Full wwPDB EM Validation Report ⓘ

Oct 8, 2024 – 01:42 AM EDT

PDB ID	:	3J7Q
EMDB ID	:	EMD-2650
Title	:	Structure of the idle mammalian ribosome-Sec61 complex
Authors	:	Voorhees, R.M.; Fernandez, I.S.; Scheres, S.H.W.; Hegde, R.S.
Deposited on	:	2014-08-01
Resolution	:	3.40 Å(reported)
Based on initial models	:	3J3B, 3J3F

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:

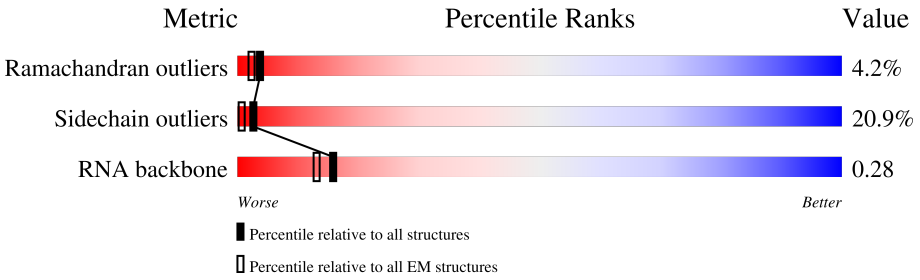
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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.



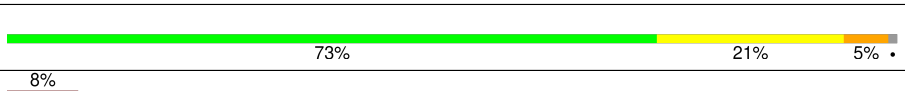
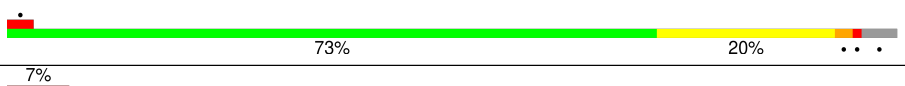
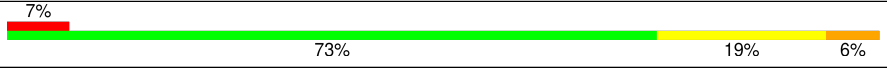
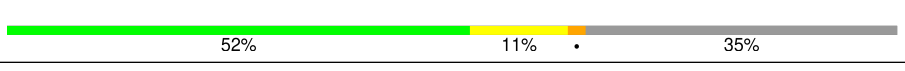
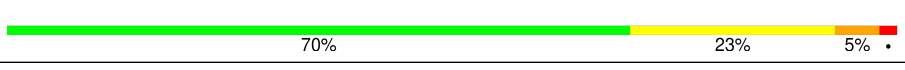
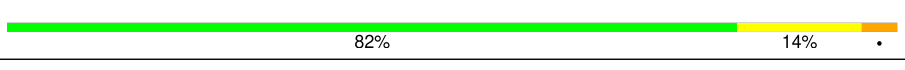
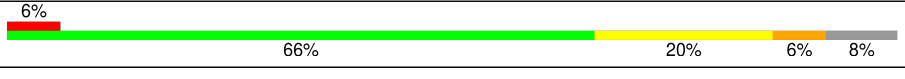
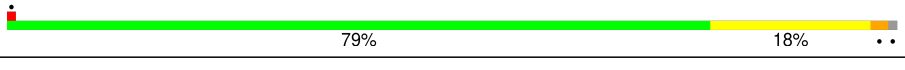
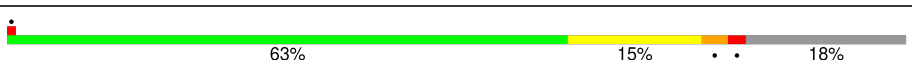
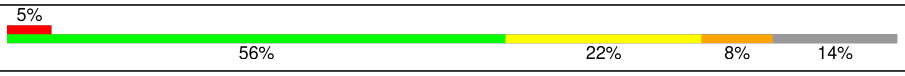
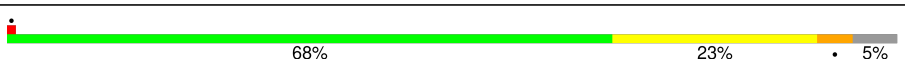
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	5	3722	9% 47% 39% 10%
2	7	120	69% 24% 6%
3	8	156	8% 53% 33% 8% 5%
4	A	257	71% 18% 5% 5%
5	B	394	74% 21%
6	C	367	77% 19%
7	D	297	68% 24% 5%
8	E	236	10% 64% 25% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	225	
10	G	266	
11	H	192	
12	I	213	
13	J	178	
14	L	211	
15	M	213	
16	N	204	
17	O	201	
18	P	153	
19	Q	188	
20	R	196	
21	S	224	
22	T	160	
23	U	128	
24	V	140	
25	W	157	
26	X	156	
27	Y	145	
28	Z	136	
29	a	148	
30	b	160	
31	c	115	
32	d	125	
33	e	135	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	f	110	
35	g	117	
36	h	123	
37	i	105	
38	j	86	
39	k	70	
40	l	51	
41	m	128	
42	n	25	
43	o	106	
44	p	91	
45	r	125	
46	1	476	
47	2	68	
48	3	36	

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 140540 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	3662	78486	34947	14363	25515	3661	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	7	120	2558	1141	456	842	119	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	244	1868	1171	382	309	6	0	0

- Molecule 5 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	394	3147	2005	591	538	13	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ILE	VAL	conflict	UNP A0A480L253
B	86	VAL	ILE	conflict	UNP A0A480L253
B	140	ALA	GLU	conflict	UNP A0A480L253

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	141	ALA	ASP	conflict	UNP A0A480L253
B	143	ALA	LYS	conflict	UNP A0A480L253
B	144	ALA	LYS	conflict	UNP A0A480L253
B	145	ALA	GLN	conflict	UNP A0A480L253
B	147	ALA	GLU	conflict	UNP A0A480L253
B	148	ALA	ARG	conflict	UNP A0A480L253
B	155	ALA	LYS	conflict	UNP A0A480L253

- Molecule 6 is a protein called Ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	367	Total	C	N	O	S	0	0
			2919	1836	582	486	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	354	ALA	-	insertion	UNP A0A287AE76
C	355	ALA	-	insertion	UNP A0A287AE76
C	356	ALA	-	insertion	UNP A0A287AE76

- Molecule 7 is a protein called Ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	292	Total	C	N	O	S	0	0
			2380	1508	434	426	12		

- Molecule 8 is a protein called Ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	236	Total	C	N	O	S	0	0
			1904	1219	364	316	5		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	62	MET	LYS	conflict	UNP Q2YGT9
E	64	MET	LEU	conflict	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	SER	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	VAL	deletion	UNP Q2YGT9
E	?	-	GLU	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	VAL	deletion	UNP Q2YGT9
E	?	-	ARG	deletion	UNP Q2YGT9
E	176	VAL	SER	conflict	UNP Q2YGT9
E	206	LYS	GLU	conflict	UNP Q2YGT9

- Molecule 9 is a protein called Ribosomal protein uL30.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	31	LYS	ARG	conflict	UNP A0A480W0U3

