L:100:ILE:HD11	1.98	0.45
49:X:30:PRO:O	49:X:32:LEU:N	2.48	0.45
57:5:118:ILE:H	57:5:119:PRO:CD	2.29	0.45
1:a:102:G:H2'	1:a:103:U:H6	1.81	0.45
1:a:1539:C:H2'	1:a:1540:U:C6	2.50	0.45
14:n:63:ARG:NH1	14:n:70:PRO:HD3	2.31	0.45
22:w:20:H2U:H51	26:A:2112:G:C2'	2.46	0.45
22:w:56:C:H41	26:A:2168:G:N2	2.14	0.45
24:y:60:U:H5''	24:y:61:C:OP2	2.17	0.45
26:A:465:G:H2'	26:A:466:A:C8	2.51	0.45
26:A:1069:A:N6	26:A:1073:A:C4	2.84	0.45
26:A:1528:A:H2'	26:A:1529:G:O4'	2.17	0.45
26:A:2379:G:H4'	40:O:21:LEU:HD11	1.98	0.45
26:A:2712:C:OP1	26:A:2714:G:H4'	2.17	0.45
29:D:40:LEU:HA	29:D:44:GLY:H	1.82	0.45
1:a:819:A:H5'	1:a:820:U:C5	2.52	0.45
1:a:1127:G:H22	1:a:1145:A:H2	1.64	0.45
1:a:1182:G:H4'	1:a:1183:U:O5'	2.16	0.45
5:e:121:ASN:O	5:e:122:VAL:HG22	2.16	0.45
22:w:73:A:N6	22:w:74:C:N3	2.64	0.45
22:w:76:A:O2'	26:A:2394:C:O2	2.35	0.45
26:A:357:C:H2'	26:A:358:U:C6	2.51	0.45
26:A:1328:A:H2'	26:A:1330:C:C4	2.52	0.45
34:I:20:SER:HB3	34:I:21:PRO:HD3	1.97	0.45
57:5:26:VAL:HG21	57:5:114:GLU:HG2	1.98	0.45
1:a:545:C:O2'	1:a:549:C:H5''	2.17	0.45
1:a:1300:G:HO2'	1:a:1301:U:H6	1.59	0.45
4:d:99:ASN:OD1	4:d:110:ARG:NH1	2.49	0.45
4:d:169:TRP:CD1	4:d:185:PRO:HG3	2.51	0.45
4:d:172:VAL:HG22	4:d:174:ALA:H	1.81	0.45
26:A:136:G:H1	26:A:143:C:H42	1.63	0.45
26:A:780:G:OP1	28:C:216:ARG:NH2	2.49	0.45
26:A:2528:U:H2'	26:A:2530:A:O5'	2.16	0.45
26:A:2638:G:H1'	26:A:2778:A:N6	2.32	0.45
27:B:87:U:H5''	27:B:88:C:OP2	2.16	0.45
27:B:114:C:H2'	27:B:115:A:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:35:THR:HG22	29:D:73:VAL:HG21	1.98	0.45
37:L:51:GLU:OE1	37:L:56:PRO:HA	2.17	0.45
46:U:42:LYS:HG2	46:U:59:GLU:OE1	2.16	0.45
1:a:1001:C:H2'	1:a:1002:G:C8	2.52	0.45
1:a:1016:A:O2'	1:a:1217:C:O2'	2.29	0.45
7:g:15:PRO:HB2	9:i:44:ARG:HH12	1.81	0.45
22:w:26:G:H2'	22:w:26:G:N3	2.31	0.45
26:A:89:A:H2'	26:A:90:U:C6	2.51	0.45
26:A:128:C:H2'	26:A:129:C:H6	1.81	0.45
26:A:1932:A:H2'	26:A:1933:G:O4'	2.17	0.45
26:A:2012:G:H8	26:A:2012:G:O5'	1.98	0.45
26:A:2208:C:H2'	26:A:2209:G:C8	2.52	0.45
26:A:2783:U:H2'	26:A:2784:U:C6	2.52	0.45
29:D:31:ALA:O	29:D:33:ARG:HG2	2.17	0.45
30:E:49:ARG:O	30:E:74:LYS:HE2	2.17	0.45
35:J:35:ARG:HB2	35:J:54:ILE:HD11	1.98	0.45
37:L:62:PRO:HG2	55:3:24:LYS:HB3	1.99	0.45
43:R:24:LYS:HD3	43:R:92:TRP:HB3	1.99	0.45
1:a:222:C:H2'	1:a:223:A:C8	2.48	0.45
1:a:424:G:H2'	1:a:425:G:O4'	2.16	0.45
5:e:108:GLY:O	5:e:110:MET:N	2.44	0.45
10:j:11:LYS:HE2	10:j:71:LEU:HG	1.97	0.45
16:p:12:LYS:C	16:p:14:ARG:H	2.25	0.45
16:p:54:LEU:HA	16:p:57:ILE:HD12	1.97	0.45
21:u:19:LYS:HD2	21:u:19:LYS:N	2.32	0.45
61:v:105:FME:O	26:A:2585:U:C2	2.69	0.45
26:A:1858:A:C2	26:A:1885:A:H1'	2.51	0.45
26:A:2313:C:H5''	31:F:87:LYS:HD2	1.98	0.45
26:A:2869:G:H2'	26:A:2870:C:O4'	2.17	0.45
30:E:18:THR:HA	30:E:106:LYS:HE3	1.99	0.45
31:F:24:VAL:O	31:F:27:VAL:HG12	2.17	0.45
31:F:97:GLU:HG2	58:6:25:ARG:HB2	1.99	0.45
34:I:18:ASN:HB2	34:I:38:CYS:HB3	1.99	0.45
35:J:56:VAL:HB	35:J:124:VAL:HG12	1.99	0.45
1:a:613:C:H2'	1:a:614:C:C6	2.51	0.45
1:a:1162:C:H2'	1:a:1163:A:C8	2.52	0.45
1:a:1225:A:H5'	1:a:1226:C:OP2	2.16	0.45
1:a:1426:G:H2'	1:a:1427:C:O4'	2.17	0.45
6:f:24:ARG:NH1	6:f:24:ARG:HB3	2.32	0.45
22:w:33:U:H2'	22:w:35:A:OP2	2.16	0.45
26:A:500:G:N1	26:A:503:A:OP2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2146:C:H4'	26:A:2147:A:C4	2.52	0.45
26:A:2514:U:H5''	35:J:81:ILE:HD11	1.99	0.45
30:E:159:LEU:C	30:E:161:ALA:H	2.25	0.45
37:L:57:LEU:HD22	55:3:53:ASP:HB3	1.98	0.45
50:Y:39:GLN:HB2	50:Y:41:HIS:CE1	2.52	0.45
1:a:668:G:H2'	1:a:669:G:H8	1.82	0.45
1:a:769:G:H4'	1:a:1513:A:H4'	1.98	0.45
1:a:1039:G:H2'	1:a:1040:U:H6	1.82	0.45
1:a:1282:C:H2'	1:a:1283:U:C6	2.51	0.45
25:z:69:TYR:HE2	25:z:78:HIS:HB2	1.81	0.45
26:A:1204:A:H4'	26:A:1205:A:H5''	1.99	0.45
26:A:1340:U:OP1	45:T:19:LYS:NZ	2.49	0.45
26:A:1637:A:H5'	26:A:1760:C:O2'	2.17	0.45
26:A:2221:G:H2'	26:A:2222:C:C6	2.52	0.45
26:A:2489:U:C4	26:A:2490:G:C6	3.05	0.45
26:A:2512:C:H2'	26:A:2513:A:O4'	2.17	0.45
26:A:2846:G:H2'	26:A:2847:U:O4'	2.17	0.45
34:I:4:VAL:HA	34:I:7:TYR:CE2	2.51	0.45
1:a:389:A:H3'	1:a:390:U:C6	2.51	0.44
3:c:87:ARG:O	3:c:91:ALA:CB	2.65	0.44
7:g:143:MET:O	7:g:147:ASN:HB3	2.16	0.44
14:n:81:ARG:HA	14:n:84:VAL:HG12	1.99	0.44
15:o:52:ARG:O	15:o:55:LEU:HB3	2.17	0.44
22:w:67:C:C4	22:w:68:C:C5	3.05	0.44
25:z:93:THR:HG21	25:z:288:ARG:NH1	2.33	0.44
26:A:529:A:OP2	35:J:113:PRO:HD3	2.17	0.44
26:A:955:PSU:H5'	38:M:86:LYS:HD3	1.99	0.44
26:A:1014:A:H2'	26:A:1015:U:C6	2.52	0.44
26:A:2793:C:H2'	26:A:2794:C:C6	2.52	0.44
29:D:36:GLN:HB3	29:D:49:GLN:HB3	1.97	0.44
31:F:153:ILE:H	31:F:153:ILE:HD12	1.82	0.44
32:G:37:ASN:OD1	32:G:38:ASP:N	2.50	0.44
1:a:624:C:O3'	16:p:10:GLY:HA2	2.17	0.44
1:a:1026:G:H2'	1:a:1027:C:C6	2.52	0.44
1:a:1323:G:H2'	1:a:1324:A:C8	2.52	0.44
3:c:141:MET:HG3	3:c:169:GLU:HB3	1.99	0.44
6:f:46:GLN:HA	6:f:56:LYS:HG2	1.98	0.44
11:k:51:PHE:CE2	11:k:64:VAL:HG11	2.52	0.44
13:m:28:ARG:O	13:m:32:ILE:HG12	2.17	0.44
22:w:15:G:OP2	22:w:16:C:C5	2.70	0.44
24:y:10:G:H8	24:y:10:G:OP1	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:z:25:THR:O	25:z:28:THR:HG22	2.16	0.44
25:z:331:TYR:CE2	25:z:377:ARG:HB2	2.52	0.44
25:z:373:ARG:HG2	25:z:387:VAL:HG12	1.98	0.44
26:A:600:G:H2'	26:A:601:C:O4'	2.17	0.44
26:A:651:G:H5'	55:3:18:LYS:HG3	1.99	0.44
26:A:973:A:H5''	43:R:81:LYS:HD2	1.99	0.44
26:A:1386:C:H2'	26:A:1387:A:H8	1.81	0.44
26:A:1525:A:H2'	26:A:1526:C:O4'	2.17	0.44
26:A:1682:G:H2'	26:A:1683:U:C6	2.52	0.44
26:A:2022:U:O4	52:0:5:ASN:ND2	2.50	0.44
33:H:2:GLN:HB3	33:H:39:ALA:HB3	1.98	0.44
33:H:30:LEU:HB3	33:H:36:ALA:HB3	2.00	0.44
56:4:22:VAL:HG11	56:4:36:ARG:HH11	1.82	0.44
57:5:87:GLU:OE2	57:5:95:LEU:HB2	2.17	0.44
1:a:1320:C:C2	19:s:71:GLY:HA3	2.52	0.44
26:A:568:U:H2'	26:A:570:G:OP2	2.17	0.44
34:I:104:GLN:O	34:I:108:ILE:HG13	2.17	0.44
38:M:69:PRO:HA	38:M:94:ALA:HB2	2.00	0.44
49:X:17:ARG:HE	49:X:23:ALA:CB	2.15	0.44
1:a:469:C:H2'	1:a:470:C:O4'	2.18	0.44
1:a:1082:A:H2'	1:a:1083:U:O4'	2.16	0.44
10:j:80:THR:HB	10:j:83:THR:HB	1.98	0.44
22:w:53:G:C6	22:w:54:5MU:C4	3.06	0.44
26:A:286:U:H2'	26:A:287:G:C8	2.52	0.44
26:A:414:C:H2'	26:A:415:A:C8	2.52	0.44
26:A:1107:G:H1'	57:5:81:LEU:HD12	1.97	0.44
26:A:2141:G:N2	26:A:2151:U:H1'	2.31	0.44
31:F:137:PHE:HA	31:F:138:PRO:HD3	1.77	0.44
35:J:63:ALA:HA	35:J:69:ARG:NH2	2.32	0.44
39:N:28:LEU:HD13	39:N:34:ILE:HG12	2.00	0.44
44:S:72:THR:HG21	44:S:108:SER:HB3	1.98	0.44
55:3:29:ARG:HD3	55:3:29:ARG:HA	1.76	0.44
1:a:429:U:H4'	1:a:430:A:OP1	2.16	0.44
1:a:1095:U:OP2	1:a:1108:G:N1	2.41	0.44
16:p:12:LYS:C	16:p:14:ARG:N	2.76	0.44
22:w:28:C:H2'	22:w:29:G:O4'	2.17	0.44
24:y:65:G:H5'	25:z:329:GLN:OE1	2.17	0.44
24:y:76:A:N3	25:z:259:GLU:HG3	2.33	0.44
26:A:19:A:H5''	42:Q:21:LYS:HG2	2.00	0.44
26:A:278:A:H2'	26:A:278:A:N3	2.32	0.44
26:A:458:G:O2'	26:A:459:U:P	2.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:598:U:H2'	26:A:599:A:C8	2.52	0.44
26:A:1610:A:OP1	26:A:1611:C:H5	2.00	0.44
26:A:1820:U:C2	28:C:200:MET:HB2	2.53	0.44
26:A:2861:U:H2'	26:A:2862:G:C8	2.52	0.44
34:I:104:GLN:O	34:I:107:GLU:HB3	2.18	0.44
1:a:50:A:H4'	1:a:51:A:H5'	2.00	0.44
1:a:89:U:H2'	1:a:90:C:O4'	2.17	0.44
1:a:237:G:H5''	17:q:26:ARG:NH2	2.31	0.44
1:a:860:A:H2'	1:a:861:G:O4'	2.18	0.44
1:a:1252:A:H2'	1:a:1253:G:O4'	2.18	0.44
1:a:1371:G:O3'	9:i:70:GLY:HA3	2.18	0.44
2:b:56:LEU:HD23	2:b:59:ILE:HD11	2.00	0.44
16:p:61:VAL:HG22	16:p:67:ILE:HD11	1.99	0.44
22:w:4:G:N2	22:w:70:G:C4	2.85	0.44
24:y:36:A:N6	24:y:37:MIA:H122	2.33	0.44
24:y:76:A:C2	25:z:277:LEU:HB2	2.52	0.44
25:z:71:THR:OG1	25:z:72:PRO:HD2	2.17	0.44
26:A:18:U:O2'	26:A:554:U:OP1	2.35	0.44
26:A:278:A:C2	26:A:362:A:H1'	2.53	0.44
26:A:789:A:N1	54:2:3:ARG:NH1	2.55	0.44
26:A:938:G:H2'	26:A:939:G:H8	1.83	0.44
26:A:1278:C:H2'	26:A:1279:G:C8	2.53	0.44
26:A:1475:G:HO2'	26:A:1476:U:H6	1.62	0.44
26:A:1783:A:N1	26:A:2587:A:H2'	2.33	0.44
26:A:2121:G:H2'	26:A:2122:U:O4'	2.18	0.44
26:A:2204:G:H4'	28:C:149:LYS:HD3	1.99	0.44
26:A:2466:C:OP1	56:4:4:ARG:HB3	2.18	0.44
26:A:2682:A:H61	26:A:2728:U:C1'	2.27	0.44
26:A:2851:A:H2'	26:A:2852:G:O4'	2.17	0.44
31:F:56:LEU:HD13	31:F:88:VAL:HG23	1.99	0.44
32:G:154:GLU:C	32:G:156:TYR:H	2.24	0.44
37:L:36:LYS:HB3	37:L:37:GLY:H	1.68	0.44
41:P:77:SER:O	41:P:80:VAL:HG22	2.18	0.44
1:a:175:C:H2'	1:a:176:C:C6	2.53	0.44
1:a:1391:U:H2'	1:a:1392:G:C8	2.52	0.44
2:b:17:HIS:HB3	2:b:18:GLN:H	1.61	0.44
3:c:187:GLU:CD	3:c:187:GLU:H	2.26	0.44
5:e:80:LEU:HD21	5:e:95:MET:HE2	1.99	0.44
6:f:86:ARG:HH11	6:f:86:ARG:HB2	1.83	0.44
12:l:115:LYS:C	12:l:117:GLY:H	2.26	0.44
25:z:7:ARG:CZ	25:z:269:ARG:HH21	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:z:243:GLU:HB2	25:z:295:PRO:HG3	1.99	0.44
25:z:323:PHE:HD2	25:z:349:MET:HG2	1.83	0.44
26:A:117:G:C6	26:A:119:A:C6	3.05	0.44
26:A:232:G:OP2	26:A:232:G:H8	2.01	0.44
26:A:1198:U:H2'	26:A:1199:U:C6	2.52	0.44
26:A:1328:A:H2'	26:A:1330:C:C5	2.53	0.44
28:C:131:MET:HE2	28:C:189:ALA:HB2	1.98	0.44
31:F:3:LEU:HD13	31:F:96:TRP:HE3	1.83	0.44
1:a:390:U:H4'	16:p:28:ARG:NH2	2.33	0.44
1:a:763:G:H2'	1:a:764:C:C6	2.53	0.44
1:a:1343:G:O2'	9:i:122:ARG:HD2	2.18	0.44
6:f:24:ARG:HB3	6:f:24:ARG:HH11	1.83	0.44
11:k:35:ASP:OD1	11:k:39:ASN:N	2.48	0.44
17:q:45:VAL:HG22	17:q:72:TRP:HB2	1.99	0.44
20:t:67:HIS:C	20:t:69:ASN:H	2.25	0.44
22:v:24:C:H2'	22:v:25:U:C6	2.52	0.44
22:w:12:G:H2'	22:w:13:C:H6	1.82	0.44
26:A:563:A:OP2	43:R:79:ARG:NH2	2.50	0.44
26:A:1103:A:H3'	26:A:1104:C:C5'	2.42	0.44
26:A:1563:U:H2'	26:A:1564:C:C6	2.53	0.44
26:A:2065:C:H2'	26:A:2066:C:C6	2.52	0.44
26:A:2427:C:C5'	26:A:2429:G:H5'	2.46	0.44
35:J:7:LYS:HB2	35:J:10:THR:OG1	2.17	0.44
51:Z:23:LEU:HD11	51:Z:53:MET:SD	2.58	0.44
1:a:751:U:H2'	1:a:752:G:O4'	2.18	0.44
1:a:909:A:OP1	12:l:17:LYS:HD3	2.18	0.44
1:a:923:A:H2'	1:a:924:C:O4'	2.18	0.44
1:a:1435:G:H2'	1:a:1436:U:C6	2.53	0.44
2:b:46:VAL:HB	2:b:47:PRO:HD3	1.99	0.44
2:b:118:THR:O	2:b:121:GLN:HG2	2.17	0.44
22:v:6:G:H1	22:v:68:C:H42	1.63	0.44
22:w:18:G:N2	22:w:58:A:C4'	2.64	0.44
22:w:27:U:H2'	22:w:43:A:N1	2.33	0.44
26:A:63:A:H2'	26:A:64:A:C8	2.53	0.44
26:A:2112:G:H5'	26:A:2113:U:C5	2.53	0.44
36:K:71:ARG:HH11	36:K:77:ILE:HD11	1.83	0.44
42:Q:57:ARG:HA	42:Q:60:TRP:CE3	2.52	0.44
1:a:79:G:N2	1:a:80:A:H1'	2.33	0.43
1:a:219:U:H2'	1:a:220:G:H8	1.83	0.43
1:a:552:U:H2'	1:a:553:A:C8	2.53	0.43
1:a:681:A:H2'	1:a:682:G:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1073:U:OP2	5:e:61:LYS:NZ	2.51	0.43
1:a:1219:A:H2'	1:a:1220:G:H8	1.83	0.43
1:a:1287:A:H2'	1:a:1288:A:C8	2.53	0.43
2:b:31:PHE:CE2	2:b:41:ASN:HB2	2.53	0.43
18:r:70:THR:HG23	18:r:71:ASP:N	2.33	0.43
22:v:1:C:H2'	22:v:2:G:H8	1.82	0.43
24:y:68:C:H2'	24:y:69:G:C8	2.53	0.43
26:A:249:C:O2	55:3:11:LYS:NZ	2.51	0.43
26:A:971:G:H2'	26:A:972:A:O4'	2.18	0.43
26:A:1094:U:H2'	26:A:1096:A:N7	2.33	0.43
26:A:1614:A:C2	44:S:93:ALA:HB2	2.53	0.43
26:A:1746:A:H2'	26:A:1747:U:C6	2.53	0.43
26:A:1806:C:H1'	28:C:43:ASN:HD21	1.83	0.43
26:A:2093:G:OP1	33:H:24:GLY:HA3	2.18	0.43
26:A:2233:U:H2'	26:A:2234:G:H8	1.80	0.43
26:A:2271:G:OP1	48:W:14:ALA:HB1	2.17	0.43
26:A:2730:C:O2'	26:A:2731:G:H5'	2.18	0.43
26:A:2848:G:O2'	26:A:2849:U:H5'	2.18	0.43
35:J:110:PRO:O	35:J:115:GLY:HA3	2.17	0.43
45:T:5:GLU:HA	45:T:8:LEU:HD12	1.98	0.43
47:V:30:ILE:HG12	47:V:91:PHE:HB2	2.00	0.43
54:2:30:VAL:O	54:2:34:ARG:HG2	2.17	0.43
1:a:1157:A:H61	1:a:1178:G:H1'	1.83	0.43
5:e:11:GLN:HE22	5:e:116:VAL:HA	1.83	0.43
6:f:9:MET:HB2	6:f:85:ILE:O	2.18	0.43
9:i:6:TYR:HE1	9:i:17:ARG:HB3	1.83	0.43
21:u:9:GLU:HB2	21:u:10:PRO:HD3	2.00	0.43
21:u:64:ALA:O	21:u:66:ARG:N	2.42	0.43
22:w:17:C:H6	22:w:17:C:H5''	1.83	0.43
22:w:20:H2U:H51	26:A:2112:G:C1'	2.44	0.43
25:z:112:MET:HE3	25:z:113:PRO:HD2	2.00	0.43
26:A:155:A:H2'	26:A:156:A:C8	2.52	0.43
26:A:1565:C:HO2'	26:A:1566:A:H2'	1.83	0.43
26:A:2019:A:H2	26:A:2035:G:H22	1.64	0.43
27:B:79:G:N7	47:V:14:LYS:NZ	2.66	0.43
43:R:79:ARG:C	43:R:81:LYS:H	2.25	0.43
44:S:23:LEU:HD22	52:0:23:ALA:HB2	2.00	0.43
49:X:32:LEU:HD22	49:X:49:ARG:HG2	1.98	0.43
51:Z:44:ARG:HD2	51:Z:47:ILE:HD12	2.00	0.43
55:3:27:ASN:O	55:3:35:LYS:HE2	2.18	0.43
1:a:192:A:H2'	1:a:193:C:O4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1190:G:O2'	3:c:2:GLN:HG3	2.19	0.43
10:j:18:ILE:HA	10:j:21:ALA:HB3	2.01	0.43
22:w:30:G:N3	22:w:30:G:H2'	2.32	0.43
22:w:50:U:O2	22:w:64:G:N2	2.37	0.43
22:w:59:A:H3'	22:w:60:U:H6	1.84	0.43
62:z:401:KIR:H441	62:z:401:KIR:H231	1.62	0.43
26:A:182:A:H2'	26:A:183:C:O4'	2.18	0.43
26:A:307:G:N1	26:A:310:A:OP2	2.50	0.43
26:A:1143:A:N7	35:J:27:ARG:NH1	2.67	0.43
26:A:1789:A:OP2	28:C:220:ARG:NH2	2.45	0.43
26:A:2286:G:H5''	26:A:2287:A:OP1	2.18	0.43
26:A:2859:G:H2'	26:A:2860:A:C8	2.53	0.43
31:F:134:GLN:OE1	31:F:147:ARG:O	2.36	0.43
34:I:56:VAL:HG13	34:I:58:ILE:HD11	2.00	0.43
1:a:280:C:H4'	1:a:281:G:OP2	2.19	0.43
1:a:305:G:H5''	1:a:306:A:OP1	2.18	0.43
1:a:709:U:H2'	1:a:710:G:H8	1.83	0.43
2:b:209:VAL:O	2:b:213:LEU:HB2	2.19	0.43
3:c:58:ARG:CZ	3:c:63:ILE:HD13	2.49	0.43
3:c:102:ILE:H	3:c:102:ILE:HG13	1.67	0.43
9:i:117:LEU:HB3	9:i:118:ARG:H	1.63	0.43
11:k:112:VAL:HG12	18:r:72:ARG:CZ	2.49	0.43
17:q:30:HIS:CD2	17:q:33:TYR:H	2.31	0.43
19:s:10:ILE:HD13	19:s:15:LEU:HD22	1.99	0.43
25:z:300:PRO:HA	25:z:367:ALA:HA	2.00	0.43
26:A:900:A:H2'	26:A:901:C:O4'	2.19	0.43
26:A:1590:A:H2'	26:A:1591:A:C8	2.53	0.43
26:A:2712:C:H3'	26:A:2714:G:H5''	1.99	0.43
30:E:102:ARG:NH1	30:E:200:LEU:O	2.51	0.43
55:3:32:LEU:HD23	55:3:35:LYS:HD2	2.00	0.43
1:a:309:A:H2'	1:a:310:G:H8	1.83	0.43
1:a:537:G:H5''	12:l:109:ARG:NH1	2.34	0.43
1:a:721:G:C2	1:a:733:G:C6	3.07	0.43
2:b:167:HIS:ND1	2:b:168:GLU:HG3	2.34	0.43
3:c:80:GLY:O	3:c:83:VAL:HB	2.18	0.43
3:c:149:LYS:O	3:c:149:LYS:HG3	2.18	0.43
12:l:35:ARG:HH12	12:l:37:TYR:HB3	1.83	0.43
17:q:59:GLU:HB2	17:q:75:VAL:HB	2.00	0.43
22:w:27:U:N3	22:w:44:A:C5	2.83	0.43
22:w:52:G:N1	22:w:53:G:C6	2.87	0.43
26:A:17:G:H4'	42:Q:24:TYR:HE1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:310:A:C2'	26:A:311:A:H5''	2.48	0.43
26:A:1213:A:H62	26:A:1236:G:H1'	1.84	0.43
26:A:1235:G:C6	26:A:1236:G:N2	2.87	0.43
26:A:1421:G:C2	26:A:1422:G:C8	3.07	0.43
26:A:1469:A:H2'	26:A:1470:A:C8	2.54	0.43
26:A:2066:C:O2'	26:A:2067:G:H5'	2.18	0.43
26:A:2325:G:C6	26:A:2326:C:N4	2.86	0.43
27:B:53:A:H2'	27:B:53:A:N3	2.33	0.43
31:F:120:SER:HB2	31:F:127:TYR:CE1	2.53	0.43
32:G:82:PHE:O	32:G:133:LYS:HA	2.19	0.43
35:J:37:ARG:NH2	35:J:110:PRO:HG3	2.33	0.43
38:M:60:GLN:NE2	38:M:108:VAL:HG12	2.33	0.43
44:S:20:VAL:HG11	44:S:44:ALA:HA	2.00	0.43
1:a:202:G:H1	1:a:215:C:H42	1.66	0.43
1:a:490:C:H2'	1:a:491:G:C8	2.53	0.43
1:a:993:G:H2'	1:a:993:G:N3	2.34	0.43
3:c:59:PRO:HD2	3:c:62:SER:O	2.19	0.43
19:s:7:GLY:HA2	19:s:8:PRO:HD3	1.91	0.43
22:w:33:U:OP2	22:w:33:U:C6	2.71	0.43
22:w:48:C:O2'	22:w:49:G:OP1	2.33	0.43
26:A:549:G:HO2'	26:A:550:C:P	2.41	0.43
26:A:1432:G:O2'	26:A:1433:A:H5'	2.18	0.43
26:A:1679:A:H2'	26:A:1680:U:C6	2.54	0.43
26:A:1807:G:H2'	26:A:1808:A:H5'	1.99	0.43
26:A:2307:G:H8	26:A:2307:G:OP1	2.00	0.43
28:C:179:GLU:HG3	28:C:269:ARG:HA	2.00	0.43
37:L:135:ILE:HB	37:L:142:ILE:HD11	2.01	0.43
45:T:64:LYS:N	45:T:64:LYS:HD2	2.34	0.43
46:U:83:GLY:O	46:U:93:ARG:HA	2.19	0.43
2:b:19:THR:HG23	2:b:20:ARG:N	2.20	0.43
10:j:22:THR:HA	10:j:25:ILE:HG22	2.01	0.43
11:k:60:PHE:O	11:k:63:GLN:HB3	2.18	0.43
13:m:56:ARG:NH2	58:6:35:ASP:OD1	2.52	0.43
20:t:28:ARG:O	20:t:32:LYS:HG2	2.19	0.43
22:w:16:C:H5''	22:w:17:C:P	2.58	0.43
22:w:72:A:H4'	26:A:1852:U:C4'	2.47	0.43
26:A:756:A:H2'	26:A:757:G:O4'	2.18	0.43
26:A:1022:G:N2	26:A:1142:A:C2	2.87	0.43
26:A:1127:A:H2'	26:A:1128:G:H5''	2.00	0.43
26:A:1527:G:N1	26:A:1544:A:OP2	2.49	0.43
26:A:1788:C:O2'	26:A:1789:A:H5'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2128:G:H2'	26:A:2129:C:O4'	2.18	0.43
26:A:2197:U:O2'	26:A:2198:A:H2'	2.17	0.43
26:A:2347:C:H2'	26:A:2348:U:C6	2.54	0.43
26:A:2494:G:O2'	38:M:79:ALA:HA	2.18	0.43
26:A:2572:A:C8	29:D:149:ASN:ND2	2.86	0.43
26:A:2747:G:O6	26:A:2755:C:H5''	2.19	0.43
39:N:79:LEU:O	39:N:81:ASN:N	2.42	0.43
1:a:216:U:H2'	1:a:217:C:C6	2.54	0.43
1:a:571:U:OP1	1:a:819:A:O2'	2.35	0.43
9:i:30:ASN:C	9:i:32:ARG:H	2.26	0.43
9:i:113:LYS:HE2	9:i:118:ARG:O	2.18	0.43
13:m:51:GLN:O	13:m:54:THR:OG1	2.32	0.43
22:v:62:C:H2'	22:v:63:C:H6	1.84	0.43
25:z:137:CYS:SG	25:z:171:ARG:HB2	2.58	0.43
26:A:242:G:N7	55:3:4:LYS:HG2	2.34	0.43
26:A:2059:A:H2'	26:A:2503:2MA:HM23	2.01	0.43
26:A:2298:A:OP1	31:F:70:ARG:NH2	2.52	0.43
26:A:2646:C:H2'	26:A:2647:U:O4'	2.19	0.43
28:C:86:ARG:HD3	28:C:104:LEU:HD21	2.01	0.43
30:E:178:VAL:O	30:E:182:ALA:HB2	2.19	0.43
38:M:50:ARG:HA	38:M:53:MET:HE2	2.01	0.43
45:T:8:LEU:HA	45:T:50:LEU:HD21	2.01	0.43
53:1:32:LYS:HB3	53:1:50:GLU:HB3	2.01	0.43
57:5:57:ASN:ND2	57:5:63:ALA:HB2	2.33	0.43
1:a:158:G:H2'	1:a:159:G:C8	2.53	0.43
1:a:508:U:H1'	1:a:509:A:N7	2.34	0.43
1:a:580:C:H2'	1:a:581:G:O4'	2.19	0.43
8:h:39:LEU:HD21	8:h:128:VAL:HG21	1.99	0.43
25:z:24:LYS:HB2	63:z:402:GDP:O1B	2.18	0.43
26:A:17:G:H4'	42:Q:24:TYR:CE1	2.54	0.43
26:A:207:A:H2'	26:A:208:C:O4'	2.19	0.43
26:A:494:G:H4'	44:S:6:LYS:O	2.18	0.43
26:A:678:C:H2'	26:A:679:C:C6	2.53	0.43
26:A:816:C:H2'	26:A:817:C:C6	2.54	0.43
26:A:1798:U:OP2	28:C:270:ARG:NH2	2.49	0.43
26:A:1872:A:H2'	26:A:1873:G:O4'	2.18	0.43
26:A:2398:U:H2'	26:A:2399:G:C8	2.54	0.43
26:A:2884:U:C6	52:0:49:ARG:HG2	2.54	0.43
30:E:128:ALA:C	30:E:130:LYS:H	2.26	0.43
34:I:112:LYS:O	34:I:116:MET:HG2	2.19	0.43
37:L:21:ARG:HD3	37:L:21:ARG:HA	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:L:23:ILE:H	37:L:23:ILE:HD12	1.84	0.43
37:L:128:THR:OG1	37:L:129:LYS:N	2.44	0.43
40:O:31:THR:HG22	40:O:33:ARG:H	1.84	0.43
1:a:142:G:O2'	1:a:196:A:N1	2.51	0.43
1:a:255:G:OP1	17:q:70:LYS:NZ	2.50	0.43
1:a:502:A:OP1	12:l:114:SER:HB2	2.19	0.43
1:a:1305:G:O2'	1:a:1306:A:P	2.77	0.43
3:c:36:PHE:O	3:c:40:GLN:HG3	2.19	0.43
4:d:145:ARG:HH21	4:d:147:LYS:HE2	1.84	0.43
5:e:106:ALA:HB2	5:e:124:ALA:HB3	2.00	0.43
12:l:3:VAL:HG23	17:q:33:TYR:HB3	2.00	0.43
22:w:18:G:H4'	22:w:19:G:OP1	2.19	0.43
25:z:175:LEU:HD12	63:z:402:GDP:C2	2.54	0.43
26:A:278:A:H2	26:A:362:A:H1'	1.83	0.43
26:A:364:C:H2'	26:A:365:U:C6	2.54	0.43
26:A:1956:U:C2'	26:A:1957:C:H5'	2.48	0.43
26:A:2530:A:N6	32:G:155:PRO:HG3	2.34	0.43
26:A:2773:C:H2'	26:A:2774:C:C6	2.53	0.43
35:J:102:GLU:HG3	35:J:119:PHE:CZ	2.52	0.43
52:O:28:SER:O	52:O:36:LYS:HA	2.18	0.43
1:a:256:U:H2'	1:a:257:G:C8	2.54	0.42
1:a:680:C:H2'	1:a:681:A:C8	2.53	0.42
1:a:709:U:H2'	1:a:710:G:C8	2.53	0.42
1:a:1273:C:H2'	1:a:1274:A:O4'	2.18	0.42
1:a:1327:C:H2'	1:a:1328:C:C6	2.53	0.42
1:a:1347:G:O2'	1:a:1348:U:OP2	2.37	0.42
5:e:160:VAL:HG13	5:e:161:GLU:N	2.34	0.42
7:g:137:ARG:NH2	7:g:138:GLU:OE2	2.52	0.42
24:y:66:U:C4	24:y:67:C:N4	2.87	0.42
26:A:191:A:H2'	26:A:192:C:C6	2.54	0.42
26:A:811:U:C4	37:L:21:ARG:NH2	2.87	0.42
26:A:1796:U:H2'	26:A:1797:G:H8	1.84	0.42
26:A:1866:A:H2'	26:A:1867:G:O4'	2.18	0.42
26:A:2682:A:N6	26:A:2728:U:H1'	2.30	0.42
33:H:114:GLU:OE1	33:H:114:GLU:N	2.51	0.42
34:I:11:GLN:NE2	34:I:56:VAL:HG12	2.34	0.42
35:J:4:PHE:HE2	35:J:43:GLU:HB2	1.84	0.42
43:R:33:VAL:HG23	43:R:61:ALA:HB3	2.01	0.42
45:T:38:ALA:HA	45:T:42:GLU:OE1	2.19	0.42
57:5:18:VAL:HG11	57:5:70:GLU:HB3	2.01	0.42
57:5:40:GLU:O	57:5:43:LYS:HB3	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:686:U:H2'	1:a:687:A:C8	2.54	0.42
1:a:751:U:H4'	15:o:23:SER:HA	2.01	0.42
1:a:1263:C:H2'	1:a:1264:U:C6	2.54	0.42
1:a:1306:A:H62	1:a:1331:G:H1'	1.82	0.42
3:c:85:LYS:O	3:c:89:VAL:HG22	2.19	0.42
4:d:191:SER:OG	4:d:192:ALA:N	2.52	0.42
5:e:12:GLU:HB3	5:e:38:VAL:HG12	2.01	0.42
7:g:49:LEU:O	7:g:53:SER:OG	2.37	0.42
8:h:4:ASP:HB2	8:h:80:PRO:HG3	2.01	0.42
9:i:74:GLN:O	9:i:78:ILE:HG13	2.19	0.42
13:m:27:THR:HA	13:m:30:LYS:HE2	2.01	0.42
25:z:16:THR:HG23	25:z:78:HIS:CE1	2.53	0.42
26:A:118:A:H2'	26:A:120:U:O4	2.19	0.42
26:A:189:G:H2'	26:A:205:G:N2	2.34	0.42
26:A:1378:A:C4	26:A:1380:G:N7	2.87	0.42
26:A:2362:C:P	55:3:27:ASN:ND2	2.92	0.42
26:A:2391:G:H5''	55:3:31:ILE:HD12	2.02	0.42
26:A:2572:A:H2'	29:D:149:ASN:ND2	2.34	0.42
26:A:2637:U:H2'	26:A:2638:G:O4'	2.19	0.42
26:A:2728:U:H2'	26:A:2729:G:H8	1.84	0.42
57:5:24:SER:HA	57:5:85:SER:O	2.19	0.42
1:a:123:U:OP1	1:a:312:C:H5'	2.18	0.42
3:c:40:GLN:NE2	3:c:40:GLN:C	2.77	0.42
12:l:86:VAL:HG21	12:l:89:LEU:HB2	2.00	0.42
17:q:30:HIS:HA	17:q:31:PRO:HD3	1.94	0.42
26:A:1509:A:H2'	26:A:1510:G:H8	1.83	0.42
26:A:2287:A:O2'	26:A:2288:A:H2'	2.20	0.42
26:A:2684:U:O4'	36:K:70:ARG:NH1	2.52	0.42
36:K:64:ARG:HB2	36:K:83:ALA:HB3	2.00	0.42
58:6:39:LYS:O	58:6:40:CYS:CB	2.67	0.42
1:a:147:G:H2'	1:a:148:G:C8	2.54	0.42
1:a:501:C:H2'	1:a:502:A:C8	2.55	0.42
1:a:502:A:H2'	1:a:503:C:O4'	2.19	0.42
1:a:696:A:H2'	1:a:697:U:C6	2.55	0.42
1:a:1010:U:H2'	1:a:1011:C:C6	2.55	0.42
1:a:1234:C:H2'	1:a:1235:U:C6	2.54	0.42
22:w:69:C:HO2'	22:w:70:G:P	2.43	0.42
22:w:69:C:C4	22:w:70:G:N7	2.87	0.42
25:z:129:TYR:HB3	25:z:198:TYR:CE2	2.54	0.42
26:A:476:G:H4'	26:A:502:A:N1	2.34	0.42
26:A:789:A:C6	54:2:3:ARG:NH1	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1447:C:H2'	26:A:1448:G:C8	2.55	0.42
26:A:1816:C:H3'	28:C:61:TYR:CE1	2.54	0.42
26:A:1996:C:H4'	26:A:1997:C:OP1	2.19	0.42
26:A:2261:C:C6	48:W:12:SER:OG	2.71	0.42
26:A:2285:C:O2'	26:A:2287:A:H1'	2.20	0.42
26:A:2572:A:H5''	26:A:2574:G:H4'	2.02	0.42
27:B:13:G:O2'	27:B:15:A:H2'	2.19	0.42
31:F:48:LEU:HA	31:F:51:ASN:ND2	2.34	0.42
39:N:67:PHE:O	39:N:71:ARG:HD2	2.19	0.42
39:N:81:ASN:N	39:N:81:ASN:OD1	2.52	0.42
42:Q:57:ARG:NH1	42:Q:61:ILE:HD11	2.34	0.42
45:T:33:LYS:HG2	45:T:80:TRP:CZ3	2.55	0.42
1:a:1478:U:H2'	1:a:1479:C:C6	2.55	0.42
7:g:131:GLY:O	7:g:134:VAL:HG22	2.19	0.42
11:k:81:LEU:HD11	11:k:99:LEU:HD23	2.01	0.42
16:p:69:ASP:OD1	16:p:70:ARG:N	2.53	0.42
22:v:73:A:H2'	22:v:74:A:O4'	2.19	0.42
26:A:156:A:H2'	26:A:157:C:O4'	2.20	0.42
26:A:366:C:H2'	26:A:367:G:O4'	2.20	0.42
26:A:723:C:H2'	26:A:724:U:O4'	2.19	0.42
26:A:822:G:OP2	26:A:946:C:H5''	2.20	0.42
26:A:1649:G:O2'	39:N:106:ASP:OD2	2.37	0.42
26:A:1857:G:H2'	26:A:1884:G:H22	1.82	0.42
26:A:2287:A:C6	26:A:2289:G:C5	3.07	0.42
26:A:2358:A:H2'	26:A:2359:C:O4'	2.19	0.42
26:A:2415:G:H2'	26:A:2416:C:C6	2.55	0.42
26:A:2526:G:H2'	26:A:2527:C:H6	1.83	0.42
26:A:2590:A:H2'	26:A:2591:C:C6	2.54	0.42
26:A:2837:A:H2'	26:A:2838:G:C8	2.54	0.42
31:F:139:GLU:HA	58:6:28:VAL:HG22	2.01	0.42
32:G:41:GLU:HB2	32:G:54:ARG:HE	1.85	0.42
42:Q:107:ALA:O	43:R:48:LYS:HE3	2.19	0.42
46:U:40:LEU:HD23	46:U:61:GLU:HG3	2.01	0.42
52:0:6:LYS:HA	52:0:7:PRO:HD3	1.87	0.42
1:a:860:A:N6	1:a:861:G:C2	2.87	0.42
4:d:173:ASP:C	4:d:175:GLY:N	2.77	0.42
8:h:63:LYS:HB3	8:h:70:VAL:HG21	2.00	0.42
22:w:26:G:OP2	22:w:27:U:OP2	2.37	0.42
26:A:546:U:H1'	26:A:548:G:C2	2.53	0.42
26:A:631:A:N3	26:A:2415:G:O2'	2.48	0.42
26:A:687:C:H5''	54:2:2:LYS:NZ	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:779:U:P	28:C:48:ILE:HG22	2.60	0.42
26:A:1747:U:H2'	26:A:1748:C:C6	2.55	0.42
27:B:16:G:C6	27:B:17:C:C4	3.08	0.42
28:C:16:VAL:H	28:C:203:VAL:HG22	1.84	0.42
31:F:7:TYR:OH	31:F:29:ARG:HB3	2.20	0.42
31:F:132:ARG:O	31:F:150:GLY:HA3	2.19	0.42
35:J:31:GLU:HG2	35:J:142:ILE:HG12	2.01	0.42
35:J:35:ARG:HD3	35:J:40:HIS:CD2	2.54	0.42
37:L:17:LYS:HE3	37:L:27:LEU:CD2	2.50	0.42
46:U:52:ASN:OD1	46:U:54:PRO:HD3	2.19	0.42
57:5:71:CYS:HB3	57:5:117:LEU:HD12	2.02	0.42
57:5:117:LEU:HD22	57:5:120:ALA:HA	2.02	0.42
1:a:621:A:H2'	1:a:622:A:C8	2.55	0.42
1:a:1460:C:H2'	1:a:1461:G:C8	2.55	0.42
3:c:27:GLU:O	3:c:31:ASN:HB2	2.19	0.42
5:e:59:ILE:O	5:e:63:MET:HG2	2.20	0.42
7:g:56:SER:HB3	7:g:59:GLU:HG2	2.02	0.42
9:i:46:VAL:HA	9:i:49:GLN:HG3	2.02	0.42
21:u:28:LEU:O	21:u:30:GLU:N	2.46	0.42
26:A:698:C:O2'	26:A:734:A:N6	2.50	0.42
26:A:919:U:H2'	26:A:920:A:O4'	2.19	0.42
26:A:1070:A:H4'	26:A:1071:G:OP2	2.19	0.42
26:A:1319:C:H2'	26:A:1320:C:O4'	2.20	0.42
26:A:1486:U:O2'	26:A:1487:U:H5'	2.19	0.42
26:A:1736:U:H2'	26:A:1737:G:O4'	2.20	0.42
26:A:1816:C:H41	28:C:34:GLU:CD	2.27	0.42
26:A:1923:U:H2'	26:A:1924:C:C6	2.55	0.42
31:F:92:GLY:N	31:F:95:MET:HG2	2.34	0.42
42:Q:5:ARG:HB2	42:Q:8:ILE:HD11	2.00	0.42
44:S:84:ARG:HB2	44:S:96:ILE:HG13	2.00	0.42
1:a:545:C:H5''	4:d:68:GLU:HG2	2.02	0.42
1:a:1162:C:H2'	1:a:1163:A:H8	1.84	0.42
1:a:1251:A:H2'	1:a:1252:A:O4'	2.19	0.42
3:c:55:VAL:HB	3:c:66:THR:HB	2.00	0.42
3:c:56:ILE:CG2	3:c:63:ILE:HD11	2.50	0.42
4:d:108:ALA:H	4:d:112:GLU:CD	2.28	0.42
17:q:58:VAL:HG22	17:q:74:LEU:HD11	2.02	0.42
25:z:236:ILE:HG13	25:z:268:GLY:O	2.20	0.42
25:z:328:PRO:HA	25:z:378:GLU:OE1	2.20	0.42
26:A:158:U:O2	26:A:169:G:N2	2.52	0.42
26:A:310:A:O2'	26:A:311:A:H5''	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:935:C:O2'	26:A:936:A:H5'	2.19	0.42
26:A:2567:G:H2'	26:A:2568:U:C6	2.54	0.42
32:G:51:PHE:CE1	32:G:71:LEU:HD22	2.54	0.42
33:H:84:ALA:HB2	33:H:90:LEU:HD12	2.02	0.42
33:H:132:PHE:HB2	33:H:140:ALA:HB3	2.02	0.42
35:J:99:ARG:HA	35:J:102:GLU:HB3	2.01	0.42
36:K:7:MET:HE1	36:K:44:LYS:HG3	2.01	0.42
39:N:54:LEU:HD21	39:N:65:LEU:HB3	2.02	0.42
1:a:25:C:H2'	1:a:26:A:C8	2.55	0.42
1:a:741:G:H2'	1:a:742:G:O4'	2.20	0.42
1:a:868:C:H2'	1:a:869:G:O4'	2.20	0.42
1:a:1212:U:H4'	1:a:1213:A:C8	2.55	0.42
1:a:1225:A:H2'	1:a:1225:A:N3	2.35	0.42
3:c:8:GLY:HA2	3:c:11:LEU:HG	2.02	0.42
4:d:8:LEU:HD12	4:d:8:LEU:HA	1.89	0.42
25:z:87:TYR:C	25:z:89:LYS:H	2.28	0.42
26:A:97:C:H2'	26:A:98:G:O4'	2.19	0.42
26:A:255:A:H2'	26:A:256:A:O4'	2.19	0.42
26:A:594:U:H2'	26:A:595:C:C6	2.54	0.42
26:A:1843:C:O2'	28:C:253:GLY:O	2.32	0.42
26:A:2141:G:H2'	26:A:2142:A:H8	1.84	0.42
26:A:2648:G:N2	26:A:2673:G:H1'	2.35	0.42
27:B:43:C:O2'	31:F:91:ARG:HG2	2.20	0.42
28:C:2:VAL:HG21	28:C:201:LEU:HD12	2.02	0.42
35:J:43:GLU:CD	35:J:43:GLU:H	2.26	0.42
36:K:108:ARG:NH1	36:K:116:ILE:HD13	2.34	0.42
39:N:31:HIS:O	39:N:32:GLU:HB2	2.20	0.42
1:a:113:G:N3	1:a:353:A:O2'	2.53	0.42
3:c:34:SER:O	3:c:37:LYS:HB2	2.20	0.42
3:c:116:ALA:HB1	3:c:186:SER:OG	2.19	0.42
5:e:165:GLY:O	8:h:113:ARG:HD2	2.20	0.42
7:g:28:ILE:O	7:g:104:VAL:HG21	2.20	0.42
25:z:19:HIS:CD2	25:z:112:MET:HB3	2.55	0.42
25:z:163:PRO:HB3	25:z:166:ASP:HB2	2.02	0.42
26:A:218:A:OP2	26:A:218:A:C8	2.67	0.42
26:A:460:A:H2'	26:A:461:C:O4'	2.20	0.42
26:A:706:A:H2'	26:A:707:G:O4'	2.20	0.42
26:A:1366:A:H2'	26:A:1367:A:O4'	2.20	0.42
26:A:1943:U:H1'	26:A:1945:G:OP2	2.20	0.42
26:A:2016:U:H1'	52:O:2:VAL:HG13	2.02	0.42
26:A:2064:C:H2'	26:A:2065:C:C6	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2884:U:C5	52:O:49:ARG:HG2	2.54	0.42
27:B:85:G:H2'	27:B:86:G:H8	1.84	0.42
35:J:17:VAL:HG22	35:J:55:ILE:HB	2.02	0.42
37:L:57:LEU:C	37:L:59:ARG:H	2.27	0.42
56:4:30:GLU:HA	56:4:31:PRO:HD3	1.89	0.42
1:a:295:C:H2'	1:a:296:U:O4'	2.20	0.41
1:a:358:U:H2'	1:a:359:G:H8	1.82	0.41
1:a:786:G:H2'	1:a:787:A:O4'	2.20	0.41
1:a:1057:G:H2'	1:a:1058:G:O4'	2.20	0.41
1:a:1067:A:N1	1:a:1108:G:O2'	2.49	0.41
1:a:1346:A:H2'	1:a:1346:A:N3	2.35	0.41
2:b:16:GLY:O	2:b:202:ASN:HB2	2.20	0.41
2:b:185:ILE:HD12	2:b:212:TYR:CD2	2.54	0.41
19:s:62:THR:HG22	19:s:63:ASP:H	1.85	0.41
22:w:10:G:H2'	22:w:11:A:O4'	2.20	0.41
25:z:329:GLN:N	25:z:329:GLN:NE2	2.61	0.41
26:A:137:U:H3	26:A:142:A:H61	1.68	0.41
26:A:1078:U:H4'	26:A:1079:C:H5''	2.02	0.41
26:A:1717:A:H2'	26:A:1718:G:O4'	2.20	0.41
26:A:1884:G:H5'	26:A:1885:A:OP1	2.20	0.41
26:A:2146:C:O2'	26:A:2147:A:N7	2.52	0.41
26:A:2545:G:H2'	26:A:2546:U:O4'	2.20	0.41
26:A:2572:A:OP1	26:A:2574:G:H4'	2.20	0.41
26:A:2619:C:O2'	26:A:2620:C:H5'	2.19	0.41
26:A:2896:C:H2'	26:A:2897:U:C6	2.54	0.41
29:D:33:ARG:HG2	29:D:33:ARG:H	1.58	0.41
30:E:128:ALA:O	30:E:130:LYS:N	2.51	0.41
33:H:3:VAL:HA	33:H:38:PRO:HA	2.02	0.41
47:V:6:ALA:HB2	47:V:42:LEU:HB3	2.01	0.41
48:W:21:ARG:HB2	48:W:33:ILE:HG23	2.02	0.41
49:X:4:CYS:HA	49:X:32:LEU:HD21	2.01	0.41
53:1:10:LEU:HD23	53:1:50:GLU:HA	2.02	0.41
56:4:1:MET:HE2	56:4:36:ARG:HB2	2.02	0.41
1:a:165:G:H2'	1:a:166:U:C6	2.55	0.41
1:a:438:U:O2'	1:a:439:U:P	2.78	0.41
1:a:564:C:P	12:l:11:ARG:HH21	2.42	0.41
1:a:1327:C:H2'	1:a:1328:C:H6	1.86	0.41
1:a:1394:A:O2'	1:a:1402:4OC:HM21	2.20	0.41
1:a:1499:A:H5'	1:a:1519:MA6:H92	2.02	0.41
3:c:39:ARG:HG3	3:c:54:ILE:HD11	2.00	0.41
6:f:18:VAL:O	6:f:19:PRO:C	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:26:ASN:HD22	16:p:26:ASN:H	1.67	0.41
17:q:4:ILE:H	17:q:4:ILE:HG13	1.71	0.41
19:s:66:VAL:HG21	58:6:57:VAL:HG22	2.01	0.41
22:w:13:C:OP2	22:w:13:C:C6	2.73	0.41
22:w:54:5MU:H3'	22:w:55:PSU:O4	2.21	0.41
22:w:76:A:C2	26:A:2421:G:N1	2.86	0.41
26:A:832:U:H2'	26:A:833:A:C8	2.55	0.41
26:A:848:C:H2'	26:A:849:A:C8	2.55	0.41
26:A:1204:A:H4'	26:A:1205:A:C5'	2.49	0.41
26:A:1222:U:H2'	26:A:1223:G:H8	1.86	0.41
26:A:1726:C:H2'	26:A:1727:C:C6	2.54	0.41
26:A:1880:U:H2'	26:A:1881:C:C6	2.55	0.41
26:A:2038:G:H2'	26:A:2039:U:O4'	2.19	0.41
28:C:259:ASN:O	28:C:261:ARG:N	2.47	0.41
34:I:20:SER:HA	34:I:24:GLY:HA3	2.02	0.41
36:K:36:GLY:HA2	36:K:62:VAL:O	2.19	0.41
1:a:618:C:H5''	1:a:619:U:H5''	2.02	0.41
1:a:736:C:H2'	1:a:737:C:C6	2.55	0.41
1:a:1432:G:O2'	1:a:1433:A:H8	2.02	0.41
1:a:1504:G:H4'	1:a:1505:G:C4	2.56	0.41
1:a:1506:U:O2'	1:a:1507:A:H5'	2.20	0.41
9:i:106:ASP:OD2	9:i:108:ARG:HD3	2.19	0.41
11:k:88:PRO:HB2	11:k:89:GLY:H	1.69	0.41
11:k:127:ARG:HB2	21:u:34:ARG:HH22	1.86	0.41
22:v:6:G:H1	22:v:68:C:N4	2.18	0.41
22:v:65:G:H2'	22:v:66:C:O4'	2.20	0.41
22:w:18:G:O2'	22:w:19:G:P	2.78	0.41
22:w:64:G:H2'	22:w:65:C:O4'	2.20	0.41
25:z:84[A]:HIS:CD2	26:A:2661:G:O2'	2.72	0.41
25:z:124:GLN:HE21	25:z:124:GLN:HB2	1.69	0.41
26:A:591:U:H2'	26:A:592:A:C8	2.55	0.41
26:A:783:A:H2'	26:A:784:G:H4'	2.02	0.41
26:A:1201:U:H2'	26:A:1202:G:C8	2.55	0.41
26:A:1511:G:H2'	26:A:1512:C:C6	2.55	0.41
26:A:1801:A:H5'	26:A:2203:U:O2'	2.20	0.41
26:A:1930:G:O2'	26:A:1931:U:OP2	2.26	0.41
26:A:2756:U:H1'	26:A:2757:A:H5''	2.02	0.41
27:B:78:A:H2'	27:B:79:G:O4'	2.20	0.41
29:D:149:ASN:CG	29:D:150:GLN:N	2.78	0.41
31:F:135:ILE:HG13	31:F:135:ILE:H	1.64	0.41
42:Q:106:THR:O	42:Q:110:GLU:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:R:16:GLU:HB2	43:R:101:ILE:HG12	2.01	0.41
12:l:4:ASN:CG	12:l:8:ARG:HH22	2.28	0.41
22:w:19:G:OP2	22:w:19:G:H3'	2.20	0.41
22:w:19:G:HO2'	22:w:20:H2U:C4	2.22	0.41
22:w:69:C:N4	22:w:70:G:N7	2.68	0.41
25:z:311:LEU:HG	25:z:384:GLY:HA2	2.03	0.41
26:A:1418:G:N1	26:A:1579:A:OP2	2.44	0.41
26:A:2556:C:H2'	26:A:2557:G:O4'	2.20	0.41
28:C:132:ARG:NH1	33:H:93:SER:OG	2.54	0.41
29:D:151:THR:HB	29:D:152:PRO:HD3	2.01	0.41
33:H:66:ASN:HB3	33:H:134:VAL:O	2.20	0.41
34:I:72:THR:HG21	34:I:112:LYS:HB3	2.02	0.41
45:T:8:LEU:HD13	50:Y:21:LEU:HB3	2.02	0.41
49:X:31:ASN:O	49:X:51:SER:HA	2.19	0.41
1:a:218:U:H2'	1:a:219:U:O4'	2.20	0.41
1:a:338:A:H2'	1:a:339:C:O4'	2.20	0.41
1:a:423:G:H3'	1:a:423:G:N3	2.36	0.41
1:a:516:PSU:O5'	1:a:516:PSU:H6	2.03	0.41
1:a:731:G:H5'	1:a:766:A:H4'	2.03	0.41
1:a:878:A:H2'	1:a:879:C:C6	2.55	0.41
1:a:1126:U:H5	10:j:73:LEU:HD11	1.85	0.41
1:a:1218:C:H2'	1:a:1219:A:C8	2.56	0.41
1:a:1293:C:H2'	1:a:1294:G:C8	2.56	0.41
2:b:22:TRP:HB3	2:b:38:HIS:CD2	2.55	0.41
5:e:63:MET:O	5:e:67:ARG:HG3	2.21	0.41
6:f:32:ALA:O	6:f:34:GLY:N	2.46	0.41
24:y:58:A:H1'	24:y:60:U:H5	1.86	0.41
26:A:463:G:N2	26:A:466:A:OP2	2.36	0.41
26:A:813:U:H2'	26:A:814:C:C6	2.55	0.41
26:A:1045:C:H5'	26:A:1046:A:C5'	2.50	0.41
26:A:1235:G:N1	26:A:1236:G:N2	2.68	0.41
26:A:2709:G:H2'	26:A:2710:C:C6	2.55	0.41
29:D:110:THR:HG21	29:D:169:ARG:HH11	1.85	0.41
37:L:123:ARG:HA	37:L:143:GLU:O	2.20	0.41
40:O:33:ARG:HG2	40:O:34:HIS:CD2	2.55	0.41
42:Q:34:ALA:O	42:Q:38:VAL:HG23	2.21	0.41
47:V:83:LYS:HA	47:V:84:PRO:HD3	1.91	0.41
56:4:5:ALA:O	56:4:38:GLY:HA2	2.21	0.41
1:a:380:G:N2	1:a:383:A:OP2	2.51	0.41
1:a:1007:U:H2'	1:a:1008:U:C6	2.55	0.41
1:a:1067:A:H4'	1:a:1068:G:O5'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1317:C:OP2	14:n:27:LYS:HE2	2.21	0.41
1:a:1329:A:H5''	13:m:24:VAL:HA	2.02	0.41
4:d:173:ASP:HB3	4:d:178:GLU:H	1.85	0.41
6:f:44:ARG:HA	6:f:57:ALA:O	2.21	0.41
7:g:85:GLN:HB2	7:g:147:ASN:ND2	2.35	0.41
21:u:18:PHE:HA	21:u:21:SER:HB3	2.03	0.41
25:z:92:ILE:CG2	62:z:401:KIR:H371	2.46	0.41
26:A:609:A:H2'	26:A:610:C:O4'	2.21	0.41
26:A:911:A:H2'	38:M:9:PHE:CZ	2.56	0.41
26:A:974:G:C8	26:A:990:A:N6	2.76	0.41
26:A:1287:A:H5'	39:N:103:ARG:NH1	2.36	0.41
26:A:1562:U:H2'	26:A:1563:U:O4'	2.20	0.41
26:A:1754:A:N1	26:A:2716:C:O2'	2.36	0.41
26:A:1826:G:OP1	28:C:222:THR:HG23	2.19	0.41
26:A:2108:A:H2'	26:A:2109:U:O4'	2.21	0.41
26:A:2746:U:H5''	32:G:137:LYS:HG2	2.01	0.41
26:A:2803:G:H2'	26:A:2804:U:C6	2.56	0.41
29:D:43:ASP:HB3	29:D:45:TYR:CE2	2.55	0.41
32:G:88:LEU:HG	32:G:161:VAL:HG22	2.03	0.41
34:I:33:ASN:HB3	34:I:36:GLU:HG2	2.01	0.41
38:M:34:LYS:HA	38:M:101:VAL:HA	2.01	0.41
42:Q:75:TYR:CZ	42:Q:79:ILE:HG13	2.55	0.41
42:Q:109:VAL:HG12	42:Q:113:LYS:HE2	2.02	0.41
45:T:80:TRP:CD1	45:T:80:TRP:H	2.38	0.41
1:a:633:G:H2'	1:a:634:C:C6	2.55	0.41
1:a:707:U:H2'	1:a:708:C:C6	2.55	0.41
1:a:945:G:N1	1:a:1337:G:C2	2.89	0.41
1:a:985:C:H2'	1:a:986:U:H6	1.85	0.41
1:a:1124:G:O2'	1:a:1145:A:N1	2.52	0.41
3:c:31:ASN:HD21	3:c:58:ARG:HD2	1.84	0.41
14:n:7:ALA:O	14:n:10:VAL:HG12	2.20	0.41
17:q:30:HIS:CD2	17:q:32:ILE:H	2.39	0.41
21:u:5:VAL:HG22	21:u:7:GLU:HG2	2.02	0.41
25:z:84[A]:HIS:CD2	25:z:85:ALA:N	2.81	0.41
26:A:340:A:H2'	26:A:341:C:O4'	2.21	0.41
26:A:833:A:H2'	26:A:834:G:H8	1.85	0.41
26:A:869:G:H1'	38:M:8:LYS:HD2	2.02	0.41
26:A:1132:U:H3'	26:A:1132:U:OP2	2.21	0.41
26:A:1413:A:H2'	26:A:1414:C:O4'	2.20	0.41
26:A:1454:C:H5'	39:N:63:ARG:NH2	2.36	0.41
26:A:1495:A:H8	26:A:1495:A:O5'	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1529:G:H2'	26:A:1530:G:O4'	2.20	0.41
26:A:1957:C:H2'	26:A:1958:C:C6	2.56	0.41
26:A:2230:G:H2'	26:A:2231:U:C6	2.56	0.41
26:A:2674:G:H5'	36:K:30:ARG:HH21	1.85	0.41
28:C:24:HIS:HB3	28:C:81:GLU:OE1	2.20	0.41
41:P:27:VAL:HG12	41:P:29:VAL:HG23	2.01	0.41
1:a:1144:G:C6	1:a:1145:A:N6	2.89	0.41
1:a:1496:C:H2'	1:a:1497:G:O4'	2.21	0.41
3:c:24:ASN:O	3:c:28:PHE:HB2	2.21	0.41
4:d:166:LYS:HA	4:d:167:PRO:HD3	1.83	0.41
9:i:27:ILE:HG23	9:i:62:LEU:HB2	2.03	0.41
22:w:8:4SU:C5'	22:w:49:G:H5''	2.27	0.41
22:w:11:A:O5'	22:w:11:A:H8	2.04	0.41
22:w:44:A:N1	22:w:45:G:C4	2.89	0.41
26:A:192:C:H2'	26:A:193:U:H5'	2.03	0.41
26:A:1292:G:H2'	26:A:1293:C:C6	2.56	0.41
26:A:2599:G:C8	28:C:235:GLU:HG2	2.56	0.41
26:A:2837:A:H2'	26:A:2838:G:H8	1.86	0.41
29:D:38:LYS:O	29:D:46:ARG:HA	2.21	0.41
38:M:33:LEU:HD12	38:M:129:THR:O	2.20	0.41
38:M:51:ARG:C	38:M:53:MET:H	2.28	0.41
39:N:82:GLU:O	39:N:86:ARG:HB2	2.21	0.41
40:O:92:PHE:HB2	40:O:117:PHE:CE1	2.56	0.41
46:U:40:LEU:HB3	46:U:59:GLU:HG3	2.03	0.41
57:5:49:GLY:H	57:5:51:TYR:HE2	1.68	0.41
1:a:228:A:H2'	1:a:229:U:O4'	2.21	0.41
1:a:530:G:O6	23:x:21:C:H1'	2.21	0.41
1:a:707:U:O2'	11:k:38:GLY:O	2.33	0.41
1:a:952:U:O4	13:m:102:LYS:HE2	2.21	0.41
1:a:1302:C:H42	13:m:13:HIS:CD2	2.38	0.41
2:b:75:ALA:HB1	2:b:163:ILE:HD13	2.03	0.41
3:c:29:ALA:HB2	14:n:76:LYS:O	2.20	0.41
4:d:77:GLU:HA	4:d:80:ARG:HG2	2.02	0.41
4:d:115:GLN:O	4:d:115:GLN:HG3	2.20	0.41
5:e:104:ILE:HG13	5:e:111:ARG:HG3	2.02	0.41
6:f:24:ARG:O	6:f:27:ALA:HB3	2.21	0.41
7:g:97:ALA:HA	7:g:100:MET:HE2	2.02	0.41
8:h:85:TYR:CD1	8:h:123:GLU:HB2	2.56	0.41
9:i:49:GLN:C	9:i:51:LEU:N	2.78	0.41
10:j:88:MET:C	10:j:90:LEU:H	2.29	0.41
15:o:17:ASP:OD1	15:o:17:ASP:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:47:ASP:N	17:q:47:ASP:OD1	2.54	0.41
18:r:41:SER:HB3	18:r:51:GLN:HE21	1.85	0.41
21:u:46:ARG:O	21:u:49:ALA:HB3	2.21	0.41
61:v:105:FME:HA	26:A:2063:C:H1'	2.03	0.41
22:w:2:G:C6	22:w:70:G:O6	2.73	0.41
22:w:11:A:N1	22:w:25:C:N4	2.68	0.41
25:z:247:ILE:O	25:z:248:LYS:HB3	2.21	0.41
26:A:306:U:H2'	26:A:307:G:O4'	2.21	0.41
26:A:329:G:OP2	46:U:68:ASN:ND2	2.54	0.41
26:A:507:A:H5''	26:A:508:A:H3'	2.02	0.41
26:A:779:U:OP1	28:C:48:ILE:HG22	2.21	0.41
26:A:859:G:H1'	26:A:860:U:H5	1.85	0.41
26:A:995:C:O2'	42:Q:92:LYS:HE2	2.20	0.41
26:A:1130:U:HO2'	26:A:1131:G:P	2.42	0.41
26:A:1739:A:H2'	26:A:1740:G:O4'	2.21	0.41
26:A:1741:C:H2'	26:A:1742:U:C6	2.56	0.41
26:A:1847:G:O2'	26:A:1848:A:H8	2.03	0.41
26:A:1993:U:H4'	29:D:133:THR:HG22	2.02	0.41
26:A:2045:C:H5''	52:O:14:MET:SD	2.61	0.41
26:A:2368:C:H2'	26:A:2369:A:H8	1.86	0.41
27:B:45:A:O4'	31:F:91:ARG:NH2	2.54	0.41
28:C:209:ALA:HA	28:C:212:TRP:CE2	2.56	0.41
28:C:252:LYS:HE3	28:C:252:LYS:HB2	1.83	0.41
29:D:14:ILE:HA	41:P:11:GLN:OE1	2.21	0.41
30:E:47:LYS:HE2	30:E:47:LYS:HB3	1.87	0.41
30:E:97:ASN:O	30:E:100:MET:N	2.51	0.41
31:F:175:PRO:HB2	31:F:176:PHE:H	1.71	0.41
43:R:7:SER:C	43:R:9:GLY:H	2.29	0.41
49:X:12:VAL:HG23	49:X:28:PHE:HB2	2.03	0.41
54:2:34:ARG:HE	54:2:39:ARG:HD2	1.86	0.41
1:a:120:A:H1'	1:a:122:G:N7	2.36	0.41
1:a:821:G:H2'	1:a:822:U:C6	2.56	0.41
4:d:58:GLN:O	4:d:59:LYS:C	2.63	0.41
7:g:110:ARG:HD3	7:g:122:GLU:OE2	2.21	0.41
14:n:73:PHE:CZ	14:n:78:GLY:HA2	2.56	0.41
21:u:3:ILE:N	21:u:19:LYS:HE3	2.36	0.41
22:v:62:C:H2'	22:v:63:C:C6	2.56	0.41
22:w:29:G:H2'	22:w:30:G:O4'	2.21	0.41
24:y:7:A:H3'	24:y:8:4SU:C5'	2.51	0.41
26:A:22:C:H2'	26:A:23:G:O4'	2.21	0.41
26:A:84:A:N7	26:A:101:A:H2	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:413:C:H2'	26:A:414:C:H6	1.85	0.41
26:A:737:C:H2'	26:A:738:G:O4'	2.21	0.41
26:A:2825:G:H5''	26:A:2825:G:N3	2.36	0.41
29:D:80:TRP:NE1	29:D:202:ILE:HD11	2.36	0.41
34:I:12:VAL:HB	34:I:13:ALA:H	1.68	0.41
42:Q:35:PHE:CZ	42:Q:39:ILE:HD11	2.56	0.41
43:R:11:GLN:OE1	43:R:11:GLN:N	2.53	0.41
45:T:8:LEU:HD11	50:Y:22:LEU:HD12	2.03	0.41
52:O:27:LEU:HD23	52:O:36:LYS:HB3	2.03	0.41
55:3:36:ALA:O	55:3:39:ARG:HB2	2.20	0.41
55:3:51:LYS:HE3	55:3:51:LYS:HB2	1.87	0.41
3:c:133:MET:HG3	3:c:150:VAL:CG2	2.51	0.40
7:g:86:VAL:HA	7:g:87:PRO:HD2	1.99	0.40
8:h:24:VAL:O	8:h:59:GLU:HA	2.22	0.40
8:h:95:MET:O	8:h:98:LEU:HG	2.21	0.40
9:i:32:ARG:HA	9:i:32:ARG:HD3	1.94	0.40
12:l:33:CYS:HA	12:l:54:VAL:HA	2.03	0.40
18:r:67:LEU:HA	18:r:68:PRO:HD3	1.90	0.40
22:w:12:G:H2'	22:w:13:C:C6	2.56	0.40
25:z:127:VAL:HA	25:z:128:PRO:HD3	1.92	0.40
25:z:190:GLU:O	25:z:193:GLY:N	2.54	0.40
25:z:211:LEU:HD13	25:z:293:ALA:HB2	2.02	0.40
26:A:1071:G:N2	26:A:1089:A:O2'	2.54	0.40
26:A:1278:C:H2'	26:A:1279:G:H8	1.86	0.40
26:A:2039:U:H2'	26:A:2040:G:C8	2.55	0.40
26:A:2040:G:H2'	26:A:2041:U:O4'	2.20	0.40
26:A:2475:C:H6	26:A:2475:C:O5'	2.04	0.40
26:A:2804:U:H2'	26:A:2805:C:C6	2.56	0.40
28:C:212:TRP:CD1	28:C:212:TRP:C	2.99	0.40
34:I:33:ASN:HB2	34:I:64:ARG:NH1	2.34	0.40
38:M:109:PRO:HD2	38:M:112:LEU:HD23	2.03	0.40
42:Q:78:PHE:HE1	42:Q:109:VAL:HA	1.85	0.40
44:S:14:ALA:HB1	44:S:18:ARG:HH21	1.85	0.40
44:S:34:ASP:HB3	52:O:27:LEU:HD22	2.03	0.40
1:a:512:U:H2'	1:a:513:C:C6	2.56	0.40
1:a:581:G:N1	1:a:759:A:OP2	2.42	0.40
1:a:608:A:H2'	1:a:609:A:O4'	2.21	0.40
1:a:626:G:H2'	1:a:627:G:C8	2.57	0.40
1:a:1333:A:H2'	1:a:1334:G:O4'	2.22	0.40
1:a:1507:A:H2'	1:a:1508:A:C8	2.57	0.40
2:b:53:LEU:HD23	2:b:56:LEU:HD12	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:3:HIS:H	6:f:92:THR:HG22	1.85	0.40
17:q:59:GLU:O	17:q:60:ILE:HG13	2.21	0.40
25:z:124:GLN:O	62:z:401:KIR:N26	2.45	0.40
25:z:154:ARG:HD3	25:z:165:ASP:HA	2.04	0.40
25:z:211:LEU:O	25:z:232:GLU:HB3	2.22	0.40
26:A:456:C:C2	45:T:73:ARG:NH2	2.87	0.40
26:A:2092:U:H4'	26:A:2093:G:O5'	2.20	0.40
26:A:2405:G:H1'	26:A:2412:A:H61	1.87	0.40
26:A:2844:G:H2'	26:A:2845:U:O4'	2.20	0.40
27:B:54:G:H2'	27:B:55:U:C6	2.56	0.40
28:C:70:LYS:HD2	28:C:73:ILE:HD12	2.03	0.40
35:J:40:HIS:CE1	35:J:41:LYS:HG3	2.56	0.40
54:2:21:ARG:O	54:2:27:GLY:HA3	2.21	0.40
56:4:7:VAL:HG22	56:4:38:GLY:HA3	2.03	0.40
1:a:411:A:H4'	1:a:412:A:OP1	2.21	0.40
1:a:500:G:H2'	1:a:501:C:C6	2.57	0.40
1:a:994:A:N7	1:a:1216:A:H4'	2.35	0.40
10:j:37:ARG:HD3	10:j:37:ARG:HA	1.89	0.40
21:u:28:LEU:C	21:u:30:GLU:N	2.76	0.40
25:z:11:HIS:O	25:z:204:ARG:NH2	2.55	0.40
25:z:298:ILE:HD13	25:z:367:ALA:HB1	2.03	0.40
26:A:78:U:OP2	50:Y:2:LYS:HD2	2.21	0.40
26:A:190:A:OP2	49:X:25:LYS:NZ	2.53	0.40
26:A:376:G:H2'	26:A:377:G:H8	1.86	0.40
26:A:739:A:H1'	26:A:740:C:H5	1.86	0.40
26:A:1443:U:H2'	26:A:1444:G:H8	1.87	0.40
26:A:1591:A:H2'	26:A:1592:C:O4'	2.21	0.40
26:A:1824:G:O3'	28:C:246:PRO:HD3	2.21	0.40
29:D:11:MET:HE2	29:D:11:MET:HB3	1.97	0.40
29:D:14:ILE:HD11	29:D:188:LEU:HD13	2.03	0.40
33:H:9:VAL:HG12	33:H:11:ASN:H	1.85	0.40
34:I:37:PHE:CZ	34:I:58:ILE:HD12	2.56	0.40
39:N:47:VAL:C	39:N:50:PRO:HD2	2.47	0.40
41:P:77:SER:HA	41:P:78:PRO:HD3	1.89	0.40
47:V:32:GLY:O	47:V:93:ARG:NH1	2.52	0.40
1:a:70:U:H4'	1:a:71:A:O5'	2.20	0.40
1:a:178:C:H2'	1:a:179:A:H8	1.86	0.40
1:a:721:G:H4'	1:a:722:G:O4'	2.21	0.40
5:e:10:LEU:H	5:e:10:LEU:HG	1.58	0.40
5:e:33:THR:HG22	5:e:51:LYS:HB3	2.04	0.40
10:j:76:ILE:C	10:j:78:GLU:H	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:58:MET:HE3	15:o:58:MET:HB2	1.86	0.40
25:z:154:ARG:HH21	25:z:165:ASP:HA	1.87	0.40
26:A:20:C:H2'	26:A:21:A:H8	1.87	0.40
26:A:758:C:O2	26:A:758:C:H2'	2.20	0.40
26:A:981:A:OP2	26:A:982:C:N4	2.43	0.40
26:A:1023:U:H4'	26:A:1123:C:OP1	2.21	0.40
26:A:1180:U:H2'	26:A:1181:U:H5'	2.03	0.40
26:A:1730:C:O2	26:A:1731:G:N1	2.54	0.40
26:A:1988:G:H2'	26:A:1989:G:O4'	2.22	0.40
26:A:2106:U:H2'	26:A:2107:G:C8	2.56	0.40
27:B:17:C:H2'	27:B:18:G:O4'	2.22	0.40
29:D:101:PHE:HA	29:D:104:VAL:HG22	2.02	0.40
38:M:41:LEU:HG	38:M:96:ILE:HG13	2.03	0.40
41:P:51:ASN:O	41:P:52:ARG:HD3	2.21	0.40
42:Q:71:ASN:N	42:Q:71:ASN:ND2	2.69	0.40
45:T:44:LYS:HG3	45:T:55:VAL:HG11	2.04	0.40
47:V:30:ILE:HG21	47:V:70:ILE:HG21	2.02	0.40
58:6:2:LYS:O	58:6:5:ILE:HG12	2.21	0.40
1:a:134:G:H2'	1:a:135:C:O4'	2.22	0.40
1:a:193:C:H2'	1:a:194:C:C6	2.57	0.40
1:a:422:C:O2'	1:a:423:G:N2	2.54	0.40
1:a:716:A:H1'	11:k:118:ASN:O	2.22	0.40
1:a:954:G:H2'	1:a:955:U:O4'	2.22	0.40
3:c:191:THR:HG23	3:c:192:TYR:CD2	2.57	0.40
4:d:58:GLN:O	4:d:62:ARG:HG2	2.22	0.40
7:g:102:TRP:CZ2	7:g:140:VAL:HG21	2.56	0.40
10:j:88:MET:O	10:j:90:LEU:N	2.55	0.40
13:m:15:VAL:O	13:m:19:THR:HG23	2.21	0.40
22:v:51:U:H2'	22:v:52:C:C6	2.57	0.40
22:w:2:G:C6	22:w:3:C:N4	2.90	0.40
22:w:8:4SU:H6	22:w:8:4SU:H3'	2.02	0.40
22:w:27:U:N3	22:w:44:A:C6	2.90	0.40
22:w:47:U:H6	22:w:47:U:P	2.45	0.40
26:A:21:A:H2'	26:A:22:C:O4'	2.21	0.40
26:A:753:A:H2'	26:A:754:U:C6	2.56	0.40
26:A:974:G:H4'	26:A:975:A:OP1	2.19	0.40
26:A:1045:C:H1'	26:A:1047:G:N3	2.36	0.40
26:A:1078:U:O2'	26:A:1088:A:H5''	2.22	0.40
26:A:1275:A:H4'	26:A:1276:A:O5'	2.20	0.40
26:A:1752:C:H2'	26:A:1753:G:C8	2.56	0.40
26:A:2060:A:H1'	26:A:2502:G:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2697:G:H2'	26:A:2698:U:O4'	2.21	0.40
29:D:6:GLY:O	29:D:201:LEU:HB2	2.21	0.40
29:D:20:VAL:HG22	36:K:72:PRO:HB2	2.03	0.40
50:Y:28:LEU:HD13	50:Y:42:LEU:HB3	2.03	0.40
50:Y:44:LYS:HA	50:Y:47:ARG:NH2	2.37	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	
2	b	216/240 (90%)	183 (85%)	23 (11%)	10 (5%)	2	7
3	c	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	12	39
4	d	203/206 (98%)	172 (85%)	21 (10%)	10 (5%)	1	6
5	e	155/167 (93%)	130 (84%)	16 (10%)	9 (6%)	1	4
6	f	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	1	4
7	g	149/179 (83%)	124 (83%)	15 (10%)	10 (7%)	1	3
8	h	127/130 (98%)	110 (87%)	14 (11%)	3 (2%)	4	18
9	i	125/130 (96%)	98 (78%)	19 (15%)	8 (6%)	1	3
10	j	96/103 (93%)	74 (77%)	16 (17%)	6 (6%)	1	3
11	k	114/129 (88%)	92 (81%)	16 (14%)	6 (5%)	1	5
12	l	121/124 (98%)	96 (79%)	20 (16%)	5 (4%)	2	9
13	m	112/118 (95%)	99 (88%)	8 (7%)	5 (4%)	2	8
14	n	99/102 (97%)	82 (83%)	12 (12%)	5 (5%)	1	6
15	o	86/89 (97%)	71 (83%)	10 (12%)	5 (6%)	1	4
16	p	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	4	17
17	q	78/84 (93%)	65 (83%)	8 (10%)	5 (6%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	r	63/75 (84%)	53 (84%)	5 (8%)	5 (8%)	1	2
19	s	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
20	t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	4	18
21	u	63/71 (89%)	44 (70%)	14 (22%)	5 (8%)	1	2
25	z	368/393 (94%)	327 (89%)	35 (10%)	6 (2%)	7	27
28	C	269/273 (98%)	243 (90%)	21 (8%)	5 (2%)	6	23
29	D	207/209 (99%)	185 (89%)	20 (10%)	2 (1%)	12	39
30	E	199/201 (99%)	172 (86%)	20 (10%)	7 (4%)	3	12
31	F	175/179 (98%)	149 (85%)	20 (11%)	6 (3%)	3	12
32	G	174/177 (98%)	148 (85%)	21 (12%)	5 (3%)	3	15
33	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	4	16
34	I	139/142 (98%)	110 (79%)	20 (14%)	9 (6%)	1	3
35	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	9	30
36	K	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	4	17
37	L	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1	2
38	M	134/136 (98%)	117 (87%)	14 (10%)	3 (2%)	5	20
39	N	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	4	17
40	O	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	14	41
41	P	112/115 (97%)	93 (83%)	18 (16%)	1 (1%)	14	41
42	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
43	R	101/103 (98%)	82 (81%)	17 (17%)	2 (2%)	6	22
44	S	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	1	4
45	T	91/100 (91%)	77 (85%)	11 (12%)	3 (3%)	3	13
46	U	100/104 (96%)	80 (80%)	17 (17%)	3 (3%)	3	14
47	V	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	5	20
48	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	9	30
49	X	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	9	32
50	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	7	27
51	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
52	0	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	6	23
53	1	48/55 (87%)	43 (90%)	5 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
55	3	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	7	27
56	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
57	5	129/165 (78%)	100 (78%)	22 (17%)	7 (5%)	1	5
58	6	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	7	27
All	All	6215/6613 (94%)	5318 (86%)	691 (11%)	206 (3%)	5	13

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	156	LEU
5	e	122	VAL
6	f	63	ASN
9	i	12	LYS
9	i	71	ILE
10	j	57	VAL
10	j	75	ASP
10	j	89	ARG
16	p	8	ARG
17	q	79	GLU
18	r	17	VAL
28	C	204	LEU
31	F	175	PRO
32	G	108	PHE
35	J	81	ILE
36	K	93	GLN
37	L	15	ALA
37	L	85	VAL
37	L	128	THR
44	S	67	ASP
46	U	6	ARG
46	U	97	SER
49	X	31	ASN
55	3	27	ASN
2	b	17	HIS
2	b	19	THR
2	b	179	GLY
3	c	13	ILE
4	d	26	ALA
4	d	108	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	e	23	THR
5	e	93	VAL
7	g	16	LYS
7	g	56	SER
7	g	63	VAL
7	g	112	ASP
7	g	145	GLU
8	h	66	GLN
9	i	57	VAL
10	j	29	ALA
10	j	77	VAL
11	k	76	TYR
11	k	77	GLY
11	k	88	PRO
12	l	75	GLU
13	m	104	ASN
14	n	54	ASP
15	o	21	THR
15	o	45	HIS
17	q	17	GLU
17	q	49	ASN
18	r	46	THR
20	t	68	LYS
21	u	12	ASP
28	C	195	GLY
28	C	231	HIS
33	H	9	VAL
34	I	64	ARG
34	I	89	SER
34	I	92	PRO
36	K	35	VAL
36	K	110	GLU
37	L	29	LYS
37	L	31	GLY
37	L	111	ILE
38	M	70	ASP
40	O	66	GLY
41	P	65	ASN
43	R	43	ASN
43	R	54	VAL
44	S	2	GLU
44	S	3	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	T	37	ASP
45	T	38	ALA
45	T	71	GLY
50	Y	24	GLU
57	5	55	VAL
2	b	73	ARG
2	b	87	ASP
2	b	153	MET
4	d	7	LYS
4	d	31	CYS
4	d	152	SER
4	d	166	LYS
4	d	174	ALA
5	e	98	ALA
5	e	99	SER
5	e	121	ASN
6	f	54	LEU
6	f	92	THR
7	g	64	ALA
7	g	95	ARG
8	h	74	ILE
9	i	90	ASP
9	i	107	ALA
9	i	125	GLN
10	j	35	GLN
11	k	14	GLN
12	l	2	THR
12	l	46	SER
13	m	6	ILE
13	m	7	ASN
13	m	113	LYS
14	n	22	LYS
14	n	38	ASP
14	n	55	SER
15	o	2	LEU
15	o	13	GLU
16	p	49	GLY
17	q	16	MET
20	t	76	ALA
21	u	29	ALA
21	u	32	ARG
21	u	34	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	C	239	PHE
30	E	89	PRO
30	E	122	GLU
32	G	44	HIS
32	G	45	ALA
33	H	15	LEU
34	I	12	VAL
37	L	88	GLY
38	M	6	ARG
39	N	59	SER
44	S	62	ASP
57	5	88	HIS
57	5	118	ILE
58	6	40	CYS
2	b	11	ALA
2	b	88	GLN
2	b	126	ASP
5	e	100	GLU
5	e	102	THR
6	f	56	LYS
6	f	86	ARG
6	f	99	ALA
7	g	29	LEU
8	h	22	ALA
9	i	99	LYS
11	k	92	ARG
12	l	23	LEU
14	n	2	LYS
15	o	75	ALA
18	r	18	GLN
18	r	71	ASP
25	z	9	LYS
29	D	32	ASN
30	E	80	SER
30	E	160	ALA
31	F	20	ASN
31	F	142	TYR
31	F	173	ASP
31	F	176	PHE
33	H	2	GLN
34	I	6	ALA
34	I	20	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L	25	SER
39	N	117	ASP
44	S	65	ASP
47	V	58	SER
48	W	8	ASN
52	0	2	VAL
57	5	22	ALA
57	5	90	GLY
57	5	130	PRO
2	b	14	HIS
4	d	34	GLU
18	r	70	THR
25	z	164	GLY
25	z	207	ASP
25	z	249	GLU
30	E	84	THR
31	F	174	PHE
32	G	70	LEU
33	H	3	VAL
34	I	22	PRO
34	I	100	ILE
35	J	82	GLY
37	L	94	THR
4	d	6	PRO
4	d	28	ASP
9	i	13	SER
25	z	14	VAL
29	D	148	GLN
30	E	83	VAL
34	I	38	CYS
37	L	119	PRO
44	S	101	SER
11	k	119	GLY
12	l	44	PRO
28	C	168	GLY
37	L	26	GLY
38	M	69	PRO
39	N	116	VAL
17	q	20	ILE
21	u	9	GLU
46	U	38	ILE
7	g	5	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	z	286	ILE
47	V	15	GLY
57	5	108	VAL
7	g	28	ILE
30	E	129	PRO
5	e	26	GLY
13	m	9	PRO
32	G	155	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/198 (91%)	173 (96%)	7 (4%)	28	63
3	c	170/190 (90%)	159 (94%)	11 (6%)	15	44
4	d	172/173 (99%)	166 (96%)	6 (4%)	32	66
5	e	114/126 (90%)	104 (91%)	10 (9%)	9	29
6	f	87/116 (75%)	82 (94%)	5 (6%)	18	49
7	g	124/147 (84%)	119 (96%)	5 (4%)	28	62
8	h	104/105 (99%)	103 (99%)	1 (1%)	68	89
9	i	105/107 (98%)	103 (98%)	2 (2%)	50	79
10	j	86/90 (96%)	82 (95%)	4 (5%)	23	56
11	k	89/99 (90%)	86 (97%)	3 (3%)	32	66
12	l	103/104 (99%)	99 (96%)	4 (4%)	28	63
13	m	92/96 (96%)	88 (96%)	4 (4%)	26	60
14	n	79/84 (94%)	75 (95%)	4 (5%)	21	53
15	o	76/77 (99%)	75 (99%)	1 (1%)	61	86
16	p	65/65 (100%)	61 (94%)	4 (6%)	16	46
17	q	74/78 (95%)	72 (97%)	2 (3%)	39	73
18	r	48/65 (74%)	47 (98%)	1 (2%)	47	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	s	70/79 (89%)	65 (93%)	5 (7%)	13	40
20	t	65/66 (98%)	63 (97%)	2 (3%)	35	69
21	u	44/61 (72%)	44 (100%)	0	100	100
25	z	311/326 (95%)	298 (96%)	13 (4%)	26	60
28	C	216/218 (99%)	210 (97%)	6 (3%)	38	72
29	D	164/164 (100%)	163 (99%)	1 (1%)	78	93
30	E	165/165 (100%)	161 (98%)	4 (2%)	43	75
31	F	148/150 (99%)	138 (93%)	10 (7%)	14	42
32	G	137/138 (99%)	136 (99%)	1 (1%)	76	92
33	H	114/114 (100%)	114 (100%)	0	100	100
34	I	109/110 (99%)	103 (94%)	6 (6%)	19	50
35	J	116/116 (100%)	114 (98%)	2 (2%)	53	82
36	K	103/104 (99%)	98 (95%)	5 (5%)	22	54
37	L	102/103 (99%)	100 (98%)	2 (2%)	48	78
38	M	109/109 (100%)	108 (99%)	1 (1%)	70	90
39	N	100/103 (97%)	97 (97%)	3 (3%)	36	70
40	O	86/87 (99%)	84 (98%)	2 (2%)	44	76
41	P	99/100 (99%)	94 (95%)	5 (5%)	21	53
42	Q	89/90 (99%)	85 (96%)	4 (4%)	24	58
43	R	84/84 (100%)	82 (98%)	2 (2%)	43	75
44	S	93/93 (100%)	90 (97%)	3 (3%)	34	68
45	T	80/84 (95%)	78 (98%)	2 (2%)	42	74
46	U	83/85 (98%)	81 (98%)	2 (2%)	43	75
47	V	78/78 (100%)	77 (99%)	1 (1%)	61	86
48	W	57/63 (90%)	56 (98%)	1 (2%)	51	80
49	X	67/68 (98%)	67 (100%)	0	100	100
50	Y	55/55 (100%)	54 (98%)	1 (2%)	51	80
51	Z	48/49 (98%)	48 (100%)	0	100	100
52	0	47/48 (98%)	45 (96%)	2 (4%)	26	60
53	1	45/49 (92%)	44 (98%)	1 (2%)	45	77
54	2	38/38 (100%)	37 (97%)	1 (3%)	40	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	3	51/52 (98%)	50 (98%)	1 (2%)	48 78
56	4	34/34 (100%)	33 (97%)	1 (3%)	37 71
57	5	100/123 (81%)	97 (97%)	3 (3%)	36 70
58	6	59/62 (95%)	58 (98%)	1 (2%)	53 82
All	All	5134/5388 (95%)	4966 (97%)	168 (3%)	34 67