- Molecule 10 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	241	Total	C	N	O	S	0	0
			1934	1232	372	326	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	53	ARG	CYS	conflict	UNP A0A4X1W808
G	172	ALA	SER	conflict	UNP A0A4X1W808
G	185	LYS	ASN	conflict	UNP A0A4X1W808
G	231	ASN	ASP	conflict	UNP A0A4X1W808

- Molecule 11 is a protein called Ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 12 is a protein called Ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	213	Total	C	N	O	S	0	0
			1713	1083	331	284	15		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	49	GLY	CYS	conflict	UNP Q29195
I	82	ARG	LYS	conflict	UNP Q29195
I	87	MET	ILE	conflict	UNP Q29195
I	145	GLU	LYS	conflict	UNP Q29195
I	187	LYS	GLU	conflict	UNP Q29195
I	189	CYS	ARG	conflict	UNP Q29195
I	200	VAL	ILE	conflict	UNP Q29195
I	203	HIS	ARG	conflict	UNP Q29195
I	211	VAL	ALA	conflict	UNP Q29195

- Molecule 13 is a protein called Ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	170	Total	C	N	O	S	0	0
			1359	856	256	241	6		

- Molecule 14 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	210	Total	C	N	O	S	0	0
			1703	1064	354	280	5		

- Molecule 15 is a protein called Ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	138	Total	C	N	O	S	0	0
			1131	727	216	181	7		

- Molecule 16 is a protein called Ribosomal protein eL15.

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

- Molecule 17 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	201	Total	C	N	O	S	0	0
			1651	1063	323	260	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	3	GLU	-	variant	UNP A0A481CAM4
O	4	GLY	-	variant	UNP A0A481CAM4

- Molecule 18 is a protein called Ribosomal protein uL22.

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

- Molecule 19 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	187	Total	C	N	O	S	0	0
			1506	941	311	249	5		

- Molecule 20 is a protein called Ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	TYR	-	variant	UNP A0A480VXS3

- Molecule 21 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	175	Total	C	N	O	S	0	0
			1454	925	284	235	10		

- Molecule 22 is a protein called Ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called Ribosomal protein eL22.

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

- Molecule 24 is a protein called Ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called Ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 26 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 27 is a protein called Ribosomal protein uL24.

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

- Molecule 28 is a protein called Ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 29 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	147	Total	C	N	O	S	0	0
			1163	735	239	185	4		

- Molecule 30 is a protein called Ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	75	Total	C	N	O	S	0	0
			610	378	130	99	3		

- Molecule 31 is a protein called Ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 32 is a protein called Ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 33 is a protein called Ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 34 is a protein called Ribosomal protein eL33.

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

- Molecule 35 is a protein called Ribosomal protein eL34.

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

- Molecule 36 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	122	Total	C	N	O	S	0	0
			1015	642	205	167	1		

- Molecule 37 is a protein called Ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 38 is a protein called Ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	86	Total	C	N	O	S	0	0
			706	436	155	110	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	82	ILE	THR	conflict	UNP A0A480UVT3

- Molecule 39 is a protein called Ribosomal protein eL38.

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

- Molecule 40 is a protein called Ribosomal protein eL39.

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

- Molecule 41 is a protein called Ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 42 is a protein called Ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 43 is a protein called Ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 44 is a protein called Ribosomal protein eL43.

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

- Molecule 45 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	125	Total	C	N	O	S	0	0
			1001	622	206	168	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	64	ILE	MET	conflict	UNP A0A480YX24

- Molecule 46 is a protein called Sec61 alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	392	Total	C	N	O	S	0	0
			3051	2007	493	532	19		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	343	HIS	TYR	conflict	UNP A0A480EHF8

- Molecule 47 is a protein called Sec61 gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 48 is a protein called Sec61 beta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	3	36	Total 180	C 108	N 36	O 36	0	0

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	5	119	Total 119	Mg 119	0
49	7	5	Total 5	Mg 5	0
49	8	4	Total 4	Mg 4	0
49	P	1	Total 1	Mg 1	0
49	V	1	Total 1	Mg 1	0

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

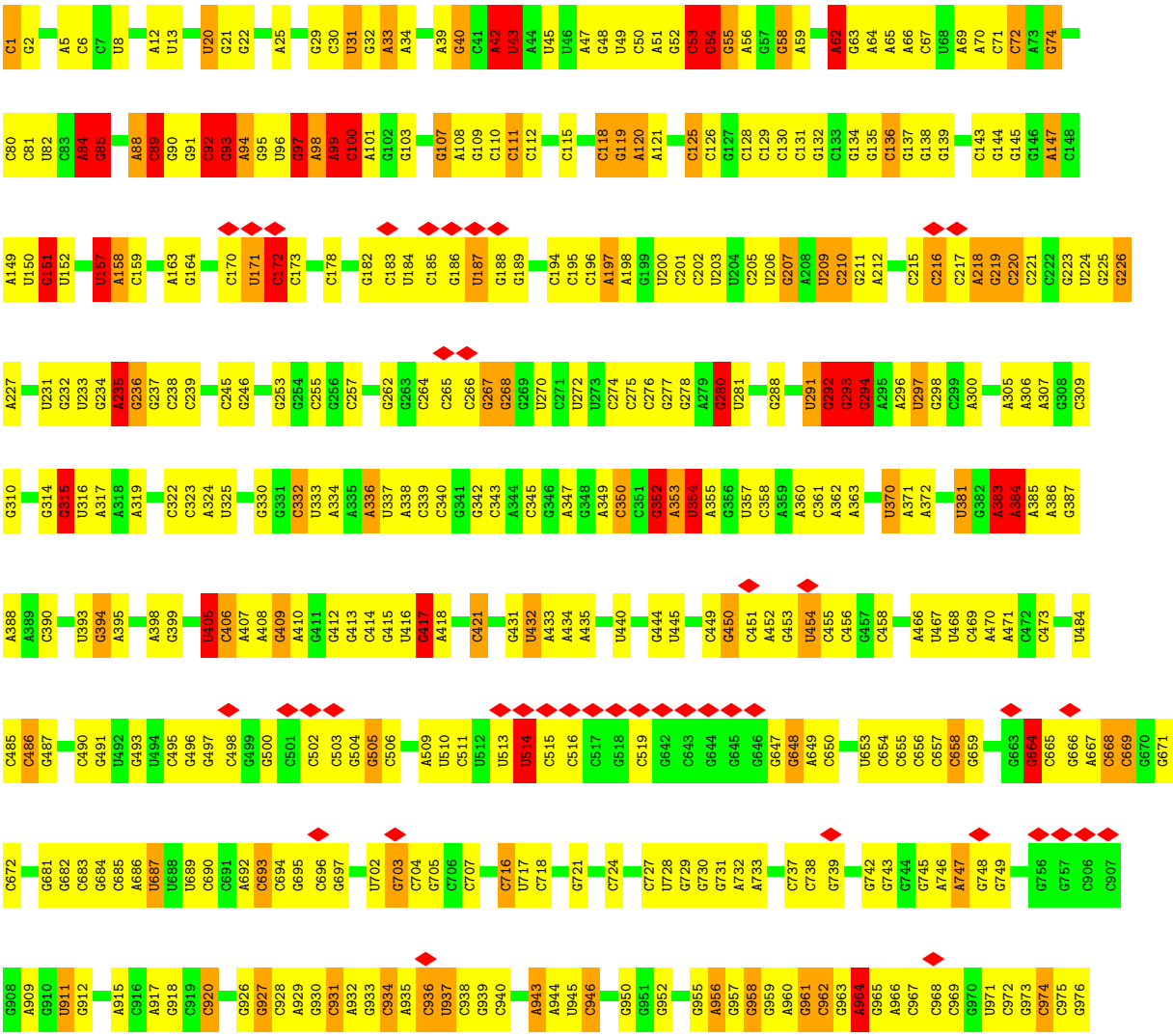
Mol	Chain	Residues	Atoms		AltConf
50	j	1	Total 1	Zn 1	0
50	m	1	Total 1	Zn 1	0
50	o	1	Total 1	Zn 1	0