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	9	LEU
2	b	35	ASN
2	b	71	THR
2	b	162	VAL
2	b	185	ILE
2	b	198	VAL
2	b	202	ASN
3	c	3	LYS
3	c	40	GLN
3	c	96	VAL
3	c	102	ILE
3	c	105	VAL
3	c	127	VAL
3	c	133	MET
3	c	149	LYS
3	c	156	LEU
3	c	161	ILE
3	c	199	VAL
4	d	16	THR
4	d	52	VAL
4	d	115	GLN
4	d	119	HIS
4	d	141	VAL
4	d	196	GLU
5	e	10	LEU
5	e	11	GLN
5	e	45	VAL
5	e	51	LYS
5	e	75	LEU
5	e	105	ILE
5	e	122	VAL
5	e	140	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	e	156	ARG
5	e	158	LYS
6	f	54	LEU
6	f	64	VAL
6	f	74	LEU
6	f	86	ARG
6	f	89	VAL
7	g	6	ILE
7	g	58	LEU
7	g	75	LYS
7	g	83	THR
7	g	134	VAL
8	h	58	LEU
9	i	54	VAL
9	i	60	LEU
10	j	10	LEU
10	j	64	GLN
10	j	77	VAL
10	j	98	VAL
11	k	30	ILE
11	k	39	ASN
11	k	109	ILE
12	l	20	VAL
12	l	28	GLN
12	l	54	VAL
12	l	63	THR
13	m	6	ILE
13	m	15	VAL
13	m	24	VAL
13	m	99	GLN
14	n	26	LEU
14	n	33	VAL
14	n	49	GLN
14	n	60	GLN
15	o	86	LEU
16	p	19	VAL
16	p	26	ASN
16	p	34	GLU
16	p	70	ARG
17	q	51	GLU
17	q	69	THR
18	r	24	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	s	10	ILE
19	s	48	ILE
19	s	57	VAL
19	s	59	VAL
19	s	62	THR
20	t	22	SER
20	t	26	MET
25	z	14	VAL
25	z	68	GLU
25	z	73	THR
25	z	79	VAL
25	z	104	VAL
25	z	183	GLU
25	z	190	GLU
25	z	238	VAL
25	z	329	GLN
25	z	337	VAL
25	z	338	THR
25	z	359	VAL
25	z	362	LEU
28	C	13	ARG
28	C	45	ASN
28	C	48	ILE
28	C	129	LEU
28	C	181	ARG
28	C	206	LYS
29	D	52	THR
30	E	7	ASP
30	E	41	GLN
30	E	96	VAL
30	E	187	VAL
31	F	3	LEU
31	F	5	ASP
31	F	9	ASP
31	F	30	VAL
31	F	39	VAL
31	F	55	ASP
31	F	90	LEU
31	F	95	MET
31	F	134	GLN
31	F	148	VAL
32	G	10	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	I	10	LEU
34	I	48	ILE
34	I	85	ILE
34	I	95	ASP
34	I	100	ILE
34	I	134	SER
35	J	57	LEU
35	J	64	VAL
36	K	8	LEU
36	K	32	TYR
36	K	58	LEU
36	K	61	VAL
36	K	73	ASP
37	L	27	LEU
37	L	110	VAL
38	M	46	ILE
39	N	15	SER
39	N	81	ASN
39	N	113	ILE
40	O	69	ASP
40	O	100	HIS
41	P	7	LEU
41	P	31	VAL
41	P	72	VAL
41	P	99	LEU
41	P	113	LEU
42	Q	36	GLN
42	Q	48	ASP
42	Q	71	ASN
42	Q	94	LEU
43	R	22	LEU
43	R	58	VAL
44	S	25	ARG
44	S	62	ASP
44	S	107	VAL
45	T	32	LEU
45	T	59	ASN
46	U	48	VAL
46	U	82	VAL
47	V	42	LEU
48	W	67	VAL
50	Y	40	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	0	22	THR
52	0	24	VAL
53	1	46	VAL
54	2	44	VAL
55	3	61	LEU
56	4	17	VAL
57	5	3	LEU
57	5	57	ASN
57	5	122	GLN
58	6	16	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	23	ASN
2	b	57	ASN
3	c	40	GLN
4	d	70	GLN
4	d	84	ASN
4	d	119	HIS
4	d	151	GLN
5	e	11	GLN
5	e	131	ASN
5	e	145	ASN
6	f	11	HIS
6	f	58	HIS
7	g	141	HIS
7	g	147	ASN
8	h	20	ASN
9	i	80	HIS
10	j	56	HIS
10	j	58	ASN
10	j	70	HIS
11	k	39	ASN
12	l	111	GLN
13	m	7	ASN
13	m	90	HIS
14	n	49	GLN
14	n	60	GLN
15	o	45	HIS
16	p	26	ASN
17	q	30	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	q	49	ASN
18	r	51	GLN
19	s	13	HIS
19	s	42	ASN
19	s	51	HIS
19	s	56	HIS
20	t	19	HIS
20	t	69	ASN
25	z	19	HIS
25	z	75	HIS
25	z	78	HIS
25	z	114	GLN
25	z	118	HIS
25	z	124	GLN
25	z	273	ASN
25	z	329	GLN
28	C	196	ASN
29	D	49	GLN
29	D	58	ASN
29	D	149	ASN
29	D	173	GLN
30	E	136	GLN
30	E	195	GLN
31	F	51	ASN
31	F	134	GLN
32	G	103	ASN
32	G	138	GLN
33	H	33	GLN
33	H	133	GLN
34	I	29	GLN
35	J	40	HIS
36	K	3	GLN
36	K	5	GLN
39	N	9	GLN
39	N	73	ASN
40	O	38	GLN
42	Q	71	ASN
44	S	7	HIS
44	S	9	HIS
44	S	40	ASN
45	T	70	HIS
46	U	53	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	U	65	GLN
47	V	75	GLN
50	Y	39	GLN
50	Y	41	HIS
52	0	4	GLN
52	0	5	ASN
54	2	29	GLN
58	6	65	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1538/1539 (99%)	244 (15%)	0
22	v	76/77 (98%)	18 (23%)	0
22	w	76/77 (98%)	43 (56%)	0
23	x	10/11 (90%)	1 (10%)	0
24	y	75/77 (97%)	19 (25%)	0
26	A	2898/2903 (99%)	549 (18%)	90 (3%)
27	B	119/120 (99%)	18 (15%)	4 (3%)
All	All	4792/4804 (99%)	892 (18%)	94 (1%)

All (892) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	14	U
1	a	22	G
1	a	30	U
1	a	32	A
1	a	39	G
1	a	47	C
1	a	49	U
1	a	51	A
1	a	71	A
1	a	85	U
1	a	86	G
1	a	87	C
1	a	94	G
1	a	95	C
1	a	120	A
1	a	121	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	130	A
1	a	174	A
1	a	175	C
1	a	181	A
1	a	183	C
1	a	184	G
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	246	A
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	281	G
1	a	283	U
1	a	289	G
1	a	306	A
1	a	321	A
1	a	328	C
1	a	345	C
1	a	346	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	355	C
1	a	367	U
1	a	368	U
1	a	372	C
1	a	373	A
1	a	387	U
1	a	392	C
1	a	398	U
1	a	406	G
1	a	412	A
1	a	413	G
1	a	414	A
1	a	422	C
1	a	423	G
1	a	424	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	429	U
1	a	430	A
1	a	439	U
1	a	467	U
1	a	468	A
1	a	482	A
1	a	484	G
1	a	485	U
1	a	486	U
1	a	496	A
1	a	497	G
1	a	500	G
1	a	511	C
1	a	527	7MG
1	a	531	U
1	a	532	A
1	a	536	C
1	a	547	A
1	a	559	A
1	a	561	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	574	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	579	A
1	a	597	G
1	a	618	C
1	a	626	G
1	a	633	G
1	a	641	U
1	a	642	A
1	a	654	G
1	a	661	G
1	a	665	A
1	a	671	G
1	a	687	A
1	a	688	G
1	a	701	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	702	A
1	a	703	G
1	a	724	G
1	a	731	G
1	a	755	G
1	a	777	A
1	a	792	A
1	a	793	U
1	a	794	A
1	a	814	A
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	832	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	871	U
1	a	874	G
1	a	884	U
1	a	890	G
1	a	902	G
1	a	914	A
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	979	C
1	a	981	U
1	a	991	U
1	a	992	U
1	a	993	G
1	a	994	A
1	a	1004	A
1	a	1026	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1028	C
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1053	G
1	a	1056	U
1	a	1065	U
1	a	1067	A
1	a	1085	U
1	a	1086	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1127	G
1	a	1129	C
1	a	1130	A
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1152	A
1	a	1159	U
1	a	1160	G
1	a	1168	U
1	a	1182	G
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1198	G
1	a	1200	C
1	a	1201	A
1	a	1202	U
1	a	1207	2MG
1	a	1212	U
1	a	1213	A
1	a	1224	U
1	a	1225	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1226	C
1	a	1227	A
1	a	1228	C
1	a	1236	A
1	a	1238	A
1	a	1240	U
1	a	1241	G
1	a	1256	A
1	a	1258	G
1	a	1260	G
1	a	1278	G
1	a	1279	G
1	a	1280	A
1	a	1281	C
1	a	1282	C
1	a	1286	U
1	a	1287	A
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1301	U
1	a	1302	C
1	a	1306	A
1	a	1312	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1331	G
1	a	1332	A
1	a	1346	A
1	a	1347	G
1	a	1348	U
1	a	1353	G
1	a	1363	A
1	a	1381	U
1	a	1395	C
1	a	1400	C
1	a	1401	G
1	a	1418	A
1	a	1429	A
1	a	1433	A
1	a	1446	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1448	C
1	a	1451	U
1	a	1452	C
1	a	1492	A
1	a	1502	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1519	MA6
1	a	1520	C
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1539	C
22	v	7	G
22	v	8	4SU
22	v	9	G
22	v	14	A
22	v	16	C
22	v	17	C
22	v	18	U
22	v	19	G
22	v	20	G
22	v	21	H2U
22	v	22	A
22	v	23	G
22	v	60	A
22	v	61	U
22	v	62	C
22	v	68	C
22	v	76	C
22	v	77	A
22	w	2	G
22	w	3	C
22	w	5	G
22	w	7	G
22	w	8	4SU
22	w	9	G
22	w	10	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	w	13	C
22	w	14	A
22	w	15	G
22	w	16	C
22	w	17	C
22	w	117	U
22	w	18	G
22	w	19	G
22	w	20	H2U
22	w	21	A
22	w	22	G
22	w	25	C
22	w	26	G
22	w	28	C
22	w	32	C
22	w	33	U
22	w	34	C
22	w	37	A
22	w	38	A
22	w	40	C
22	w	43	A
22	w	44	A
22	w	48	C
22	w	49	G
22	w	53	G
22	w	59	A
22	w	60	U
22	w	64	G
22	w	66	C
22	w	67	C
22	w	69	C
22	w	70	G
22	w	71	C
22	w	73	A
22	w	75	C
22	w	76	A
23	x	13	A
24	y	7	A
24	y	8	4SU
24	y	9	A
24	y	10	G
24	y	16	H2U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	y	17	C
24	y	18	G
24	y	19	G
24	y	20	H2U
24	y	21	A
24	y	22	G
24	y	44	G
24	y	45	U
24	y	46	7MG
24	y	48	C
24	y	59	U
24	y	61	C
24	y	75	C
24	y	76	A
26	A	10	A
26	A	12	U
26	A	23	G
26	A	27	G
26	A	28	A
26	A	34	U
26	A	35	G
26	A	42	A
26	A	46	G
26	A	49	A
26	A	51	G
26	A	52	A
26	A	60	G
26	A	63	A
26	A	71	A
26	A	73	A
26	A	74	A
26	A	75	G
26	A	91	A
26	A	92	U
26	A	103	A
26	A	110	G
26	A	118	A
26	A	119	A
26	A	120	U
26	A	127	A
26	A	138	U
26	A	139	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	140	C
26	A	141	G
26	A	142	A
26	A	158	U
26	A	162	U
26	A	163	C
26	A	181	A
26	A	196	A
26	A	199	A
26	A	204	A
26	A	205	G
26	A	215	G
26	A	216	A
26	A	218	A
26	A	219	A
26	A	221	A
26	A	222	A
26	A	227	A
26	A	228	C
26	A	242	G
26	A	243	U
26	A	248	G
26	A	249	C
26	A	255	A
26	A	265	A
26	A	266	G
26	A	267	C
26	A	272	A
26	A	276	U
26	A	278	A
26	A	281	C
26	A	294	A
26	A	301	G
26	A	302	C
26	A	311	A
26	A	312	G
26	A	321	U
26	A	322	A
26	A	323	C
26	A	324	A
26	A	329	G
26	A	330	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	333	G
26	A	334	C
26	A	345	A
26	A	346	A
26	A	353	C
26	A	361	G
26	A	362	A
26	A	370	G
26	A	371	A
26	A	372	G
26	A	373	U
26	A	386	G
26	A	387	U
26	A	390	U
26	A	391	A
26	A	404	A
26	A	405	U
26	A	406	G
26	A	411	G
26	A	422	A
26	A	424	G
26	A	442	G
26	A	446	G
26	A	454	A
26	A	455	C
26	A	457	A
26	A	458	G
26	A	459	U
26	A	467	G
26	A	479	A
26	A	480	A
26	A	481	G
26	A	490	C
26	A	491	G
26	A	504	A
26	A	505	A
26	A	506	G
26	A	508	A
26	A	518	G
26	A	527	C
26	A	529	A
26	A	530	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	532	A
26	A	533	G
26	A	542	C
26	A	543	G
26	A	545	U
26	A	547	A
26	A	550	C
26	A	555	G
26	A	563	A
26	A	572	A
26	A	573	U
26	A	575	A
26	A	603	A
26	A	614	A
26	A	616	A
26	A	627	A
26	A	637	A
26	A	645	C
26	A	646	U
26	A	654	A
26	A	655	A
26	A	659	G
26	A	668	A
26	A	669	G
26	A	670	A
26	A	677	A
26	A	685	A
26	A	686	U
26	A	687	C
26	A	694	U
26	A	695	G
26	A	717	C
26	A	726	G
26	A	730	A
26	A	740	C
26	A	747	5MC
26	A	748	G
26	A	752	A
26	A	753	A
26	A	765	C
26	A	772	C
26	A	775	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	776	G
26	A	777	G
26	A	782	A
26	A	784	G
26	A	785	G
26	A	789	A
26	A	791	C
26	A	801	G
26	A	802	A
26	A	805	G
26	A	806	C
26	A	812	C
26	A	819	A
26	A	822	G
26	A	827	U
26	A	828	U
26	A	830	G
26	A	831	G
26	A	845	A
26	A	846	U
26	A	847	U
26	A	858	G
26	A	859	G
26	A	860	U
26	A	878	A
26	A	896	A
26	A	897	C
26	A	907	G
26	A	910	A
26	A	932	U
26	A	941	A
26	A	946	C
26	A	953	G
26	A	958	U
26	A	961	C
26	A	974	G
26	A	975	A
26	A	982	C
26	A	983	A
26	A	985	C
26	A	989	G
26	A	990	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	995	C
26	A	996	A
26	A	999	U
26	A	1011	G
26	A	1012	U
26	A	1013	C
26	A	1021	A
26	A	1022	G
26	A	1023	U
26	A	1026	G
26	A	1033	U
26	A	1046	A
26	A	1053	C
26	A	1054	A
26	A	1057	A
26	A	1060	U
26	A	1061	U
26	A	1062	G
26	A	1064	C
26	A	1065	U
26	A	1066	U
26	A	1068	G
26	A	1069	A
26	A	1070	A
26	A	1071	G
26	A	1072	C
26	A	1075	C
26	A	1076	C
26	A	1079	C
26	A	1084	A
26	A	1088	A
26	A	1089	A
26	A	1090	A
26	A	1104	C
26	A	1111	A
26	A	1112	G
26	A	1119	U
26	A	1130	U
26	A	1131	G
26	A	1132	U
26	A	1134	A
26	A	1135	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	1142	A
26	A	1143	A
26	A	1151	A
26	A	1174	U
26	A	1175	A
26	A	1176	U
26	A	1179	G
26	A	1180	U
26	A	1206	G
26	A	1212	G
26	A	1213	A
26	A	1218	G
26	A	1237	A
26	A	1238	G
26	A	1247	A
26	A	1248	G
26	A	1250	G
26	A	1251	C
26	A	1253	A
26	A	1256	G
26	A	1271	G
26	A	1272	A
26	A	1273	U
26	A	1276	A
26	A	1289	C
26	A	1298	C
26	A	1300	G
26	A	1301	A
26	A	1302	A
26	A	1311	G
26	A	1315	C
26	A	1321	A
26	A	1329	U
26	A	1330	C
26	A	1332	G
26	A	1341	G
26	A	1345	C
26	A	1352	U
26	A	1365	A
26	A	1368	G
26	A	1378	A
26	A	1379	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	1380	G
26	A	1383	A
26	A	1385	A
26	A	1395	A
26	A	1397	U
26	A	1416	G
26	A	1419	A
26	A	1420	A
26	A	1428	C
26	A	1454	C
26	A	1458	U
26	A	1461	C
26	A	1482	G
26	A	1483	G
26	A	1490	A
26	A	1491	G
26	A	1493	C
26	A	1504	A
26	A	1515	A
26	A	1524	G
26	A	1533	C
26	A	1535	A
26	A	1536	C
26	A	1537	G
26	A	1555	G
26	A	1559	U
26	A	1560	G
26	A	1567	G
26	A	1569	A
26	A	1578	U
26	A	1581	G
26	A	1585	C
26	A	1607	C
26	A	1611	C
26	A	1616	A
26	A	1627	G
26	A	1647	U
26	A	1648	U
26	A	1651	G
26	A	1654	A
26	A	1664	A
26	A	1665	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	1667	G
26	A	1674	G
26	A	1694	C
26	A	1695	G
26	A	1715	G
26	A	1729	U
26	A	1730	C
26	A	1738	G
26	A	1756	G
26	A	1758	U
26	A	1764	C
26	A	1773	A
26	A	1780	A
26	A	1781	U
26	A	1782	U
26	A	1784	A
26	A	1787	A
26	A	1800	C
26	A	1801	A
26	A	1808	A
26	A	1816	C
26	A	1818	U
26	A	1829	A
26	A	1833	C
26	A	1847	G
26	A	1858	A
26	A	1865	U
26	A	1871	A
26	A	1885	A
26	A	1896	G
26	A	1900	A
26	A	1901	A
26	A	1906	G
26	A	1907	G
26	A	1913	A
26	A	1914	C
26	A	1927	A
26	A	1929	G
26	A	1930	G
26	A	1931	U
26	A	1937	A
26	A	1938	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	1940	U
26	A	1941	C
26	A	1955	U
26	A	1960	A
26	A	1962	5MC
26	A	1963	U
26	A	1967	C
26	A	1970	A
26	A	1971	U
26	A	1972	G
26	A	1981	A
26	A	1991	U
26	A	1992	G
26	A	1993	U
26	A	1997	C
26	A	2022	U
26	A	2023	C
26	A	2031	A
26	A	2033	A
26	A	2043	C
26	A	2049	G
26	A	2052	A
26	A	2055	C
26	A	2056	G
26	A	2060	A
26	A	2061	G
26	A	2062	A
26	A	2069	7MG
26	A	2093	G
26	A	2095	A
26	A	2096	C
26	A	2098	U
26	A	2108	A
26	A	2110	G
26	A	2111	U
26	A	2112	G
26	A	2113	U
26	A	2118	U
26	A	2119	A
26	A	2127	G
26	A	2131	U
26	A	2132	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	2133	G
26	A	2145	C
26	A	2146	C
26	A	2157	G
26	A	2162	G
26	A	2164	C
26	A	2172	U
26	A	2173	A
26	A	2189	U
26	A	2192	U
26	A	2198	A
26	A	2199	A
26	A	2204	G
26	A	2211	A
26	A	2212	A
26	A	2213	U
26	A	2225	A
26	A	2238	G
26	A	2239	G
26	A	2250	G
26	A	2268	A
26	A	2273	A
26	A	2278	A
26	A	2282	G
26	A	2283	C
26	A	2287	A
26	A	2288	A
26	A	2296	U
26	A	2297	A
26	A	2305	U
26	A	2309	A
26	A	2311	A
26	A	2312	U
26	A	2320	U
26	A	2325	G
26	A	2327	A
26	A	2334	U
26	A	2336	A
26	A	2337	G
26	A	2345	G
26	A	2347	C
26	A	2350	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	2382	G
26	A	2383	G
26	A	2385	C
26	A	2391	G
26	A	2392	A
26	A	2402	U
26	A	2406	A
26	A	2407	A
26	A	2423	U
26	A	2424	C
26	A	2426	A
26	A	2427	C
26	A	2428	G
26	A	2429	G
26	A	2430	A
26	A	2435	A
26	A	2441	U
26	A	2445	2MG
26	A	2447	G
26	A	2448	A
26	A	2449	H2U
26	A	2459	A
26	A	2468	A
26	A	2476	A
26	A	2478	A
26	A	2484	G
26	A	2494	G
26	A	2497	A
26	A	2498	OMC
26	A	2502	G
26	A	2503	2MA
26	A	2504	PSU
26	A	2505	G
26	A	2506	U
26	A	2517	C
26	A	2518	A
26	A	2519	U
26	A	2529	G
26	A	2547	A
26	A	2554	U
26	A	2567	G
26	A	2572	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	2573	C
26	A	2585	U
26	A	2602	A
26	A	2603	G
26	A	2608	G
26	A	2609	U
26	A	2613	U
26	A	2614	A
26	A	2636	C
26	A	2645	G
26	A	2646	C
26	A	2655	G
26	A	2656	U
26	A	2682	A
26	A	2689	U
26	A	2690	U
26	A	2707	U
26	A	2712	C
26	A	2713	U
26	A	2714	G
26	A	2718	G
26	A	2722	G
26	A	2726	A
26	A	2731	G
26	A	2732	G
26	A	2733	A
26	A	2739	U
26	A	2744	G
26	A	2748	A
26	A	2757	A
26	A	2764	A
26	A	2765	A
26	A	2769	U
26	A	2778	A
26	A	2779	U
26	A	2791	G
26	A	2794	C
26	A	2797	U
26	A	2799	A
26	A	2800	A
26	A	2801	G
26	A	2808	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	2809	A
26	A	2818	U
26	A	2820	A
26	A	2821	A
26	A	2823	A
26	A	2833	U
26	A	2834	G
26	A	2835	A
26	A	2848	G
26	A	2849	U
26	A	2866	U
26	A	2867	G
26	A	2868	A
26	A	2872	A
26	A	2873	A
26	A	2880	C
26	A	2884	U
27	B	4	C
27	B	12	C
27	B	13	G
27	B	24	G
27	B	25	U
27	B	35	C
27	B	40	U
27	B	44	G
27	B	45	A
27	B	56	G
27	B	57	A
27	B	67	G
27	B	88	C
27	B	89	U
27	B	91	C
27	B	108	A
27	B	109	A
27	B	116	G