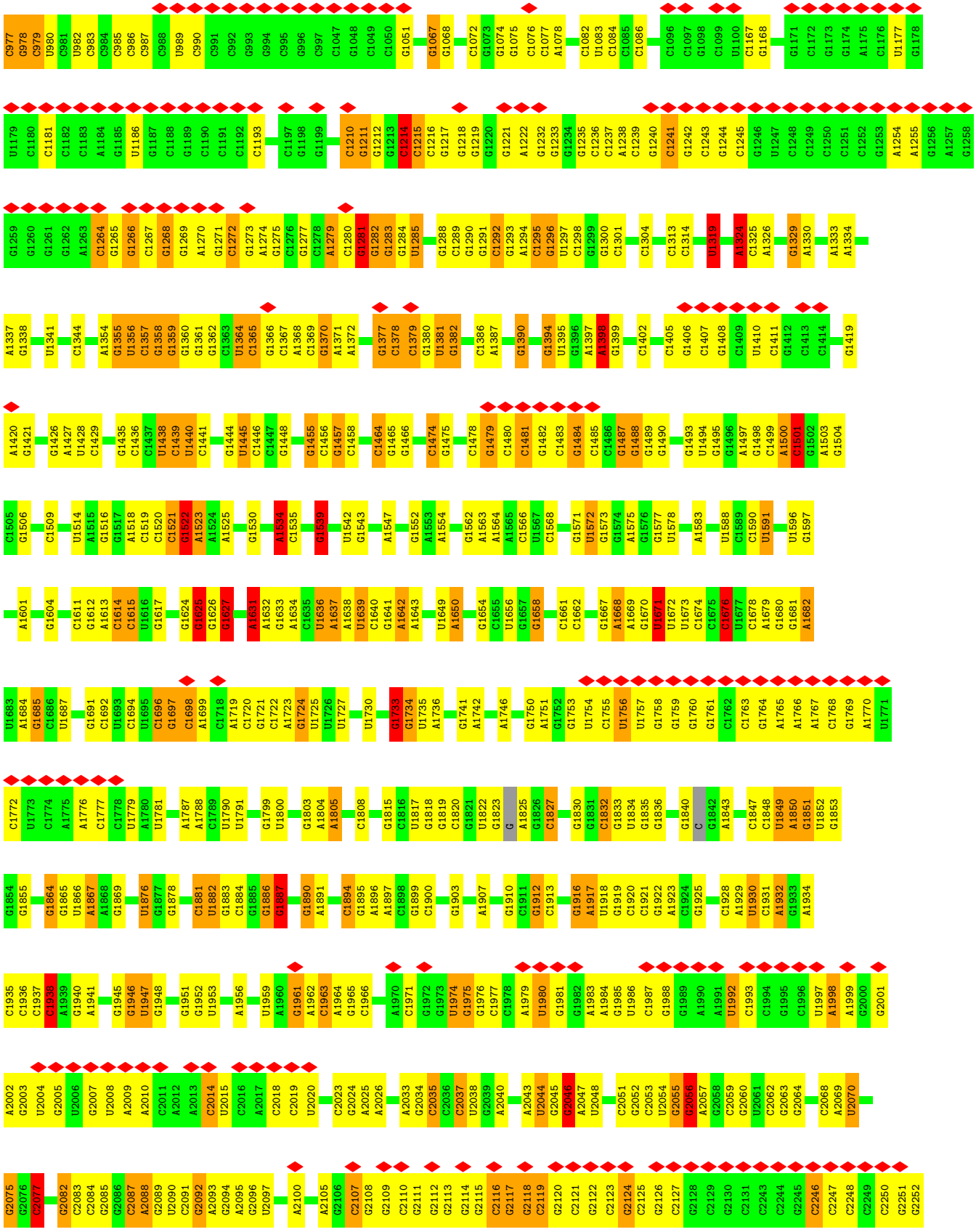
3 Residue-property plots (i)

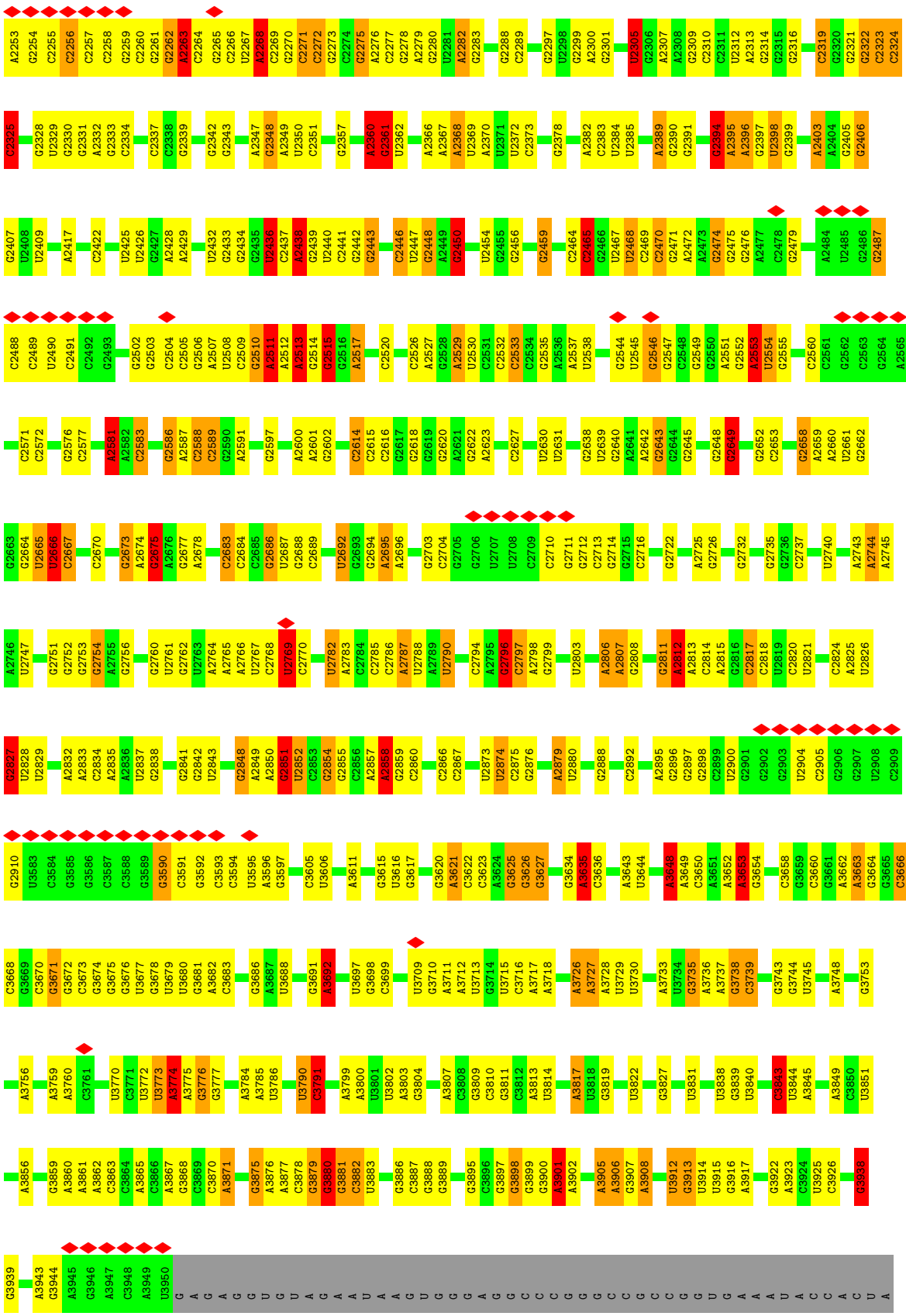
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