All (94) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	51	G
26	A	86	G
26	A	204	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	227	A
26	A	242	G
26	A	265	A
26	A	271	G
26	A	301	G
26	A	311	A
26	A	321	U
26	A	332	A
26	A	345	A
26	A	372	G
26	A	386	G
26	A	390	U
26	A	446	G
26	A	454	A
26	A	458	G
26	A	479	A
26	A	480	A
26	A	490	C
26	A	503	A
26	A	549	G
26	A	571	U
26	A	637	A
26	A	685	A
26	A	686	U
26	A	747	5MC
26	A	752	A
26	A	774	G
26	A	776	G
26	A	800	A
26	A	830	G
26	A	858	G
26	A	859	G
26	A	974	G
26	A	1012	U
26	A	1020	A
26	A	1022	G
26	A	1070	A
26	A	1089	A
26	A	1111	A
26	A	1124	G
26	A	1130	U
26	A	1133	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	1134	A
26	A	1141	U
26	A	1142	A
26	A	1182	G
26	A	1190	G
26	A	1210	G
26	A	1212	G
26	A	1275	A
26	A	1288	G
26	A	1300	G
26	A	1331	G
26	A	1378	A
26	A	1399	C
26	A	1432	G
26	A	1626	A
26	A	1693	U
26	A	1713	A
26	A	1783	A
26	A	1799	G
26	A	1857	G
26	A	1930	G
26	A	1940	U
26	A	2060	A
26	A	2092	U
26	A	2197	U
26	A	2210	U
26	A	2282	G
26	A	2286	G
26	A	2296	U
26	A	2326	C
26	A	2333	A
26	A	2391	G
26	A	2405	G
26	A	2406	A
26	A	2517	C
26	A	2518	A
26	A	2566	A
26	A	2614	A
26	A	2655	G
26	A	2712	C
26	A	2756	U
26	A	2798	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	A	2808	G
26	A	2820	A
26	A	2866	U
27	B	24	G
27	B	56	G
27	B	66	A
27	B	88	C

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

52 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
26	2MG	A	1835	26	23,26,27	1.30	4 (17%)	33,38,41	2.24	8 (24%)
26	1MG	A	745	26	23,26,27	1.19	1 (4%)	33,39,42	1.86	7 (21%)
26	OMG	A	2251	22,26	23,26,27	1.26	3 (13%)	32,38,41	1.81	5 (15%)
24	5MU	y	54	24	19,22,23	1.38	5 (26%)	27,32,35	2.24	7 (25%)
26	6MZ	A	2030	26	22,25,26	1.60	4 (18%)	29,36,39	2.26	10 (34%)
1	5MC	a	1407	1	19,22,23	1.54	3 (15%)	26,32,35	1.16	3 (11%)
26	PSU	A	2504	26	18,21,22	1.35	2 (11%)	21,30,33	1.98	3 (14%)
24	PSU	y	32	24	18,21,22	1.35	2 (11%)	21,30,33	2.04	4 (19%)
26	7MG	A	2069	26	23,26,27	1.36	4 (17%)	27,39,42	2.63	7 (25%)
26	PSU	A	955	26	18,21,22	1.44	4 (22%)	21,30,33	2.17	4 (19%)
1	MA6	a	1519	1	23,26,27	1.52	5 (21%)	33,38,41	2.35	14 (42%)
1	4OC	a	1402	1	20,23,24	0.77	0	25,32,35	0.93	0
1	PSU	a	516	1,59	18,21,22	1.47	4 (22%)	21,30,33	2.31	5 (23%)
22	5MU	w	54	22	19,22,23	1.27	3 (15%)	27,32,35	2.36	10 (37%)
24	7MG	y	46	24	23,26,27	1.31	3 (13%)	27,39,42	2.64	7 (25%)
26	PSU	A	746	26,59	18,21,22	1.35	3 (16%)	21,30,33	1.98	4 (19%)
22	PSU	w	55	22	18,21,22	1.51	3 (16%)	21,30,33	2.32	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	2MG	A	2445	26	23,26,27	1.33	4 (17%)	33,38,41	1.95	6 (18%)
26	H2U	A	2449	26	18,21,22	0.92	2 (11%)	19,30,33	1.11	2 (10%)
24	H2U	y	20	24	18,21,22	0.95	2 (11%)	19,30,33	0.89	1 (5%)
26	PSU	A	2580	26	18,21,22	1.44	3 (16%)	21,30,33	2.19	4 (19%)
22	5MU	v	55	22	19,22,23	1.37	5 (26%)	27,32,35	2.26	5 (18%)
26	3TD	A	1915	26	19,22,23	1.35	3 (15%)	23,32,35	2.07	4 (17%)
1	2MG	a	966	1	23,26,27	1.26	4 (17%)	33,38,41	2.30	8 (24%)
26	PSU	A	1911	26	18,21,22	1.35	2 (11%)	21,30,33	2.12	4 (19%)
24	4SU	y	8	24	18,21,22	1.86	4 (22%)	25,30,33	2.45	5 (20%)
1	2MG	a	1516	1	23,26,27	1.27	4 (17%)	33,38,41	2.15	7 (21%)
26	6MZ	A	1618	26	22,25,26	1.68	5 (22%)	29,36,39	2.31	9 (31%)
24	PSU	y	39	24	18,21,22	1.33	2 (11%)	21,30,33	2.04	4 (19%)
22	4SU	w	8	22	18,21,22	1.89	4 (22%)	25,30,33	2.42	4 (16%)
1	MA6	a	1518	1	23,26,27	1.67	5 (21%)	33,38,41	2.26	9 (27%)
1	2MG	a	1207	1	23,26,27	1.27	4 (17%)	33,38,41	2.25	8 (24%)
26	OMU	A	2552	26	19,22,23	1.24	3 (15%)	25,31,34	2.28	7 (28%)
24	H2U	y	16	24	18,21,22	0.97	2 (11%)	19,30,33	0.98	1 (5%)
26	PSU	A	1917	26	18,21,22	1.38	2 (11%)	21,30,33	2.00	3 (14%)
22	H2U	v	21	22	18,21,22	0.92	2 (11%)	19,30,33	1.03	2 (10%)
26	OMC	A	2498	26,59	19,22,23	0.81	1 (5%)	25,31,34	0.88	0
26	5MC	A	747	26	19,22,23	1.53	3 (15%)	26,32,35	1.38	3 (11%)
26	PSU	A	2605	26	18,21,22	1.43	3 (16%)	21,30,33	1.96	5 (23%)
1	UR3	a	1498	1	19,22,23	0.93	1 (5%)	26,32,35	1.95	4 (15%)
1	7MG	a	527	1	23,26,27	1.34	4 (17%)	27,39,42	2.57	7 (25%)
22	4SU	v	8	22	18,21,22	1.77	4 (22%)	25,30,33	2.36	6 (24%)
24	PSU	y	55	24	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
26	PSU	A	2604	26	18,21,22	1.38	3 (16%)	21,30,33	2.05	5 (23%)
26	5MU	A	1939	26	19,22,23	1.36	4 (21%)	27,32,35	2.28	6 (22%)
1	5MC	a	967	1	19,22,23	1.52	2 (10%)	26,32,35	1.08	2 (7%)
26	2MA	A	2503	26,59	22,25,26	1.47	5 (22%)	32,37,40	2.32	9 (28%)
24	MIA	y	37	24	28,31,32	2.36	6 (21%)	38,44,47	3.05	15 (39%)
22	PSU	v	56	22	18,21,22	1.38	3 (16%)	21,30,33	2.00	4 (19%)
26	5MC	A	1962	26	19,22,23	1.58	3 (15%)	26,32,35	1.10	2 (7%)
26	PSU	A	2457	26	18,21,22	1.36	3 (16%)	21,30,33	2.23	4 (19%)
22	H2U	w	20	22	18,21,22	1.35	3 (16%)	19,30,33	1.87	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	2MG	A	1835	26	-	0/9/27/28	0/3/3/3
26	1MG	A	745	26	-	0/7/25/26	0/3/3/3
26	OMG	A	2251	22,26	-	0/9/27/28	0/3/3/3
24	5MU	y	54	24	-	0/7/25/26	0/2/2/2
26	6MZ	A	2030	26	-	2/9/27/28	0/3/3/3
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
26	PSU	A	2504	26	-	2/7/25/26	0/2/2/2
24	PSU	y	32	24	-	0/7/25/26	0/2/2/2
26	7MG	A	2069	26	-	0/7/37/38	0/3/3/3
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	2/11/29/30	0/3/3/3
1	4OC	a	1402	1	-	0/9/29/30	0/2/2/2
1	PSU	a	516	1,59	-	2/7/25/26	0/2/2/2
22	5MU	w	54	22	-	2/7/25/26	0/2/2/2
24	7MG	y	46	24	-	3/7/37/38	0/3/3/3
26	PSU	A	746	26,59	-	1/7/25/26	0/2/2/2
22	PSU	w	55	22	-	2/7/25/26	0/2/2/2
26	2MG	A	2445	26	-	2/9/27/28	0/3/3/3
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
24	H2U	y	20	24	-	5/7/38/39	0/2/2/2
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2
22	5MU	v	55	22	-	0/7/25/26	0/2/2/2
26	3TD	A	1915	26	-	3/7/25/26	0/2/2/2
1	2MG	a	966	1	-	2/9/27/28	0/3/3/3
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
24	4SU	y	8	24	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
26	6MZ	A	1618	26	-	0/9/27/28	0/3/3/3
24	PSU	y	39	24	-	0/7/25/26	0/2/2/2
22	4SU	w	8	22	-	5/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	6/11/29/30	0/3/3/3
1	2MG	a	1207	1	-	2/9/27/28	0/3/3/3
26	OMU	A	2552	26	-	2/9/27/28	0/2/2/2
24	H2U	y	16	24	-	0/7/38/39	0/2/2/2
26	PSU	A	1917	26	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	H2U	v	21	22	-	1/7/38/39	0/2/2/2
26	OMC	A	2498	26,59	-	1/9/27/28	0/2/2/2
26	5MC	A	747	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
1	7MG	a	527	1	-	3/7/37/38	0/3/3/3
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
24	PSU	y	55	24	-	0/7/25/26	0/2/2/2
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
26	2MA	A	2503	26,59	-	2/7/25/26	0/3/3/3
24	MIA	y	37	24	-	3/15/33/34	0/3/3/3
22	PSU	v	56	22	-	2/7/25/26	0/2/2/2
26	5MC	A	1962	26	-	1/7/25/26	0/2/2/2
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
22	H2U	w	20	22	-	1/7/38/39	0/2/2/2

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	37	MIA	C2-S10	-7.43	1.69	1.75
24	y	37	MIA	C13-C14	6.90	1.53	1.32
26	A	1618	6MZ	C5-C4	5.73	1.49	1.39
26	A	1962	5MC	C5-C4	5.55	1.48	1.44
1	a	1407	5MC	C5-C4	5.41	1.48	1.44
26	A	2030	6MZ	C5-C4	5.31	1.48	1.39
26	A	747	5MC	C5-C4	5.30	1.48	1.44
24	y	8	4SU	C4-S4	-5.25	1.59	1.68
1	a	967	5MC	C5-C4	5.19	1.48	1.44
1	a	1518	MA6	C5-C4	5.13	1.48	1.39
22	w	8	4SU	C4-S4	-5.09	1.59	1.68
22	v	8	4SU	C4-S4	-4.90	1.60	1.68
24	y	37	MIA	C5-C4	4.42	1.47	1.39
26	A	2503	2MA	C5-C4	4.33	1.46	1.39
1	a	1519	MA6	C5-C4	4.30	1.46	1.39
26	A	2069	7MG	C4-N9	-3.74	1.33	1.37
24	y	55	PSU	C6-C5	3.62	1.39	1.35
1	a	527	7MG	C4-N9	-3.59	1.33	1.37
26	A	1915	3TD	C10-N3	3.50	1.53	1.47
22	v	56	PSU	C6-C5	3.49	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	w	20	H2U	C2-N3	-3.48	1.31	1.38
22	w	8	4SU	C4-N3	-3.43	1.34	1.37
26	A	1911	PSU	C6-C5	3.40	1.39	1.35
1	a	1516	2MG	C5-C4	3.31	1.47	1.38
24	y	46	7MG	C5-C4	3.28	1.47	1.37
1	a	1207	2MG	C5-C4	3.28	1.47	1.38
26	A	2605	PSU	C6-C5	3.24	1.38	1.35
26	A	1917	PSU	C6-C5	3.24	1.38	1.35
26	A	745	1MG	C5-C4	3.24	1.47	1.38
24	y	39	PSU	C6-C5	3.20	1.38	1.35
22	w	8	4SU	C5-C4	-3.18	1.38	1.42
24	y	32	PSU	C6-C5	3.17	1.38	1.35
24	y	8	4SU	C5-C4	-3.12	1.38	1.42
1	a	966	2MG	C5-C4	3.11	1.47	1.38
1	a	516	PSU	C4-N3	-3.09	1.33	1.38
26	A	955	PSU	C4-N3	-3.09	1.33	1.38
26	A	1835	2MG	C6-N1	-3.08	1.33	1.38
26	A	2580	PSU	C4-N3	-3.08	1.33	1.38
22	v	8	4SU	C4-N3	-3.08	1.34	1.37
26	A	2251	OMG	C6-N1	-3.06	1.33	1.38
1	a	527	7MG	C5-C4	3.03	1.47	1.37
26	A	2030	6MZ	C5-C6	3.00	1.49	1.41
26	A	1618	6MZ	C5-C6	3.00	1.49	1.41
1	a	967	5MC	C6-C5	2.98	1.39	1.34
22	w	55	PSU	C4-N3	-2.98	1.33	1.38
22	w	20	H2U	C2-N1	-2.97	1.31	1.35
26	A	2605	PSU	C4-N3	-2.95	1.33	1.38
26	A	746	PSU	C6-C5	2.94	1.38	1.35
24	y	8	4SU	C4-N3	-2.93	1.34	1.37
26	A	1939	5MU	C4-N3	-2.92	1.33	1.38
26	A	2604	PSU	C4-N3	-2.91	1.33	1.38
26	A	1939	5MU	C6-N1	-2.89	1.33	1.38
22	w	55	PSU	C6-C5	2.89	1.38	1.35
1	a	1518	MA6	C4-N9	-2.88	1.31	1.37
22	w	55	PSU	C2-N1	-2.86	1.32	1.36
26	A	2445	2MG	C5-N7	-2.83	1.33	1.39
24	y	54	5MU	C4-N3	-2.82	1.33	1.38
26	A	2251	OMG	C5-C4	2.82	1.46	1.38
24	y	37	MIA	C5-C6	2.81	1.48	1.41
26	A	2504	PSU	C6-C5	2.80	1.38	1.35
26	A	746	PSU	C4-N3	-2.79	1.33	1.38
26	A	2069	7MG	C5-C4	2.78	1.46	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	46	7MG	C4-N9	-2.78	1.34	1.37
1	a	1518	MA6	C5-N7	-2.75	1.34	1.39
1	a	1518	MA6	C5-C6	2.74	1.48	1.41
26	A	2504	PSU	C4-N3	-2.74	1.33	1.38
1	a	516	PSU	C6-C5	2.73	1.38	1.35
22	v	55	5MU	C6-C5	2.73	1.39	1.34
26	A	2457	PSU	C4-N3	-2.73	1.33	1.38
26	A	1962	5MC	C6-N1	-2.71	1.33	1.38
26	A	1835	2MG	C5-C4	2.71	1.46	1.38
26	A	2604	PSU	C6-C5	2.70	1.38	1.35
24	y	32	PSU	C4-N3	-2.68	1.33	1.38
26	A	2445	2MG	C6-N1	-2.68	1.33	1.38
22	v	56	PSU	C4-N3	-2.67	1.33	1.38
26	A	2552	OMU	C4-N3	-2.66	1.34	1.38
1	a	1407	5MC	C6-N1	-2.65	1.33	1.38
26	A	2605	PSU	C2-N3	-2.65	1.33	1.37
26	A	2457	PSU	C6-C5	2.63	1.38	1.35
26	A	2604	PSU	C2-N3	-2.63	1.33	1.37
22	w	54	5MU	C6-N1	-2.63	1.33	1.38
1	a	1519	MA6	C4-N9	-2.62	1.32	1.37
26	A	1917	PSU	C4-N3	-2.62	1.33	1.38
26	A	2503	2MA	C5-C6	2.61	1.48	1.41
24	y	39	PSU	C4-N3	-2.59	1.34	1.38
22	v	55	5MU	C4-N3	-2.57	1.34	1.38
26	A	747	5MC	C6-C5	2.56	1.38	1.34
1	a	1519	MA6	C5-C6	2.56	1.48	1.41
26	A	2069	7MG	C5-N7	-2.56	1.32	1.35
26	A	2251	OMG	C5-N7	-2.53	1.34	1.39
26	A	1915	3TD	C4-N3	-2.52	1.35	1.40
1	a	1519	MA6	C5-N7	-2.52	1.34	1.39
24	y	20	H2U	C2-N3	-2.52	1.33	1.38
26	A	2580	PSU	C6-C5	2.51	1.38	1.35
1	a	966	2MG	C6-N1	-2.51	1.34	1.38
24	y	55	PSU	C4-N3	-2.51	1.34	1.38
26	A	2449	H2U	C2-N3	-2.51	1.33	1.38
26	A	1939	5MU	C2-N3	-2.50	1.33	1.38
26	A	2445	2MG	C5-C4	2.49	1.45	1.38
24	y	16	H2U	C2-N3	-2.48	1.33	1.38
22	v	8	4SU	C5-C4	-2.48	1.39	1.42
22	v	21	H2U	C2-N3	-2.48	1.33	1.38
22	v	55	5MU	C2-N1	2.47	1.42	1.38
26	A	1939	5MU	C6-C5	2.46	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	w	20	H2U	C4-N3	-2.45	1.33	1.37
24	y	54	5MU	C6-N1	-2.45	1.33	1.38
26	A	747	5MC	C6-N1	-2.45	1.33	1.38
1	a	1207	2MG	C6-N1	-2.45	1.34	1.38
24	y	54	5MU	C2-N3	-2.44	1.33	1.38
26	A	1915	3TD	C4-C5	-2.43	1.42	1.47
1	a	1519	MA6	C8-N7	2.43	1.36	1.31
22	w	54	5MU	C4-N3	-2.41	1.34	1.38
26	A	1911	PSU	C4-N3	-2.41	1.34	1.38
26	A	2445	2MG	C4-N9	-2.40	1.31	1.38
1	a	516	PSU	C2-N3	-2.40	1.33	1.37
1	a	1516	2MG	C2-N3	2.40	1.36	1.32
26	A	955	PSU	C2-N3	-2.40	1.33	1.37
22	w	8	4SU	C2-N3	-2.40	1.33	1.38
26	A	1835	2MG	C5-N7	-2.40	1.34	1.39
1	a	527	7MG	C6-N1	-2.39	1.34	1.38
1	a	1407	5MC	C6-C5	2.38	1.38	1.34
1	a	1518	MA6	C8-N7	2.35	1.36	1.31
22	v	21	H2U	C4-N3	-2.34	1.33	1.37
26	A	2449	H2U	C4-N3	-2.33	1.33	1.37
1	a	966	2MG	C2-N3	2.32	1.36	1.32
26	A	955	PSU	C2-N1	-2.31	1.33	1.36
22	v	8	4SU	C2-N1	2.31	1.42	1.38
26	A	1962	5MC	C6-C5	2.31	1.38	1.34
24	y	54	5MU	C6-C5	2.28	1.38	1.34
24	y	54	5MU	C4-C5	2.28	1.48	1.44
24	y	20	H2U	C4-N3	-2.28	1.33	1.37
1	a	1207	2MG	C2-N3	2.27	1.36	1.32
24	y	16	H2U	C4-N3	-2.27	1.33	1.37
24	y	37	MIA	C8-N7	2.25	1.36	1.31
26	A	955	PSU	C6-C5	2.25	1.37	1.35
26	A	1618	6MZ	C5-N7	-2.25	1.35	1.39
24	y	8	4SU	C2-N3	-2.23	1.34	1.38
26	A	2069	7MG	C6-N1	-2.22	1.34	1.38
24	y	37	MIA	C5-N7	-2.21	1.35	1.39
24	y	46	7MG	C6-N1	-2.19	1.34	1.38
26	A	2503	2MA	C5-N7	-2.19	1.35	1.39
22	v	55	5MU	C6-N1	-2.19	1.34	1.38
1	a	516	PSU	O4'-C1'	-2.19	1.40	1.43
1	a	1207	2MG	C5-N7	-2.18	1.34	1.39
26	A	2503	2MA	C8-N7	2.17	1.35	1.31
26	A	2552	OMU	C2-N3	-2.16	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1516	2MG	C6-N1	-2.16	1.34	1.38
22	w	54	5MU	C4-C5	2.16	1.48	1.44
26	A	2498	OMC	C6-N1	-2.15	1.33	1.38
26	A	1835	2MG	C2-N3	2.15	1.36	1.32
26	A	1618	6MZ	C8-N7	2.14	1.35	1.31
1	a	1516	2MG	C5-N7	-2.14	1.34	1.39
26	A	2552	OMU	C2-N1	2.13	1.41	1.38
1	a	966	2MG	C5-N7	-2.13	1.34	1.39
26	A	2030	6MZ	C5-N7	-2.12	1.35	1.39
26	A	2503	2MA	C4-N9	-2.11	1.33	1.37
26	A	2580	PSU	C2-N3	-2.05	1.34	1.37
26	A	746	PSU	C2-N3	-2.03	1.34	1.37
26	A	2030	6MZ	C8-N7	2.03	1.35	1.31
22	v	55	5MU	C2-N3	-2.03	1.34	1.38
26	A	1618	6MZ	C8-N9	-2.03	1.34	1.37
1	a	1498	UR3	C5-C4	-2.02	1.38	1.43
22	v	56	PSU	C2-N3	-2.01	1.34	1.37
1	a	527	7MG	C5-N7	-2.00	1.33	1.35
26	A	2457	PSU	C2-N1	-2.00	1.34	1.36

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	37	MIA	C12-C13-C14	-9.96	109.14	127.01
24	y	46	7MG	N9-C4-N3	9.02	138.69	125.46
26	A	2069	7MG	N9-C4-N3	8.77	138.32	125.46
1	a	527	7MG	N9-C4-N3	8.73	138.26	125.46
24	y	37	MIA	C5-C4-N3	-8.31	118.43	127.18
1	a	966	2MG	C2-N3-C4	7.60	121.50	112.00
1	a	1207	2MG	C2-N3-C4	7.51	121.39	112.00
26	A	2503	2MA	C5-C4-N3	-7.38	119.41	127.18
1	a	516	PSU	N1-C2-N3	7.24	122.81	115.17
26	A	1835	2MG	C2-N3-C4	7.16	120.95	112.00
1	a	1516	2MG	C2-N3-C4	7.10	120.88	112.00
22	w	8	4SU	C4-N3-C2	-7.07	120.54	127.31
1	a	1498	UR3	C4-N3-C2	-7.05	118.90	124.58
26	A	1915	3TD	N1-C2-N3	7.04	121.25	116.13
22	w	55	PSU	N1-C2-N3	7.00	122.55	115.17
26	A	2580	PSU	N1-C2-N3	6.93	122.48	115.17
22	v	8	4SU	C4-N3-C2	-6.92	120.68	127.31
26	A	2457	PSU	N1-C2-N3	6.81	122.36	115.17
24	y	8	4SU	C4-N3-C2	-6.73	120.86	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	955	PSU	N1-C2-N3	6.67	122.20	115.17
1	a	1207	2MG	C5-C4-N3	-6.61	117.87	128.39
24	y	8	4SU	C5-C4-N3	6.57	120.86	114.75
1	a	966	2MG	C5-C4-N3	-6.54	117.98	128.39
24	y	37	MIA	N3-C4-N9	6.53	135.28	126.99
26	A	1835	2MG	C5-C4-N3	-6.49	118.06	128.39
26	A	1911	PSU	N1-C2-N3	6.49	122.01	115.17
26	A	1917	PSU	N1-C2-N3	6.39	121.90	115.17
24	y	32	PSU	N1-C2-N3	6.28	121.79	115.17
24	y	55	PSU	N1-C2-N3	6.27	121.78	115.17
26	A	2445	2MG	C2-N3-C4	6.26	119.84	112.00
26	A	2504	PSU	N1-C2-N3	6.25	121.76	115.17
26	A	2503	2MA	N3-C4-N9	6.24	134.90	126.99
24	y	39	PSU	N1-C2-N3	6.23	121.74	115.17
26	A	2604	PSU	N1-C2-N3	6.21	121.72	115.17
26	A	2605	PSU	N1-C2-N3	6.16	121.66	115.17
22	v	56	PSU	N1-C2-N3	6.14	121.65	115.17
26	A	746	PSU	N1-C2-N3	6.06	121.56	115.17
26	A	1618	6MZ	C5-C4-N3	-6.00	118.45	126.72
1	a	1516	2MG	C5-C4-N3	-6.00	118.84	128.39
22	w	8	4SU	C5-C4-N3	5.93	120.27	114.75
26	A	2069	7MG	N9-C8-N7	-5.88	95.05	103.37
1	a	1518	MA6	C10-N6-C6	-5.70	106.03	120.52
22	v	8	4SU	C5-C4-N3	5.66	120.02	114.75
26	A	745	1MG	C5-C4-N3	-5.65	119.39	128.39
26	A	2251	OMG	C5-C4-N3	-5.65	119.39	128.39
26	A	1939	5MU	C4-N3-C2	-5.65	119.94	127.34
24	y	54	5MU	C4-N3-C2	-5.53	120.09	127.34
22	v	55	5MU	O4-C4-C5	-5.48	118.64	124.92
24	y	46	7MG	C5-C4-N3	-5.48	117.84	128.13
26	A	2552	OMU	C4-N3-C2	-5.48	119.81	126.61
1	a	527	7MG	N9-C8-N7	-5.44	95.67	103.37
22	w	55	PSU	O2-C2-N1	-5.42	117.20	122.79
24	y	8	4SU	C5-C4-S4	-5.42	118.12	124.31
22	v	55	5MU	C4-N3-C2	-5.34	120.34	127.34
26	A	1618	6MZ	N3-C4-N9	5.26	136.11	127.17
24	y	46	7MG	N9-C8-N7	-5.25	95.94	103.37
24	y	37	MIA	C11-S10-C2	-5.11	98.42	102.25
26	A	1939	5MU	N3-C2-N1	5.07	121.49	114.89
26	A	2445	2MG	C5-C4-N3	-5.06	120.33	128.39
22	w	8	4SU	C5-C4-S4	-5.06	118.52	124.31
24	y	54	5MU	C5-C4-N3	5.04	119.70	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	966	2MG	N9-C4-N3	5.03	136.02	125.95
1	a	527	7MG	C5-C4-N3	-5.01	118.73	128.13
26	A	1835	2MG	N9-C4-N3	4.95	135.86	125.95
1	a	1519	MA6	C5-C4-N3	-4.95	119.90	126.72
22	v	55	5MU	C5-C4-N3	4.95	119.62	115.32
26	A	2069	7MG	C5-C4-N3	-4.94	118.85	128.13
24	y	54	5MU	N3-C2-N1	4.93	121.31	114.89
22	v	55	5MU	N3-C2-N1	4.91	121.29	114.89
22	w	54	5MU	C4-N3-C2	-4.91	120.90	127.34
26	A	1939	5MU	C5-C4-N3	4.89	119.57	115.32
26	A	2552	OMU	N3-C2-N1	4.83	121.18	114.89
1	a	1207	2MG	N9-C4-N3	4.83	135.61	125.95
26	A	2030	6MZ	C5-C4-N3	-4.77	120.15	126.72
26	A	745	1MG	N9-C4-N3	4.73	135.41	125.95
26	A	2030	6MZ	C6-C5-N7	4.72	137.58	132.43
1	a	516	PSU	C4-N3-C2	-4.72	119.87	126.37
1	a	1518	MA6	C5-C4-N3	-4.66	120.30	126.72
22	v	8	4SU	C5-C4-S4	-4.66	118.98	124.31
26	A	1618	6MZ	C9-N6-C6	-4.66	118.53	122.85
26	A	2552	OMU	C1'-N1-C2	4.65	125.94	117.59
22	w	20	H2U	C5-C4-N3	4.61	121.59	116.69
26	A	955	PSU	C4-N3-C2	-4.59	120.05	126.37
1	a	1518	MA6	C2-N1-C6	4.56	122.97	111.83
26	A	2604	PSU	C4-N3-C2	-4.55	120.10	126.37
24	y	46	7MG	C2-N3-C4	4.55	120.14	112.30
26	A	1939	5MU	O4-C4-C5	-4.54	119.72	124.92
26	A	2030	6MZ	C9-N6-C6	-4.50	118.67	122.85
1	a	1519	MA6	C10-N6-C6	-4.50	109.07	120.52
22	w	20	H2U	C5-C6-N1	-4.47	98.00	111.52
26	A	2457	PSU	C4-N3-C2	-4.47	120.22	126.37
26	A	2457	PSU	O2-C2-N1	-4.46	118.19	122.79
22	w	54	5MU	N3-C2-N1	4.45	120.69	114.89
1	a	1516	2MG	N9-C4-N3	4.45	134.85	125.95
26	A	1911	PSU	C4-N3-C2	-4.44	120.26	126.37
1	a	1519	MA6	C2-N1-C6	4.44	122.67	111.83
1	a	1519	MA6	C9-N6-C6	-4.43	109.25	120.52
26	A	2251	OMG	N9-C4-N3	4.42	134.80	125.95
22	w	8	4SU	N3-C2-N1	4.40	120.61	114.89
22	v	8	4SU	N3-C2-N1	4.36	120.57	114.89
26	A	745	1MG	C2-N3-C4	4.35	121.77	111.98
26	A	1939	5MU	C5-C6-N1	-4.34	118.60	123.31
26	A	2552	OMU	C5-C4-N3	4.30	120.82	114.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1498	UR3	C5-C4-N3	4.29	120.70	115.04
22	w	54	5MU	C5-C4-N3	4.28	119.05	115.32
26	A	746	PSU	C4-N3-C2	-4.28	120.47	126.37
22	w	55	PSU	C4-N3-C2	-4.28	120.47	126.37
26	A	2445	2MG	N9-C4-N3	4.27	134.50	125.95
24	y	39	PSU	C4-N3-C2	-4.27	120.48	126.37
26	A	1915	3TD	C4-N3-C2	-4.26	120.11	124.61
24	y	32	PSU	C4-N3-C2	-4.25	120.51	126.37
26	A	2251	OMG	C2-N3-C4	4.20	119.53	112.30
22	w	54	5MU	O4-C4-C5	-4.15	120.17	124.92
26	A	2069	7MG	C2-N3-C4	4.14	119.43	112.30
26	A	2030	6MZ	N3-C4-N9	4.13	134.19	127.17
26	A	955	PSU	O2-C2-N1	-4.13	118.53	122.79
24	y	54	5MU	C5-C6-N1	-4.09	118.87	123.31
1	a	1518	MA6	C9-N6-C6	-4.07	110.17	120.52
1	a	1519	MA6	N1-C2-N3	-4.05	122.45	128.58
24	y	37	MIA	C16-C14-C13	-4.03	110.56	122.66
24	y	54	5MU	O4-C4-C5	-4.03	120.31	124.92
22	w	54	5MU	C5M-C5-C4	4.00	123.05	118.78
26	A	2580	PSU	C4-N3-C2	-4.00	120.86	126.37
24	y	55	PSU	C4-N3-C2	-3.99	120.87	126.37
22	v	56	PSU	C4-N3-C2	-3.99	120.88	126.37
1	a	527	7MG	C2-N3-C4	3.98	119.15	112.30
1	a	516	PSU	O2-C2-N1	-3.98	118.69	122.79
22	w	20	H2U	N3-C2-N1	-3.94	112.68	116.65
24	y	37	MIA	C4-C5-N7	-3.90	106.12	110.58
22	w	54	5MU	C1'-N1-C6	-3.90	114.73	121.15
26	A	2504	PSU	O2-C2-N1	-3.90	118.77	122.79
26	A	1917	PSU	C4-N3-C2	-3.86	121.05	126.37
26	A	1618	6MZ	C2-N3-C4	3.82	121.17	111.83
22	w	54	5MU	C1'-N1-C2	3.82	124.45	117.59
26	A	2504	PSU	C4-N3-C2	-3.82	121.11	126.37
26	A	2605	PSU	C4-N3-C2	-3.80	121.13	126.37
1	a	1519	MA6	C2-N3-C4	3.79	121.08	111.83
26	A	2580	PSU	O2-C2-N1	-3.77	118.90	122.79
26	A	2503	2MA	C4-N9-C8	3.76	109.69	105.74
26	A	2030	6MZ	C4-C5-N7	-3.74	106.30	110.58
26	A	1618	6MZ	C6-C5-N7	3.73	136.49	132.43
24	y	55	PSU	O2-C2-N1	-3.71	118.96	122.79
26	A	1939	5MU	O2-C2-N1	-3.70	117.97	122.80
24	y	37	MIA	C15-C14-C13	-3.68	111.60	122.66
26	A	1911	PSU	O2-C2-N1	-3.68	119.00	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	55	5MU	C5-C6-N1	-3.59	119.41	123.31
1	a	1518	MA6	N1-C2-N3	-3.58	123.16	128.58
1	a	1519	MA6	N3-C4-N9	3.57	133.24	127.17
26	A	1917	PSU	O2-C2-N1	-3.51	119.17	122.79
1	a	1518	MA6	C2-N3-C4	3.50	120.37	111.83
26	A	746	PSU	O2-C2-N1	-3.48	119.20	122.79
24	y	8	4SU	N3-C2-N1	3.44	119.38	114.89
24	y	32	PSU	O2-C2-N1	-3.42	119.26	122.79
24	y	39	PSU	O2-C2-N1	-3.42	119.26	122.79
26	A	2503	2MA	C4-C5-N7	-3.37	106.73	110.58
26	A	2552	OMU	O4-C4-C5	-3.35	119.38	125.16
1	a	1519	MA6	C4-C5-N7	-3.34	106.76	110.58
26	A	2030	6MZ	C4-N9-C8	3.34	109.24	105.74
1	a	1407	5MC	C5-C6-N1	-3.30	119.73	123.31
24	y	37	MIA	C2-N3-C4	3.29	120.92	112.29
26	A	1618	6MZ	C4-C5-N7	-3.29	106.82	110.58
1	a	1518	MA6	N1-C6-N6	3.28	120.85	116.86
26	A	747	5MC	C5-C6-N1	-3.27	119.76	123.31
26	A	2503	2MA	N6-C6-N1	3.27	121.43	117.03
22	v	56	PSU	O2-C2-N1	-3.24	119.45	122.79
26	A	2030	6MZ	C2-N3-C4	3.20	119.66	111.83
26	A	1962	5MC	C5-C4-N3	-3.18	118.50	121.75
24	y	37	MIA	C4-N9-C8	3.16	109.06	105.74
1	a	1518	MA6	N3-C4-N9	3.15	132.52	127.17
24	y	37	MIA	C6-C5-N7	3.14	135.86	132.43
1	a	1498	UR3	C1'-N1-C2	3.13	122.16	117.04
26	A	1618	6MZ	N1-C2-N3	-3.08	123.92	128.58
1	a	966	2MG	C6-C5-N7	3.02	135.79	130.29
26	A	2503	2MA	C2-N1-C6	3.00	122.71	118.10
24	y	37	MIA	C5-N7-C8	2.95	108.09	103.45
22	w	54	5MU	C5M-C5-C6	-2.93	118.89	122.85
26	A	2030	6MZ	N1-C2-N3	-2.92	124.16	128.58
1	a	1519	MA6	C10-N6-C9	-2.90	106.86	116.18
1	a	1516	2MG	C6-C5-N7	2.90	135.56	130.29
24	y	8	4SU	C1'-N1-C2	2.85	122.71	117.59
24	y	46	7MG	C5-C6-N1	2.84	115.94	110.94
1	a	1207	2MG	C6-C5-N7	2.83	135.44	130.29
26	A	1915	3TD	C10-N3-C4	2.83	122.02	117.64
1	a	1518	MA6	C4-C5-N7	-2.83	107.35	110.58
26	A	2604	PSU	C5-C6-N1	-2.78	118.28	122.14
1	a	1407	5MC	C5-C4-N3	-2.77	118.91	121.75
1	a	1519	MA6	N1-C6-N6	2.76	120.22	116.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1835	2MG	C6-C5-N7	2.76	135.32	130.29
26	A	2069	7MG	C5-C4-N9	-2.75	102.81	106.33
26	A	747	5MC	C5-C4-N3	-2.74	118.95	121.75
26	A	2503	2MA	C5-N7-C8	2.74	107.75	103.45
26	A	2552	OMU	C1'-N1-C6	-2.70	115.01	120.78
1	a	967	5MC	C5-C6-N1	-2.70	120.38	123.31
26	A	1915	3TD	C1'-C5-C4	2.69	121.69	117.61
26	A	2580	PSU	C5-C6-N1	-2.69	118.41	122.14
26	A	745	1MG	C4-C5-N7	-2.68	106.42	110.67
26	A	2503	2MA	N9-C8-N7	-2.67	110.14	113.94
24	y	54	5MU	O2-C2-N1	-2.66	119.34	122.80
26	A	2251	OMG	C6-C5-N7	2.65	135.12	130.29
26	A	2030	6MZ	C5-N7-C8	2.64	107.59	103.45
26	A	2445	2MG	C6-C5-N7	2.61	135.04	130.29
26	A	1962	5MC	C5-C6-N1	-2.61	120.48	123.31
1	a	527	7MG	C5-C4-N9	-2.60	103.00	106.33
26	A	2604	PSU	O2-C2-N1	-2.60	120.11	122.79
1	a	967	5MC	C5-C4-N3	-2.58	119.11	121.75
26	A	2457	PSU	C5-C6-N1	-2.57	118.57	122.14
26	A	745	1MG	C6-C5-N7	2.54	135.01	129.36
1	a	527	7MG	C5-C6-N1	2.54	115.42	110.94
26	A	2445	2MG	O6-C6-C5	-2.54	119.82	126.53
26	A	1618	6MZ	C4-N9-C8	2.54	108.40	105.74
26	A	1835	2MG	C2-N1-C6	-2.54	121.48	124.55
22	w	54	5MU	C5-C6-N1	-2.53	120.56	123.31
26	A	2605	PSU	O2-C2-N1	-2.49	120.22	122.79
26	A	1835	2MG	O6-C6-C5	-2.48	119.99	126.53
24	y	37	MIA	N9-C8-N7	-2.47	110.43	113.94
24	y	39	PSU	C5-C6-N1	-2.46	118.72	122.14
24	y	37	MIA	C2-N1-C6	2.44	122.18	117.54
1	a	1516	2MG	N1-C2-N2	2.42	119.03	116.56
26	A	2449	H2U	C5-C6-N1	-2.40	104.26	111.52
1	a	966	2MG	C4-C5-N7	-2.40	106.87	110.67
1	a	1516	2MG	O6-C6-C5	-2.39	120.21	126.53
26	A	746	PSU	C5-C6-N1	-2.39	118.83	122.14
1	a	516	PSU	C5-C6-N1	-2.38	118.83	122.14
26	A	2069	7MG	O6-C6-C5	-2.38	121.78	127.62
26	A	2449	H2U	O4-C4-N3	2.36	123.94	120.30
26	A	2445	2MG	N1-C2-N2	2.36	118.97	116.56
22	w	55	PSU	O4'-C1'-C2'	2.34	108.38	105.15
1	a	516	PSU	O4'-C1'-C2'	2.34	108.38	105.15
1	a	1519	MA6	C4-N9-C8	2.33	108.19	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2605	PSU	C6-C5-C4	-2.33	116.60	118.17
22	w	55	PSU	C5-C6-N1	-2.33	118.91	122.14
1	a	1207	2MG	C4-C5-N7	-2.33	106.98	110.67
24	y	16	H2U	C5-C6-N1	-2.32	104.49	111.52
22	v	8	4SU	C1'-N1-C2	2.31	121.73	117.59
1	a	1519	MA6	C6-C5-N7	2.31	137.11	133.43
26	A	2069	7MG	C5-C6-N1	2.30	115.00	110.94
1	a	527	7MG	O6-C6-C5	-2.30	121.97	127.62
26	A	955	PSU	C5-C6-N1	-2.30	118.95	122.14
26	A	1911	PSU	C5-C6-N1	-2.28	118.98	122.14
24	y	54	5MU	C5M-C5-C4	2.28	121.21	118.78
26	A	2030	6MZ	C2-N1-C6	2.26	122.75	115.24
22	w	54	5MU	O2-C2-N1	-2.25	119.87	122.80
24	y	46	7MG	C5-C4-N9	-2.24	103.46	106.33
26	A	745	1MG	C8-N9-C4	2.23	110.21	106.03
26	A	2503	2MA	C6-C5-N7	2.23	136.39	132.09
26	A	1835	2MG	C4-C5-N7	-2.23	107.14	110.67
26	A	1618	6MZ	C5-N7-C8	2.21	106.93	103.45
26	A	2251	OMG	C4-C5-N7	-2.21	107.16	110.67
1	a	1516	2MG	C4-C5-N7	-2.20	107.18	110.67
26	A	1835	2MG	C5-C6-N1	2.20	118.84	113.25
1	a	1207	2MG	O6-C6-C5	-2.19	120.75	126.53
22	v	21	H2U	N3-C2-N1	2.19	118.85	116.65
1	a	966	2MG	O6-C6-C5	-2.19	120.75	126.53
1	a	966	2MG	C2-N1-C6	-2.16	121.94	124.55
24	y	37	MIA	N3-C2-N1	-2.13	123.11	127.00
24	y	37	MIA	N6-C6-N1	2.12	121.18	118.33
1	a	1519	MA6	C5-C6-N6	-2.11	121.99	125.33
26	A	2605	PSU	O2-C2-N3	-2.11	118.12	121.86
26	A	745	1MG	C8-N7-C5	2.10	108.00	104.26
22	v	21	H2U	C5-C6-N1	-2.09	105.21	111.52
24	y	32	PSU	C5-C6-N1	-2.08	119.25	122.14
24	y	46	7MG	O6-C6-C5	-2.08	122.52	127.62
26	A	2604	PSU	O2-C2-N3	-2.08	118.17	121.86
1	a	1407	5MC	O2-C2-N3	-2.07	119.06	122.33
1	a	1207	2MG	N1-C2-N2	2.06	118.66	116.56
24	y	20	H2U	O4-C4-N3	2.04	123.45	120.30
1	a	966	2MG	C5-C6-N1	2.04	118.44	113.25
22	v	56	PSU	C6-C5-C4	-2.04	116.80	118.17
26	A	747	5MC	C3'-C2'-C1'	2.03	105.31	101.46
1	a	1207	2MG	C2-N1-C6	-2.03	122.09	124.55
22	v	8	4SU	O2-C2-N1	-2.03	120.15	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2552	OMU	O2-C2-N3	-2.02	117.76	121.49
1	a	1519	MA6	C5-N7-C8	2.01	106.61	103.45
1	a	1498	UR3	C3U-N3-C2	2.01	120.83	117.33

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1207	2MG	O4'-C4'-C5'-O5'
1	a	1207	2MG	C3'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	C5-C6-N6-C10
1	a	1518	MA6	N1-C6-N6-C9
1	a	1518	MA6	N1-C6-N6-C10
1	a	1519	MA6	C5-C6-N6-C9
22	v	56	PSU	O4'-C1'-C5-C4
22	v	56	PSU	O4'-C1'-C5-C6
22	w	8	4SU	O4'-C4'-C5'-O5'
22	w	55	PSU	O4'-C1'-C5-C4
22	w	55	PSU	O4'-C1'-C5-C6
24	y	20	H2U	O4'-C1'-N1-C2
24	y	20	H2U	O4'-C1'-N1-C6
24	y	37	MIA	C5-C6-N6-C12
24	y	37	MIA	C12-C13-C14-C15
26	A	1915	3TD	C2'-C1'-C5-C4
26	A	1915	3TD	O4'-C1'-C5-C4
26	A	1915	3TD	O4'-C1'-C5-C6
26	A	2445	2MG	O4'-C4'-C5'-O5'
26	A	2552	OMU	O4'-C1'-N1-C2
26	A	2552	OMU	O4'-C1'-N1-C6
1	a	1498	UR3	O4'-C1'-N1-C2
1	a	527	7MG	C3'-C4'-C5'-O5'
24	y	20	H2U	O4'-C4'-C5'-O5'
26	A	2445	2MG	C3'-C4'-C5'-O5'
26	A	2504	PSU	O4'-C4'-C5'-O5'
1	a	1518	MA6	O4'-C1'-N9-C8
1	a	966	2MG	O4'-C4'-C5'-O5'
1	a	1518	MA6	O4'-C1'-N9-C4
24	y	46	7MG	C2'-C1'-N9-C8
22	w	8	4SU	C3'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C6
1	a	966	2MG	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	A	2030	6MZ	O4'-C4'-C5'-O5'
1	a	527	7MG	O4'-C4'-C5'-O5'
24	y	20	H2U	C3'-C4'-C5'-O5'
26	A	2030	6MZ	C3'-C4'-C5'-O5'
26	A	2504	PSU	C3'-C4'-C5'-O5'
24	y	37	MIA	N1-C6-N6-C12
1	a	1519	MA6	N1-C6-N6-C9
22	w	54	5MU	O4'-C4'-C5'-O5'
22	w	20	H2U	C4'-C5'-O5'-P
26	A	1962	5MC	C4'-C5'-O5'-P
22	w	8	4SU	C2'-C1'-N1-C6
1	a	516	PSU	O4'-C1'-C5-C4
22	w	8	4SU	O4'-C1'-N1-C6
26	A	2503	2MA	O4'-C4'-C5'-O5'
22	v	21	H2U	C4'-C5'-O5'-P
1	a	527	7MG	C4'-C5'-O5'-P
24	y	20	H2U	C4'-C5'-O5'-P
1	a	516	PSU	O4'-C1'-C5-C6
26	A	746	PSU	O4'-C1'-C5-C6
22	w	8	4SU	O4'-C1'-N1-C2
24	y	46	7MG	O4'-C4'-C5'-O5'
24	y	46	7MG	O4'-C1'-N9-C8
26	A	2503	2MA	O4'-C1'-N9-C8
26	A	2498	OMC	C4'-C5'-O5'-P
22	w	54	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	2030	6MZ	1	0
26	A	955	PSU	1	0
1	a	1519	MA6	2	0
1	a	1402	4OC	2	0
1	a	516	PSU	1	0
22	w	54	5MU	2	0
22	w	55	PSU	3	0
26	A	2445	2MG	1	0
26	A	2449	H2U	1	0
22	v	55	5MU	1	0
24	y	8	4SU	2	0
22	w	8	4SU	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1518	MA6	1	0
1	a	1207	2MG	2	0
26	A	2552	OMU	1	0
24	y	16	H2U	1	0
26	A	1917	PSU	1	0
26	A	2498	OMC	1	0
26	A	747	5MC	1	0
1	a	1498	UR3	1	0
24	y	55	PSU	1	0
26	A	2503	2MA	1	0
24	y	37	MIA	1	0
22	v	56	PSU	1	0
26	A	1962	5MC	1	0
22	w	20	H2U	12	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 342 ligands modelled in this entry, 339 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	GDP	z	402	59	29,30,30	1.11	2 (6%)	45,47,47	1.82	7 (15%)
61	FME	v	105	-	8,9,10	0.87	0	8,9,11	1.41	2 (25%)
62	KIR	z	401	-	56,59,59	0.97	4 (7%)	60,84,84	1.74	11 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	GDP	z	402	59	-	1/16/32/32	0/3/3/3
61	FME	v	105	-	-	2/7/9/11	-
62	KIR	z	401	-	-	24/54/98/98	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	z	401	KIR	C3-C4	4.00	1.49	1.41
63	z	402	GDP	C5-C4	3.03	1.47	1.38
63	z	402	GDP	C6-N1	-2.33	1.34	1.38
62	z	401	KIR	C3-C2	2.32	1.49	1.44
62	z	401	KIR	C6-C5	2.26	1.40	1.35
62	z	401	KIR	C2-N1	-2.16	1.34	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	z	401	KIR	C23-C22-C21	-6.12	118.50	127.37
63	z	402	GDP	C5-C4-N3	-5.90	119.00	128.39
63	z	402	GDP	C2-N3-C4	4.96	120.84	112.30
63	z	402	GDP	N9-C4-N3	4.69	135.33	125.95
62	z	401	KIR	C15-C14-C13	-4.44	107.29	114.60
62	z	401	KIR	C6-N1-C2	-3.86	122.25	124.54
62	z	401	KIR	C16-C15-C14	3.70	106.04	101.84
63	z	402	GDP	C6-C5-N7	3.29	136.28	130.29
62	z	401	KIR	C44-C21-C22	-2.71	119.55	123.85
62	z	401	KIR	C3-C2-N1	2.65	119.59	114.65
61	v	105	FME	CA-N-CN	-2.46	119.04	122.82
63	z	402	GDP	C4-C5-N7	-2.45	106.78	110.67
62	z	401	KIR	C44-C21-C20	2.40	120.70	115.96
62	z	401	KIR	C10-C9-C8	-2.39	119.90	126.64
62	z	401	KIR	C41-C8-C7	2.27	119.31	115.68
63	z	402	GDP	O6-C6-C5	-2.23	120.65	126.53
62	z	401	KIR	C15-C16-C17	2.18	105.45	102.35
63	z	402	GDP	O3A-PB-O1B	-2.07	100.13	111.04
62	z	401	KIR	C39-C38-C37	-2.04	118.60	125.56
61	v	105	FME	O1-CN-N	-2.00	120.15	125.32

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	v	105	FME	O1-CN-N-CA
62	z	401	KIR	C2-C3-C7-C8
62	z	401	KIR	C4-C3-C7-C8
62	z	401	KIR	C3-C7-C8-C41
62	z	401	KIR	C17-C19-C20-C21
62	z	401	KIR	C42-C19-C20-C21
62	z	401	KIR	C17-C19-C20-O20
62	z	401	KIR	C42-C19-C20-O20
62	z	401	KIR	C12-C13-C14-C15
62	z	401	KIR	C16-C17-C19-C20
62	z	401	KIR	C16-C17-C19-C42
62	z	401	KIR	O18-C17-C19-C20
62	z	401	KIR	O18-C17-C19-C42
62	z	401	KIR	C45-C28-C29-O29
62	z	401	KIR	C45-C28-C29-O34
63	z	402	GDP	C5'-O5'-PA-O1A
62	z	401	KIR	O27-C27-N26-C25
62	z	401	KIR	C36-C37-C38-C39
62	z	401	KIR	C35-C36-C37-C38
61	v	105	FME	CB-CG-SD-CE
62	z	401	KIR	C28-C27-N26-C25
62	z	401	KIR	C12-C13-C14-O18
62	z	401	KIR	O7-C7-C8-C9
62	z	401	KIR	N26-C27-C28-C45
62	z	401	KIR	C27-C28-C45-C46
62	z	401	KIR	C10-C11-C12-C13
62	z	401	KIR	O7-C7-C8-C41

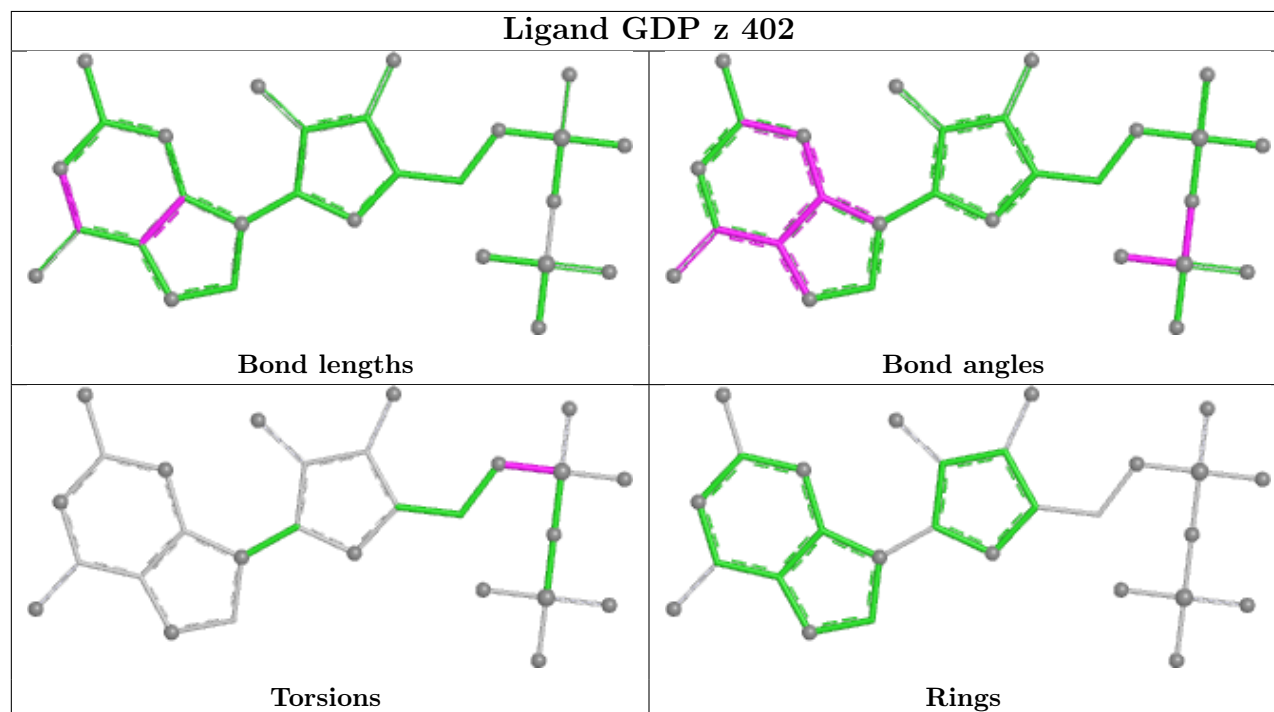
There are no ring outliers.

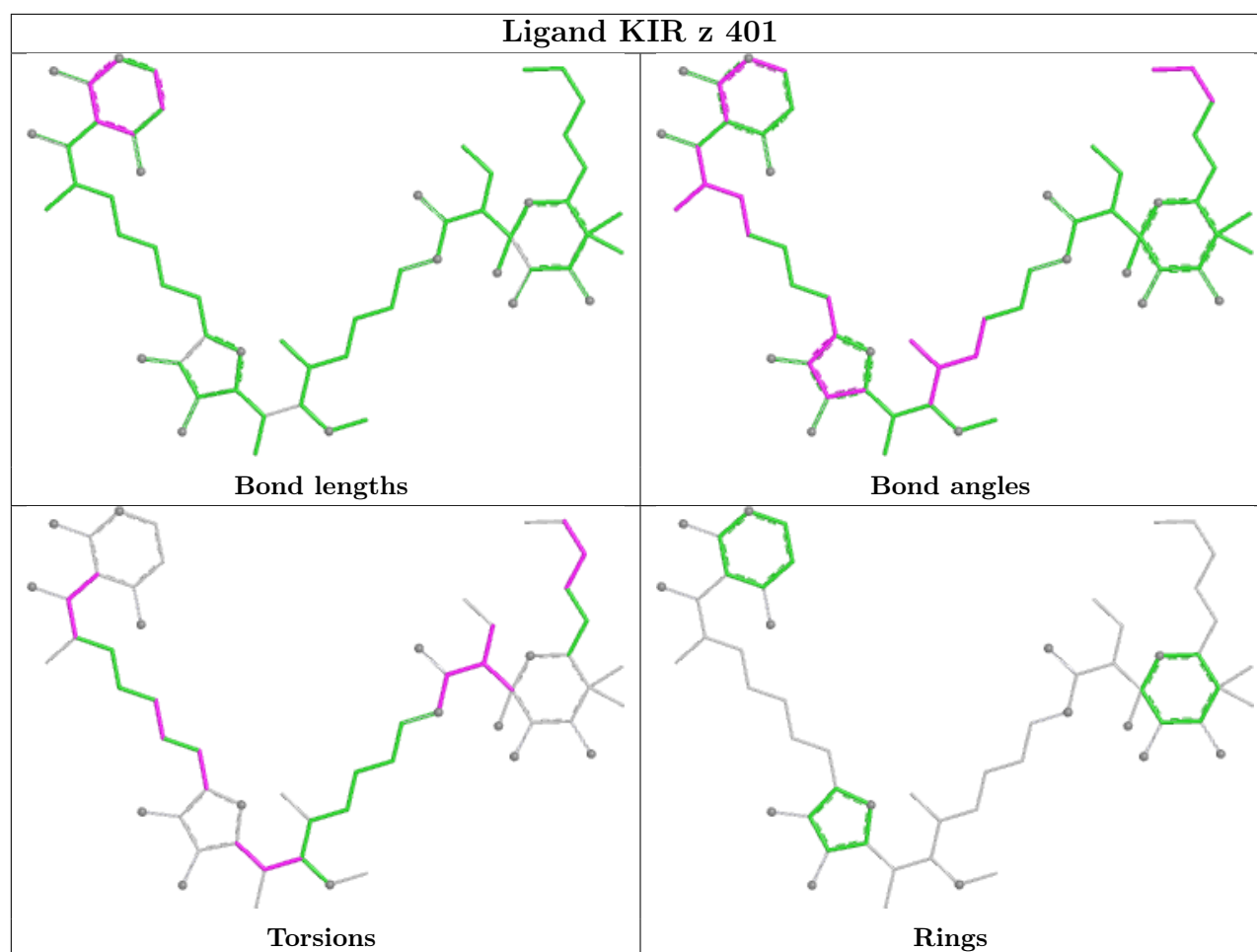
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	z	402	GDP	3	0
61	v	105	FME	7	0
62	z	401	KIR	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

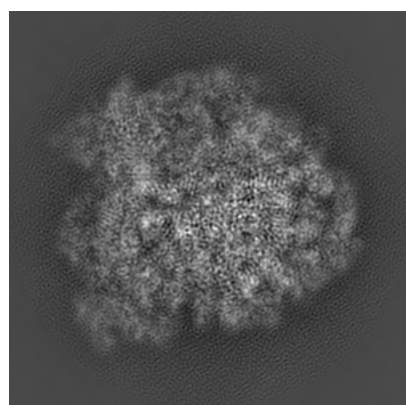
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2847. These allow visual inspection of the internal detail of the map and identification of artifacts.

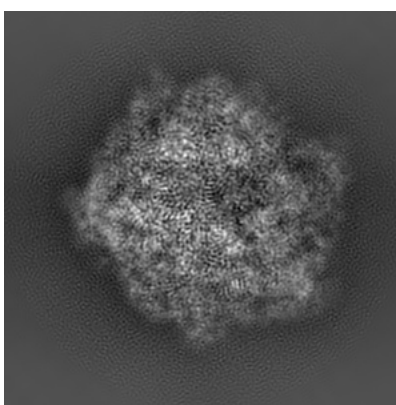
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

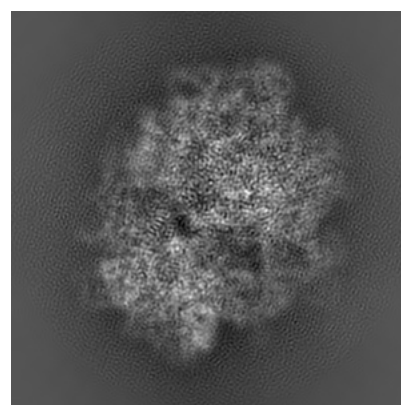
6.1.1 Primary map



X



Y

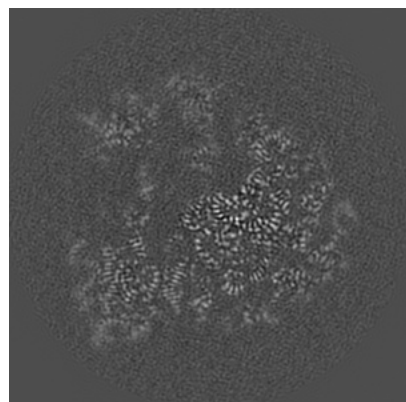


Z

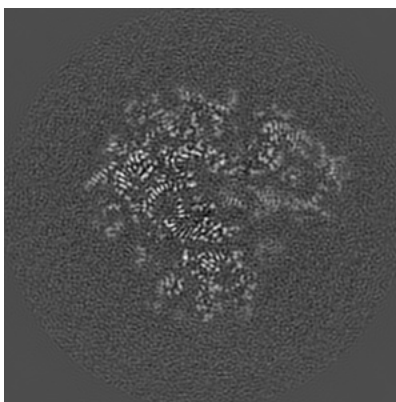
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

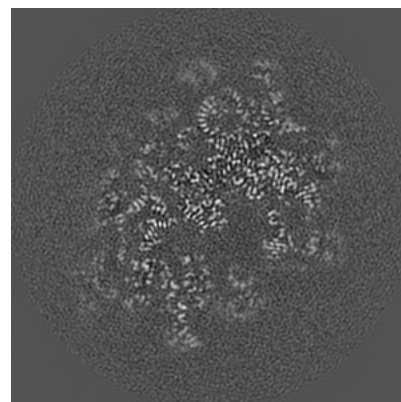
6.2.1 Primary map



X Index: 210



Y Index: 210

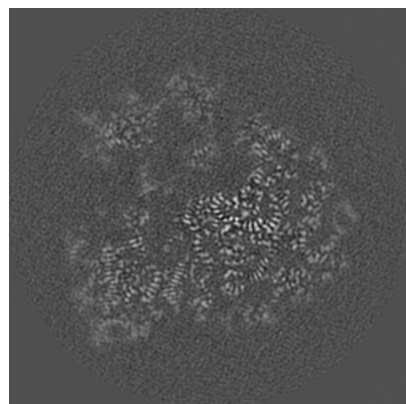


Z Index: 210

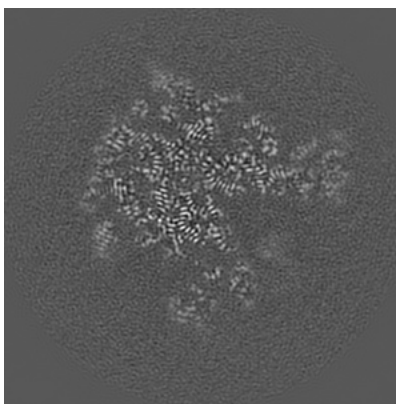
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

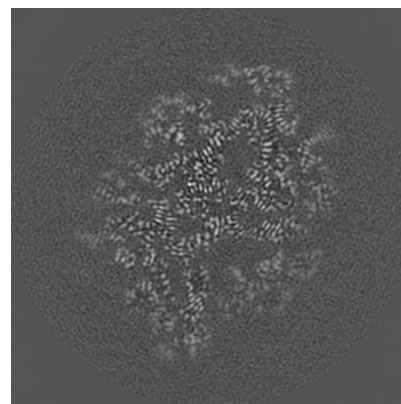
6.3.1 Primary map



X Index: 209



Y Index: 228

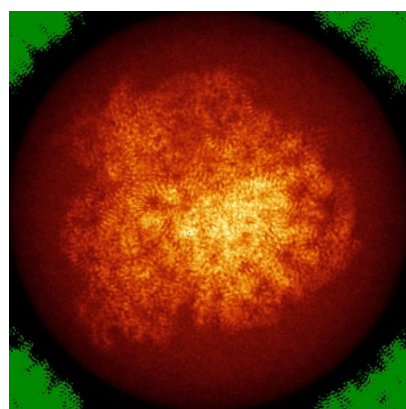


Z Index: 189

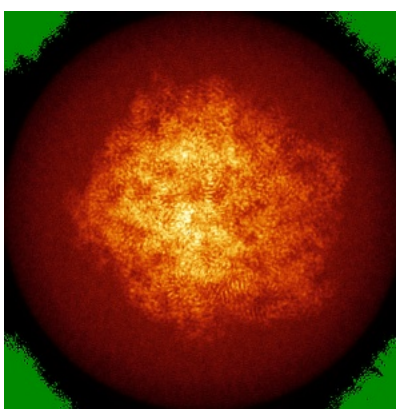
The images above show the largest variance slices of the map in three orthogonal directions.

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

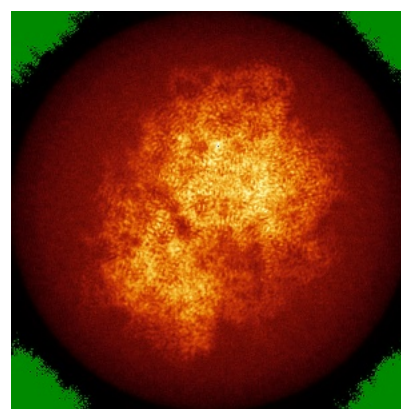
6.4.1 Primary map



X



Y

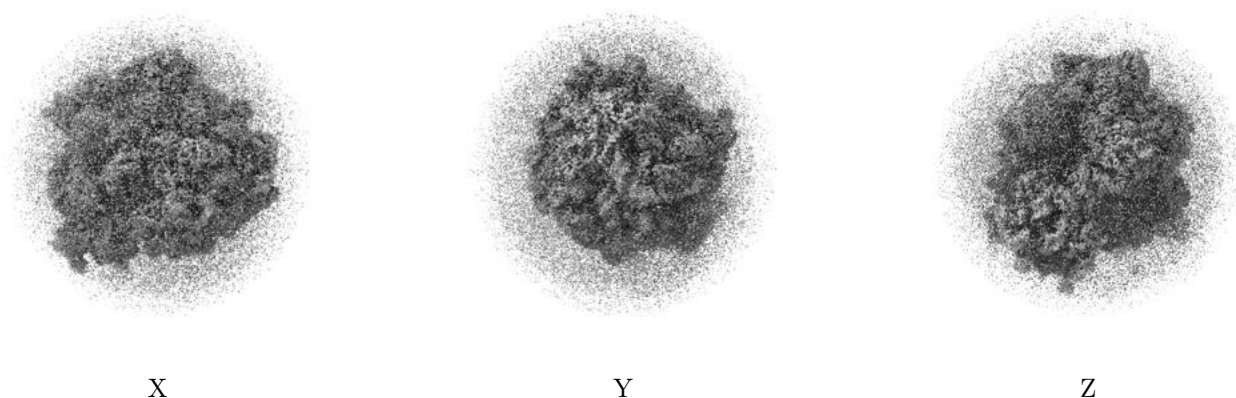


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

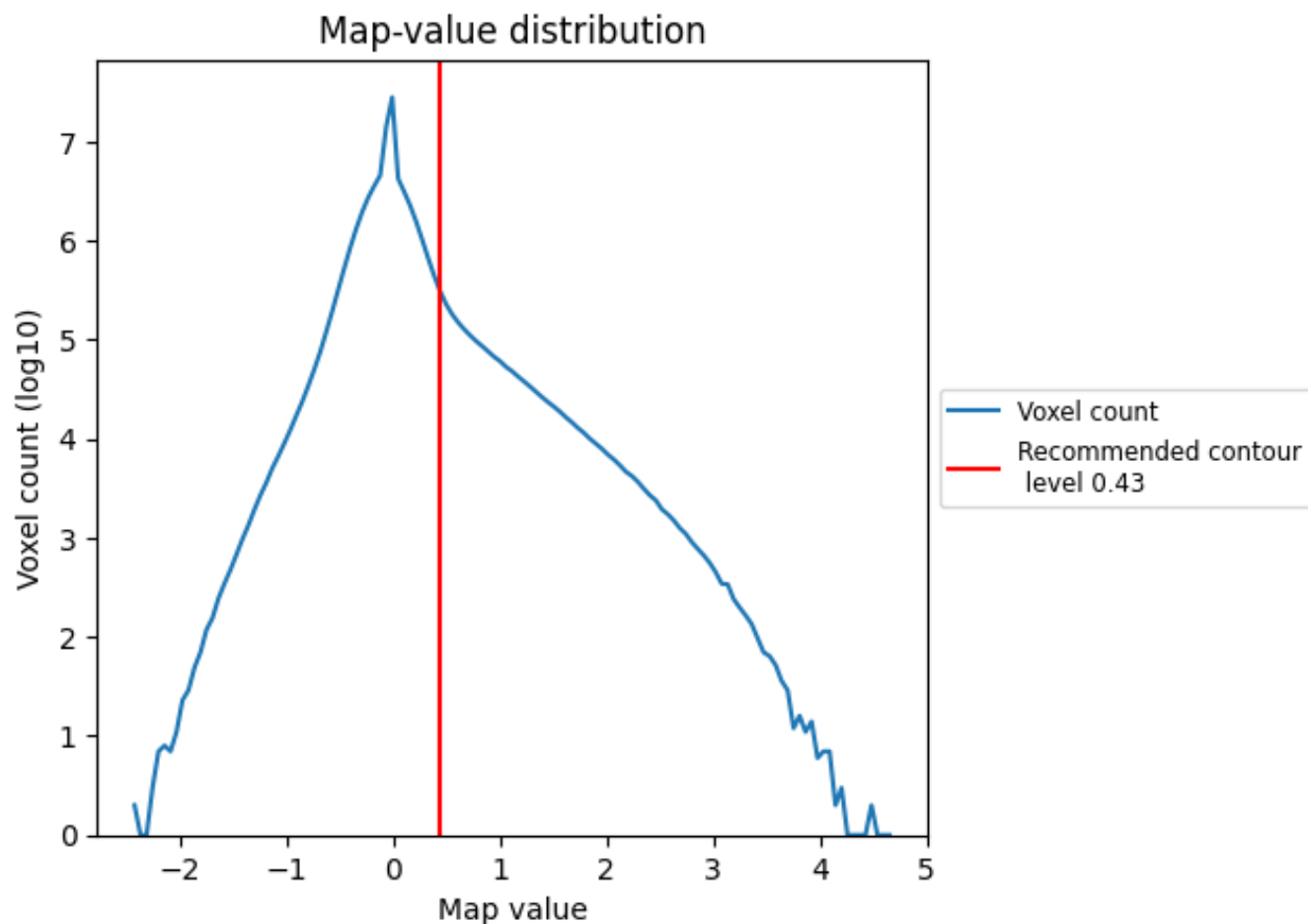
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

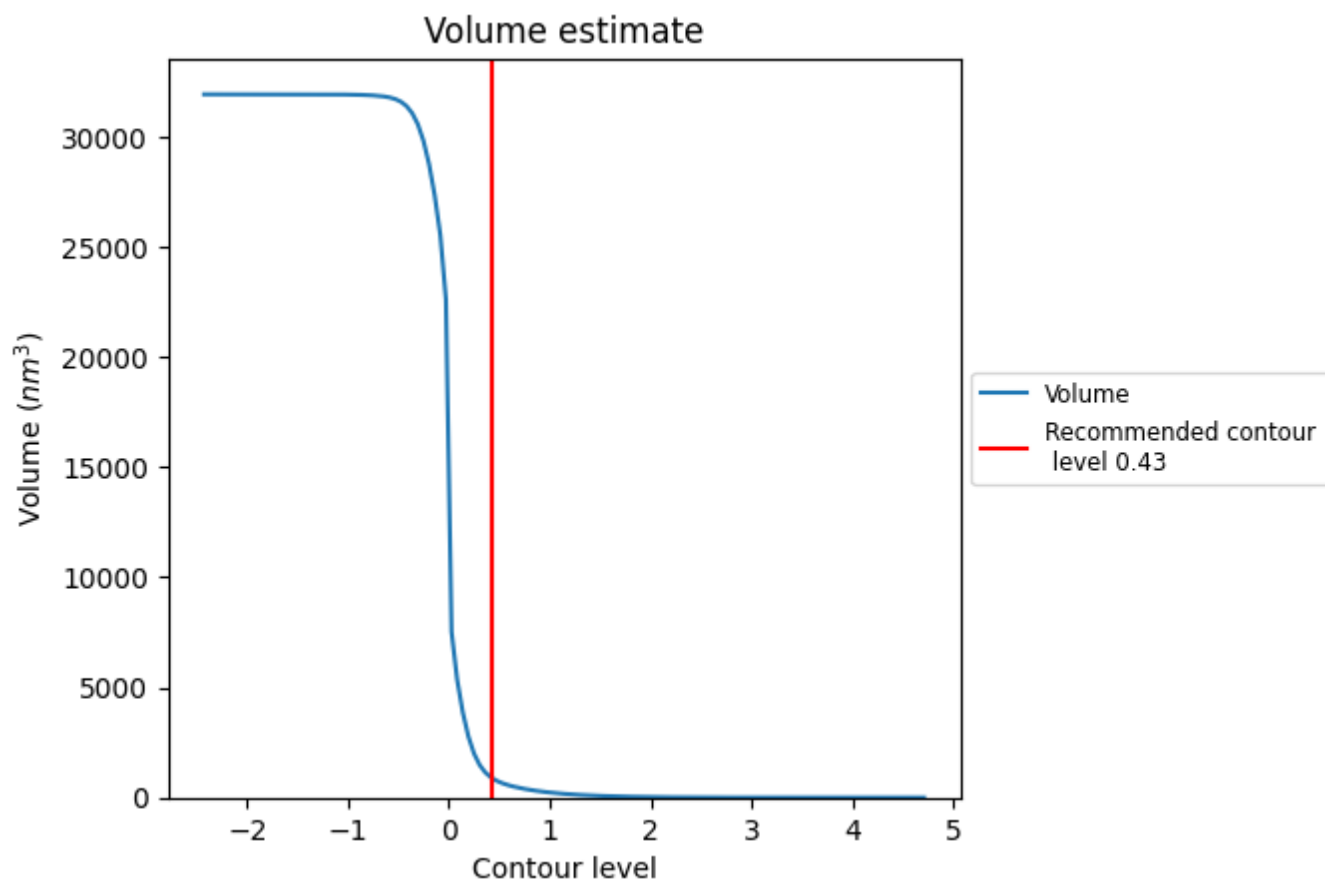
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

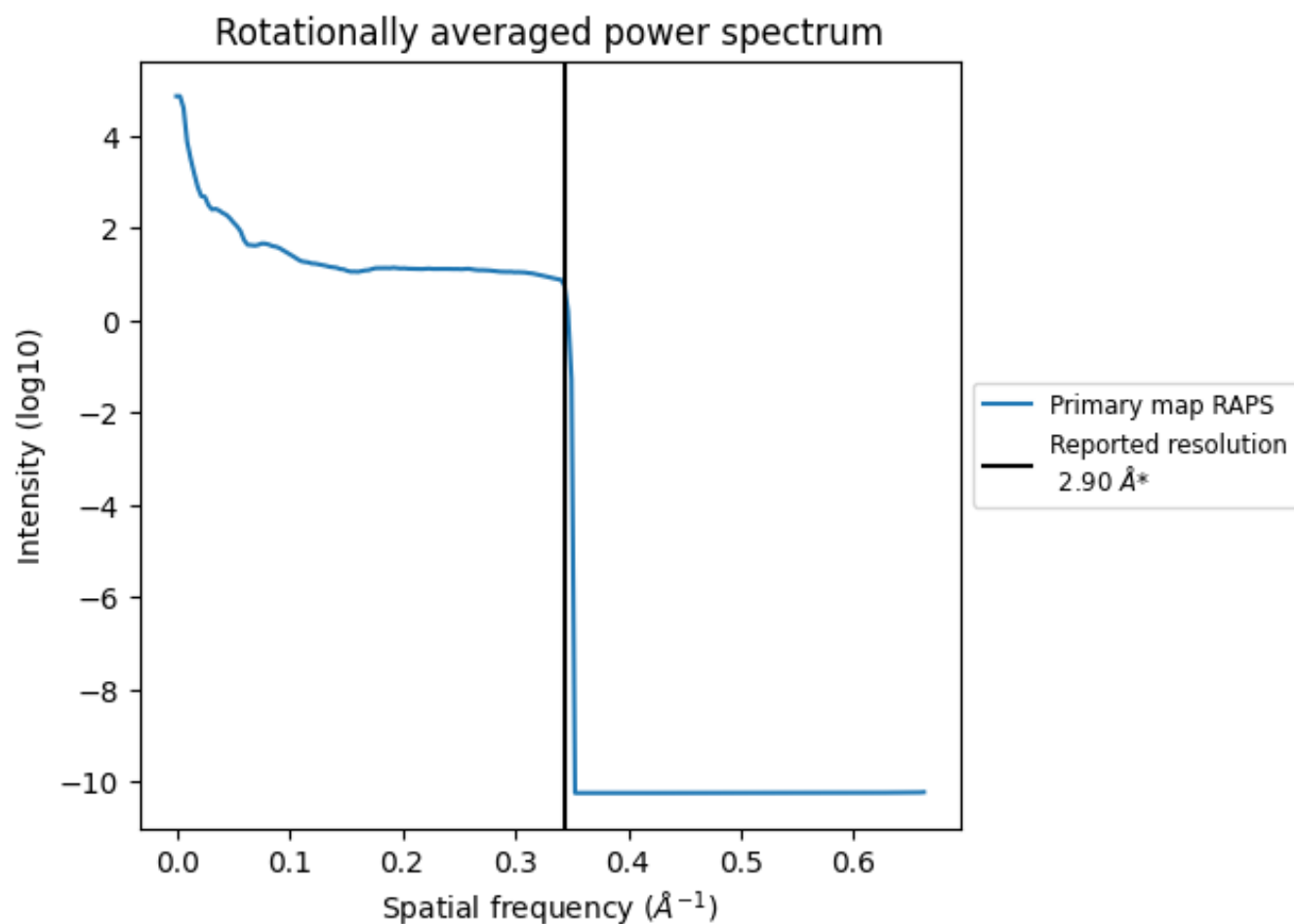
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 882 nm³; this corresponds to an approximate mass of 797 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

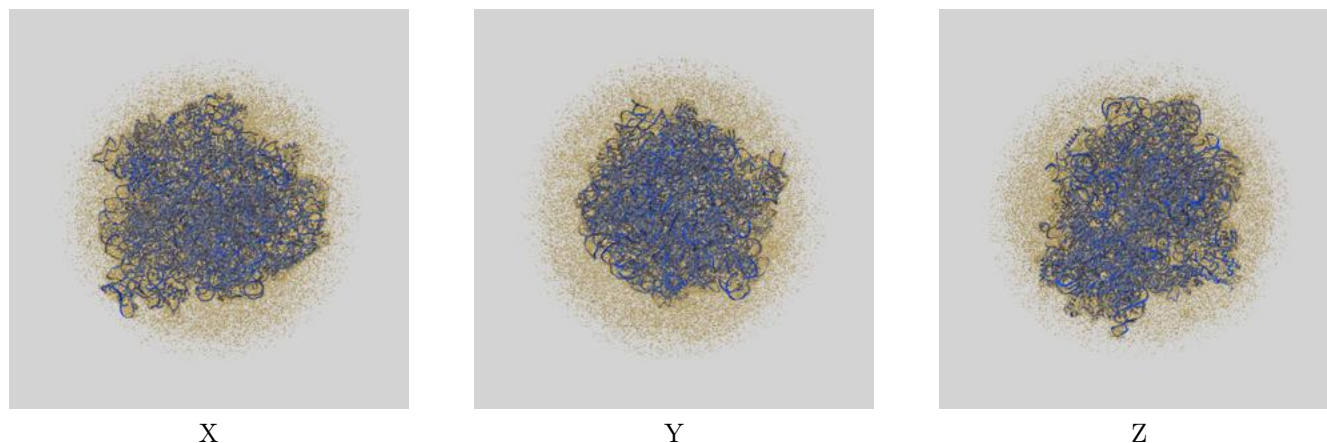
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

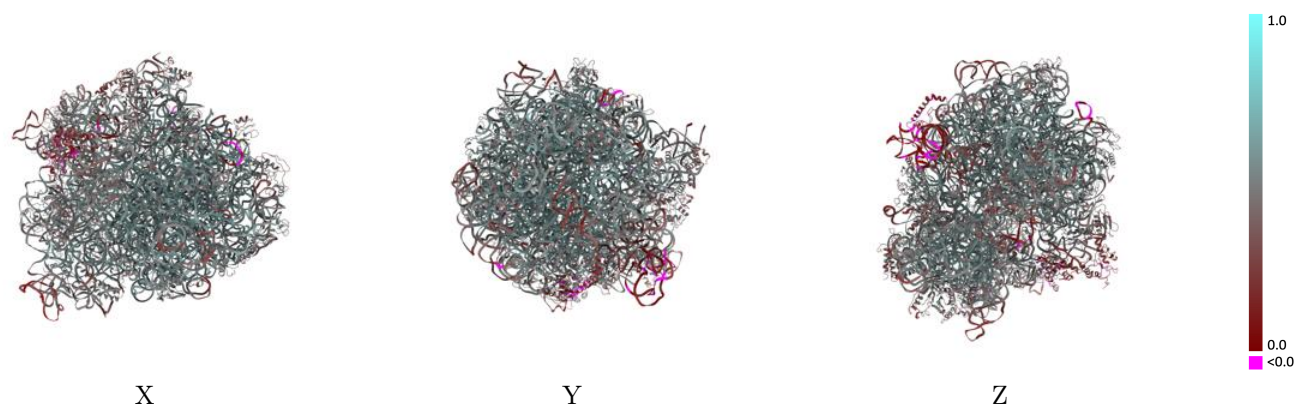
This section contains information regarding the fit between EMDB map EMD-2847 and PDB model 5AFI. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



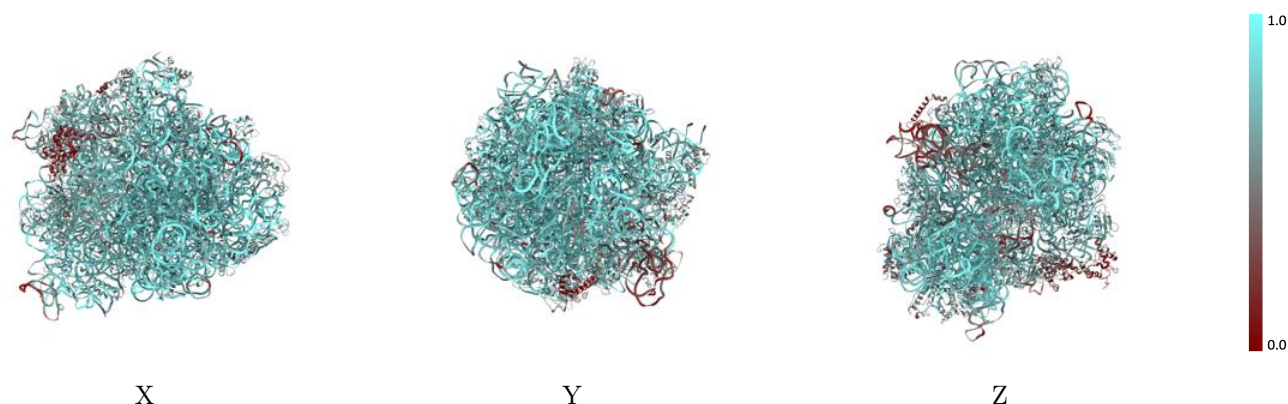
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



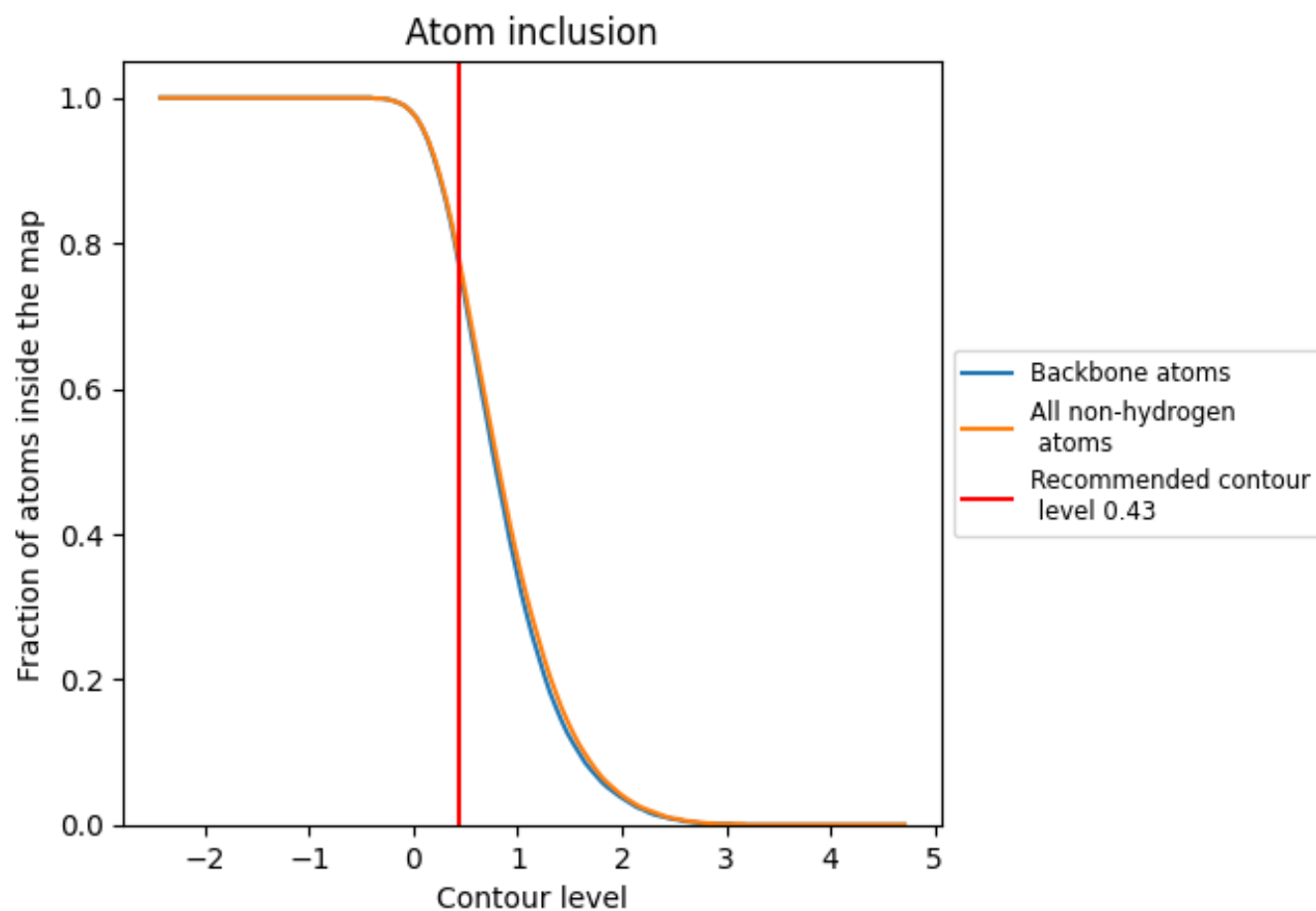
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.43).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7830	 0.4980
0	 0.7530	 0.5130
1	 0.6360	 0.4690
2	 0.8060	 0.5360
3	 0.7900	 0.5620
4	 0.7620	 0.5050
5	 0.1590	 0.1980
6	 0.4510	 0.3410
A	 0.8600	 0.5270
B	 0.8250	 0.4790
C	 0.7710	 0.5200
D	 0.7480	 0.5180
E	 0.6730	 0.4760
F	 0.5920	 0.4100
G	 0.6110	 0.4260
H	 0.2150	 0.1780
I	 0.2040	 0.2050
J	 0.7470	 0.5070
K	 0.7400	 0.5320
L	 0.7170	 0.4870
M	 0.7390	 0.5040
N	 0.7740	 0.5320
O	 0.6560	 0.4530
P	 0.7060	 0.4940
Q	 0.7770	 0.5360
R	 0.7130	 0.4760
S	 0.7390	 0.5170
T	 0.6840	 0.4660
U	 0.6210	 0.4460
V	 0.6730	 0.4530
W	 0.7460	 0.5280
X	 0.7190	 0.4930
Y	 0.6300	 0.4170
Z	 0.7070	 0.4910
a	 0.8650	 0.5260



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.4970	 0.3890
c	 0.6730	 0.4720
d	 0.6460	 0.4540
e	 0.7340	 0.4940
f	 0.6390	 0.3820
g	 0.6320	 0.4330
h	 0.7180	 0.4990
i	 0.6570	 0.4350
j	 0.5900	 0.4150
k	 0.7340	 0.4820
l	 0.7450	 0.5170
m	 0.6380	 0.4230
n	 0.6860	 0.4650
o	 0.7300	 0.4770
p	 0.6790	 0.4660
q	 0.6800	 0.4650
r	 0.7300	 0.4930
s	 0.6600	 0.4580
t	 0.6720	 0.4770
u	 0.5290	 0.3610
v	 0.7680	 0.4980
w	 0.4290	 0.3010
x	 0.7610	 0.4850
y	 0.7630	 0.4810
z	 0.6080	 0.4350