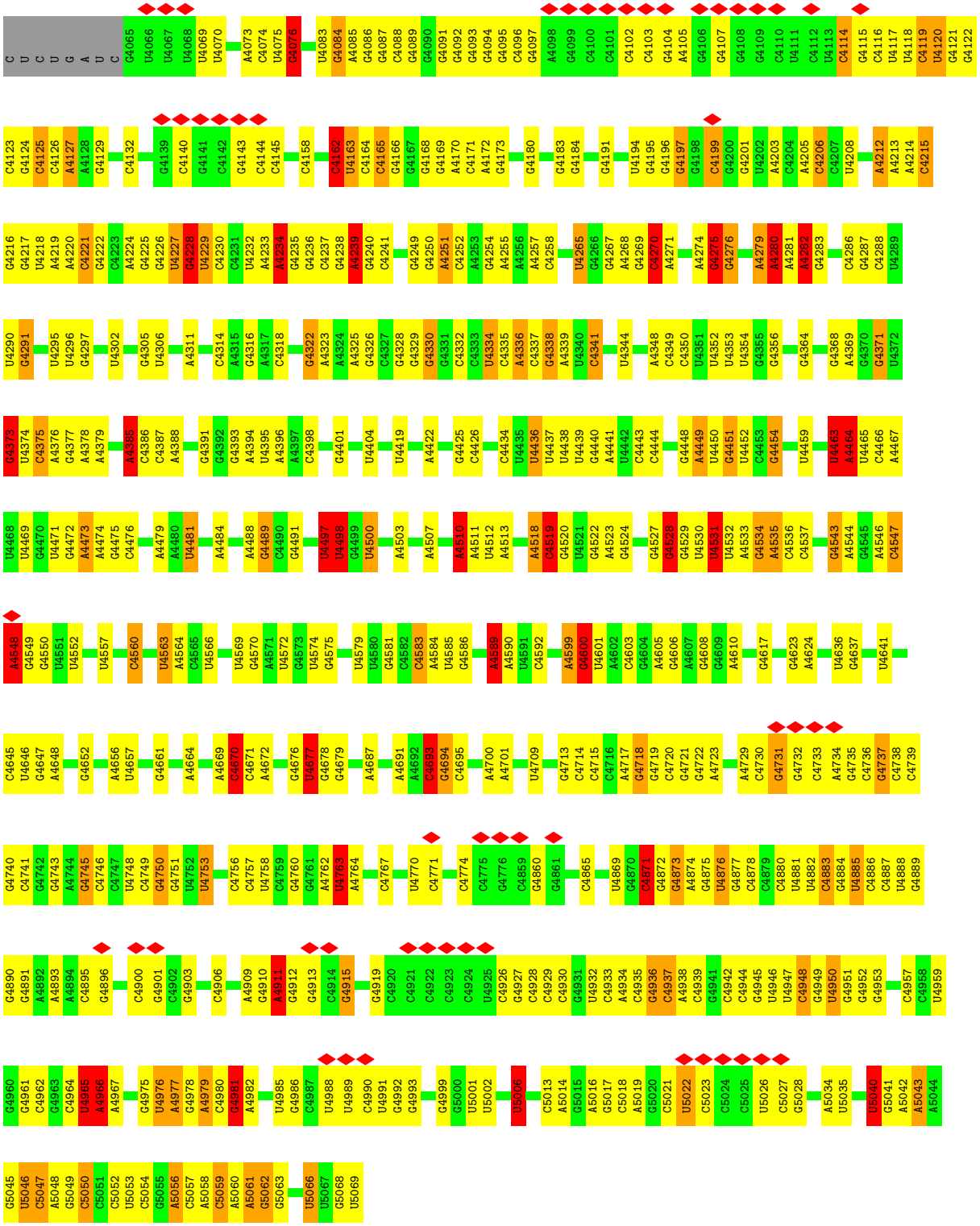
- Molecule 1: 28S ribosomal RNA

Chain 5:



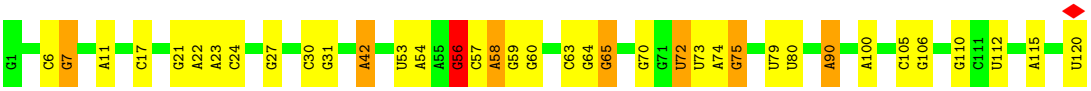






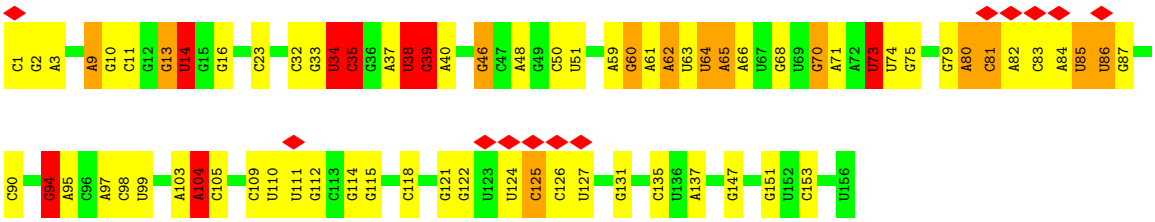
• Molecule 2: 5S ribosomal RNA

Chain 7:



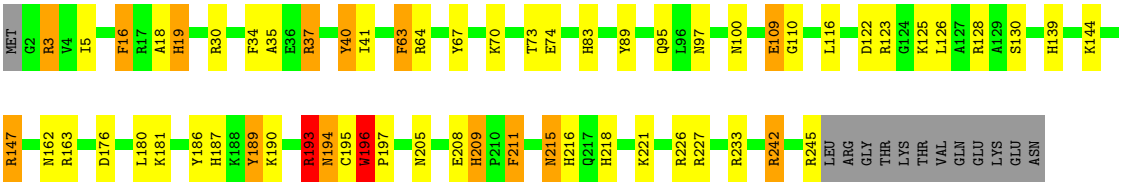
• Molecule 3: 5.8S ribosomal RNA

Chain 8:



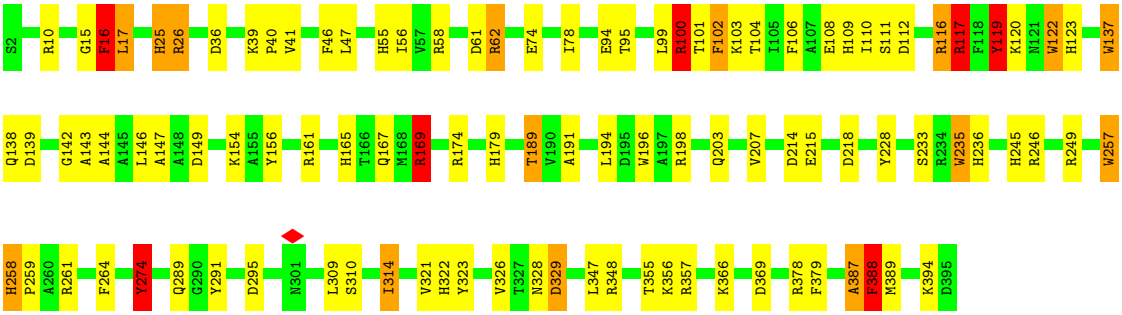
• Molecule 4: Ribosomal protein uL2

Chain A:



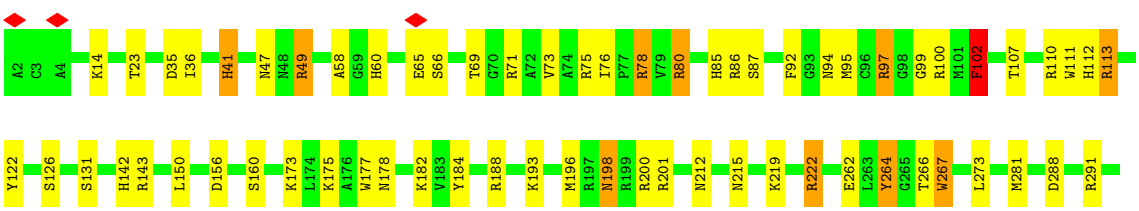
• Molecule 5: Ribosomal protein uL3

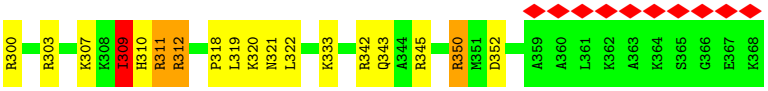
Chain B:



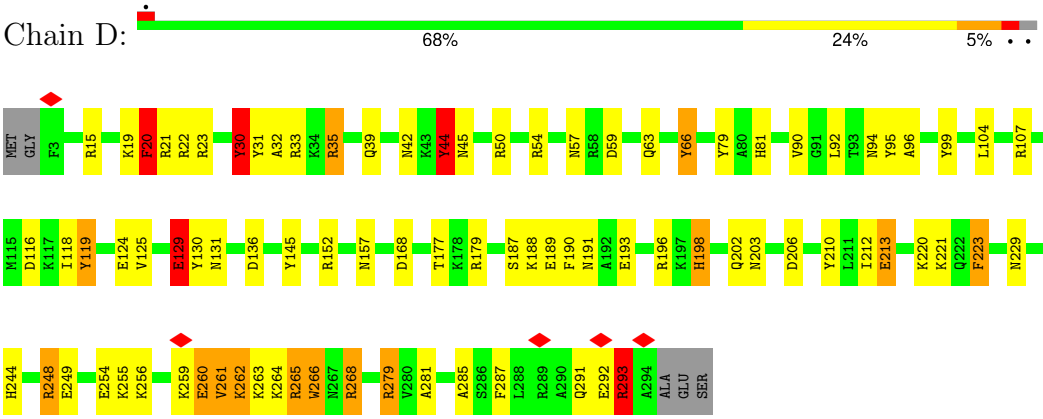
• Molecule 6: Ribosomal protein uL4

Chain C:

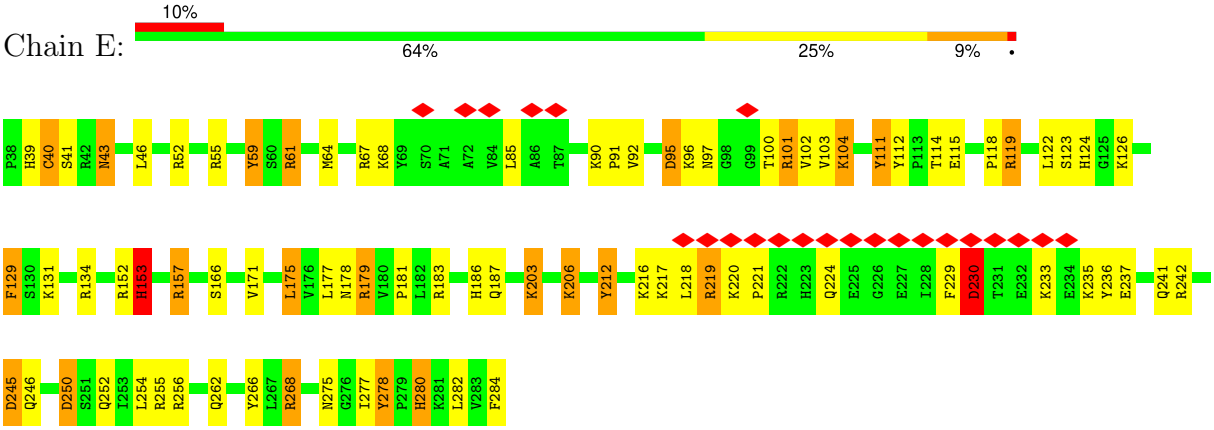




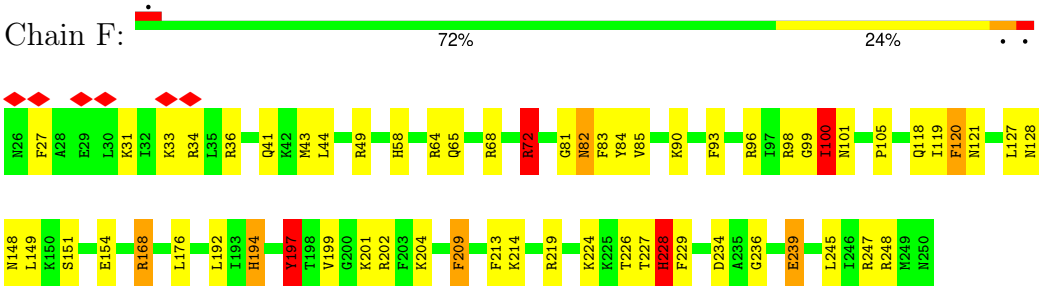
• Molecule 7: Ribosomal protein uL18



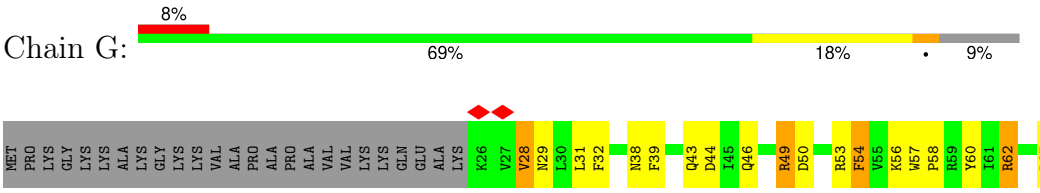
• Molecule 8: Ribosomal protein eL6

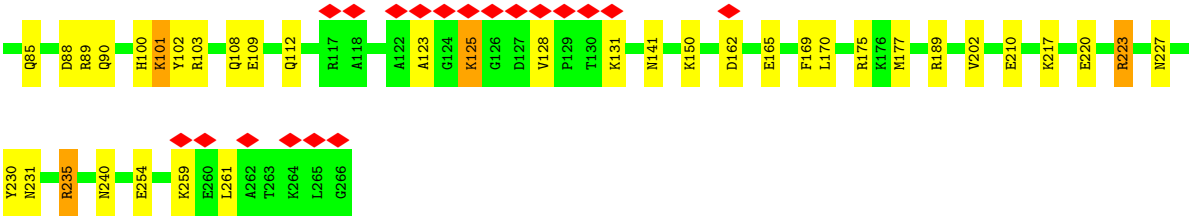


• Molecule 9: Ribosomal protein uL30



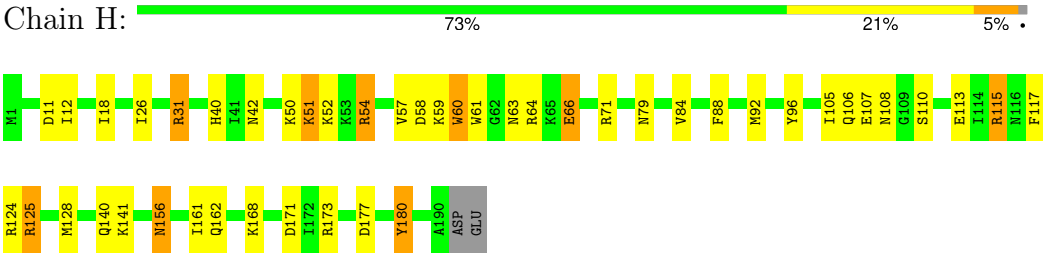
• Molecule 10: Ribosomal protein eL8





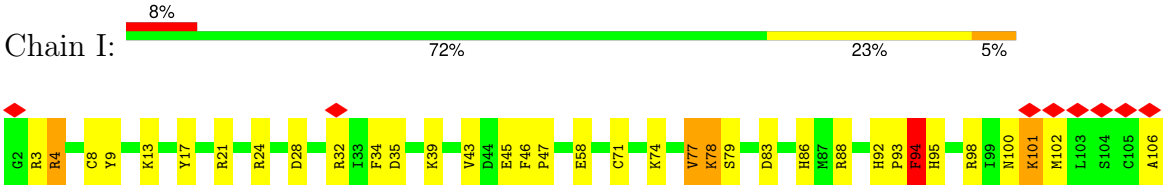
• Molecule 11: Ribosomal protein uL6

Chain H:



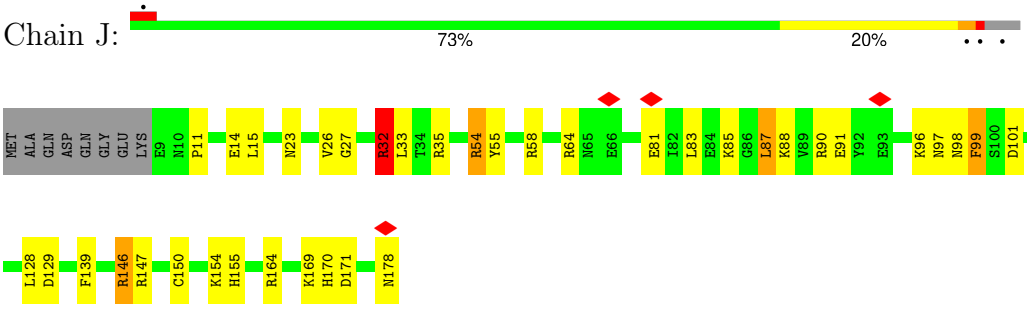
• Molecule 12: Ribosomal protein uL16

Chain I:



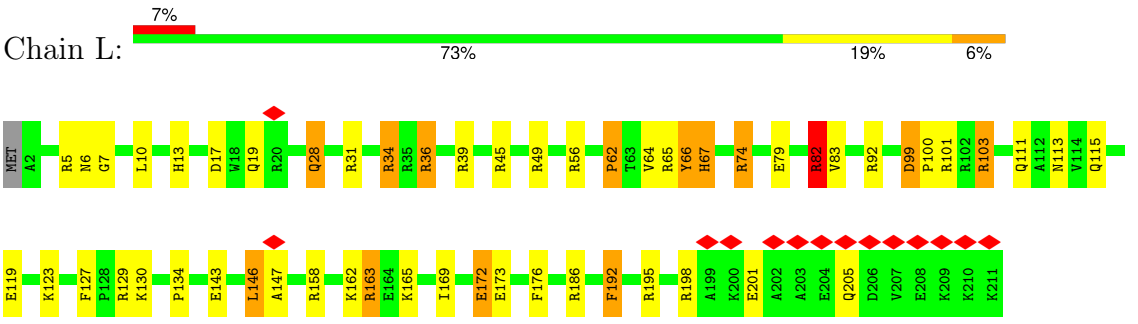
• Molecule 13: Ribosomal protein uL5

Chain J:



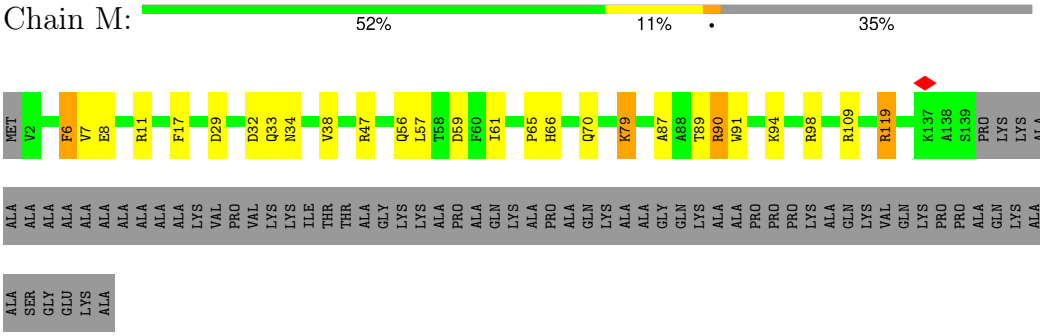
• Molecule 14: Ribosomal protein eL13

Chain L:



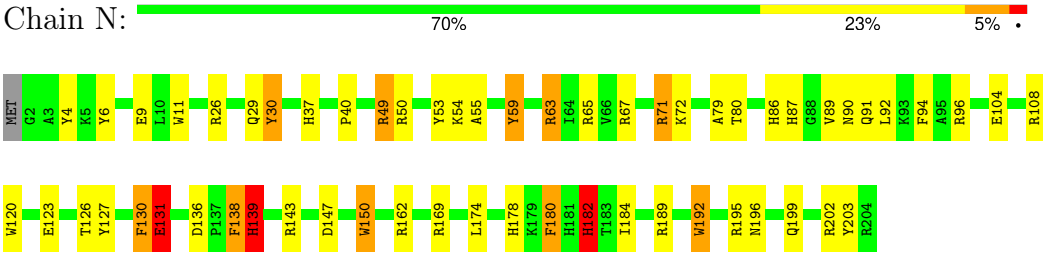
• Molecule 15: Ribosomal protein eL14

Chain M:



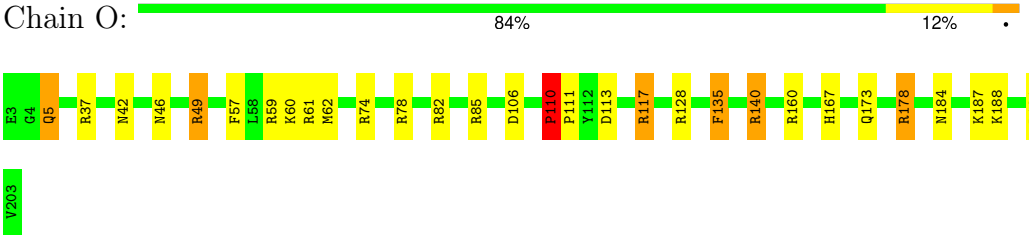
• Molecule 16: Ribosomal protein eL15

Chain N:



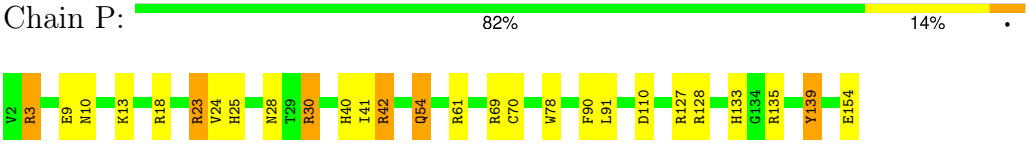
• Molecule 17: Ribosomal protein uL13

Chain O:



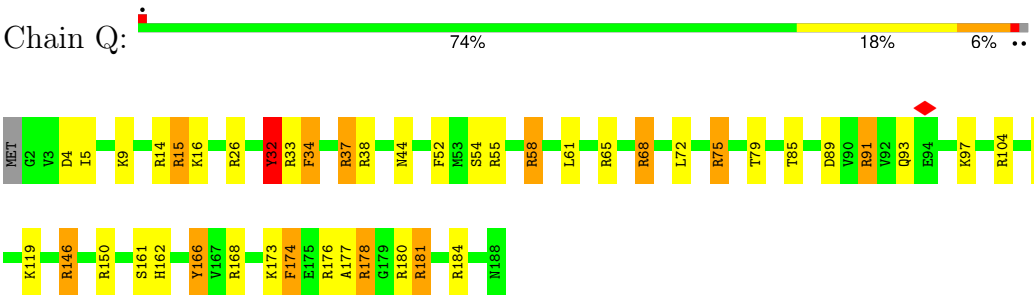
• Molecule 18: Ribosomal protein uL22

Chain P:



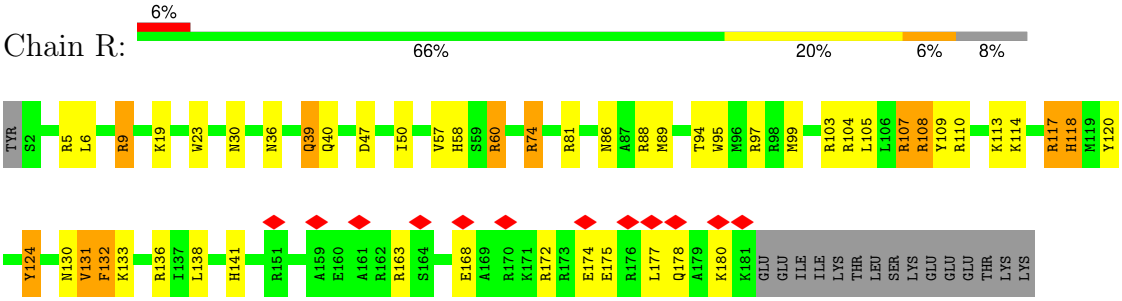
• Molecule 19: Ribosomal protein eL18

Chain Q:



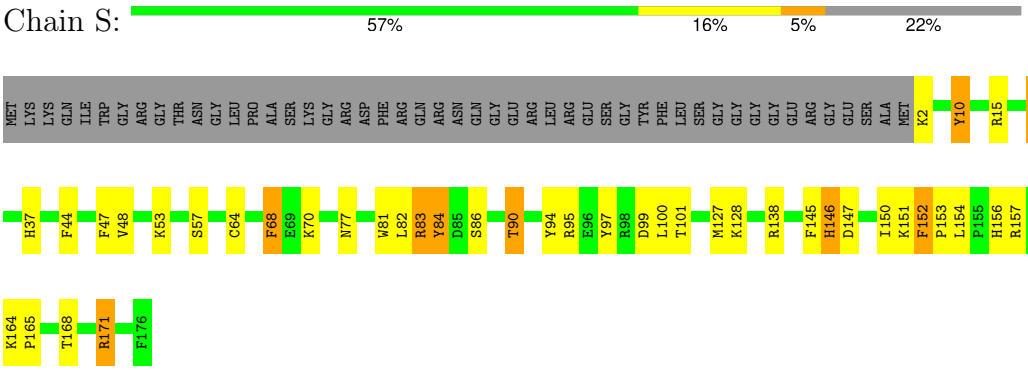
• Molecule 20: Ribosomal protein eL19

Chain R:



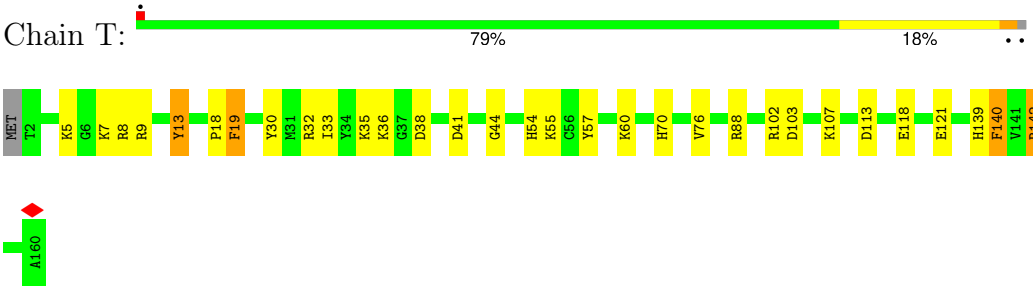
• Molecule 21: Ribosomal protein eL20

Chain S:



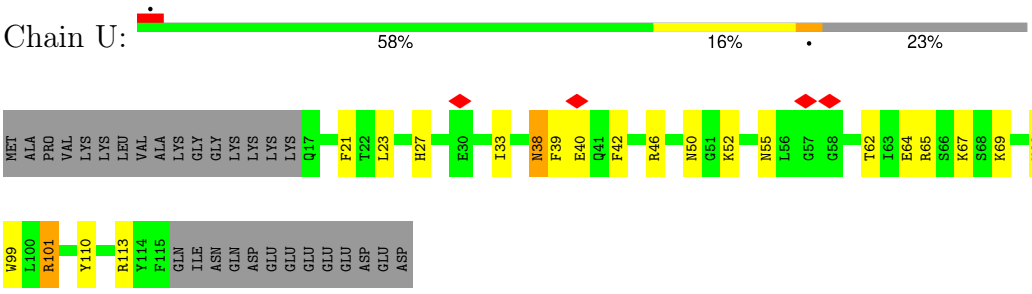
• Molecule 22: Ribosomal protein eL21

Chain T:



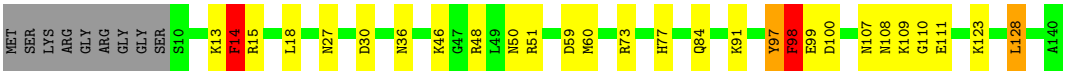
• Molecule 23: Ribosomal protein eL22

Chain U:



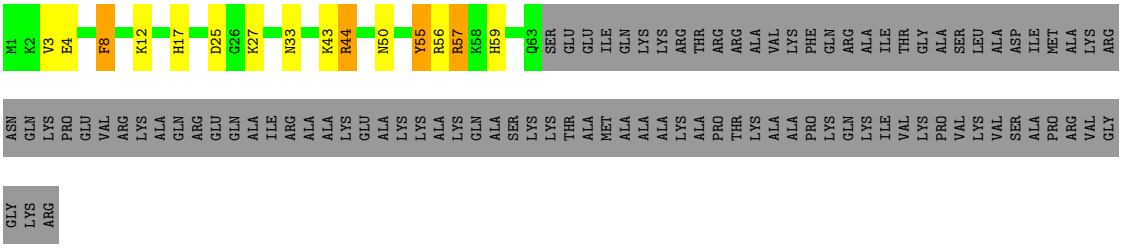
• Molecule 24: Ribosomal protein uL14

Chain V:



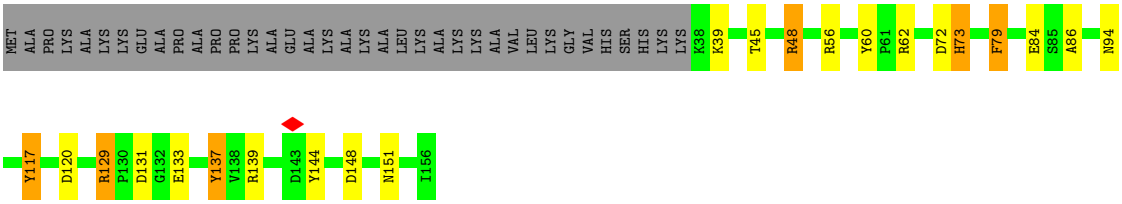
• Molecule 25: Ribosomal protein eL24

Chain W:



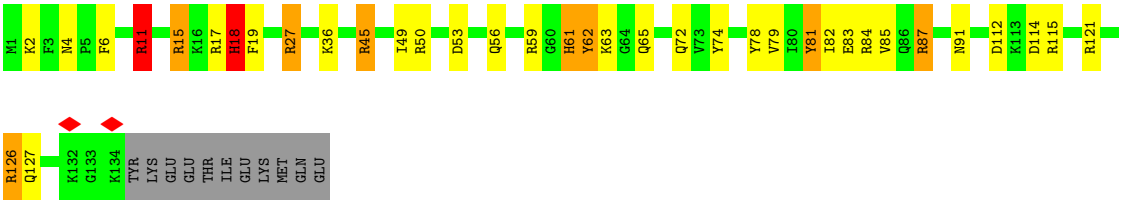
• Molecule 26: Ribosomal protein uL23

Chain X:



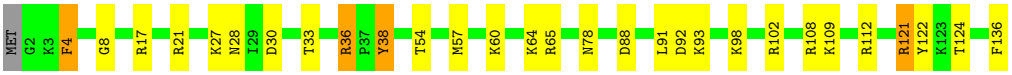
• Molecule 27: Ribosomal protein uL24

Chain Y:



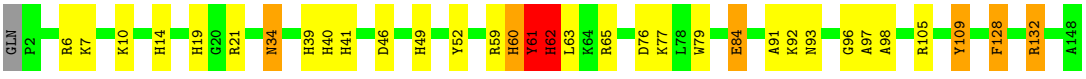
• Molecule 28: Ribosomal protein eL27

Chain Z:



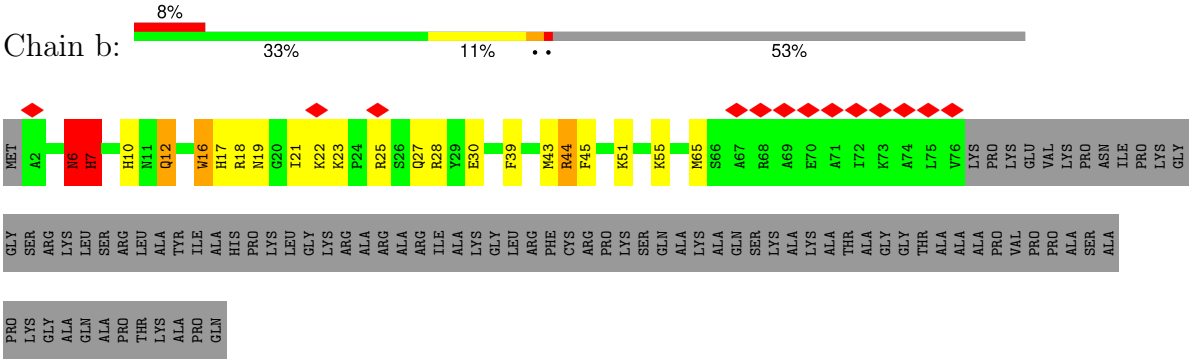
• Molecule 29: Ribosomal protein uL15

Chain a:



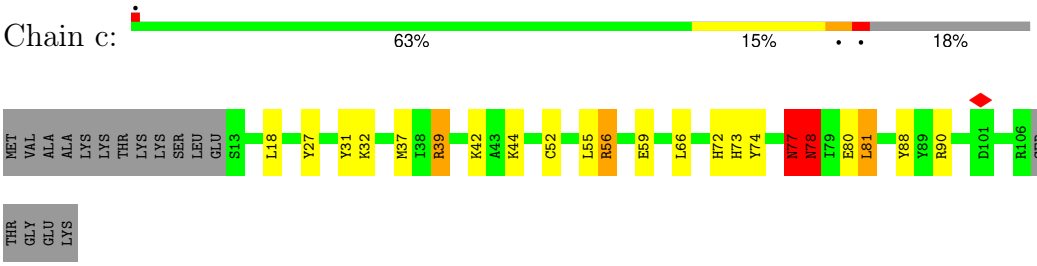
• Molecule 30: Ribosomal protein eL29

Chain b:



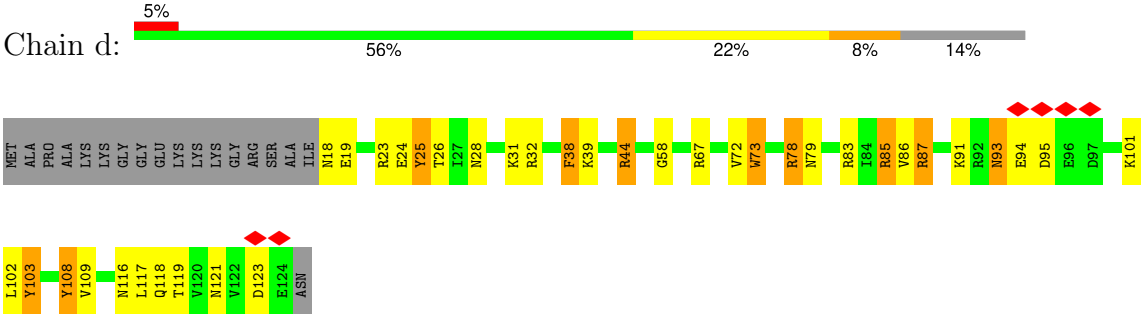
• Molecule 31: Ribosomal protein eL30

Chain c:



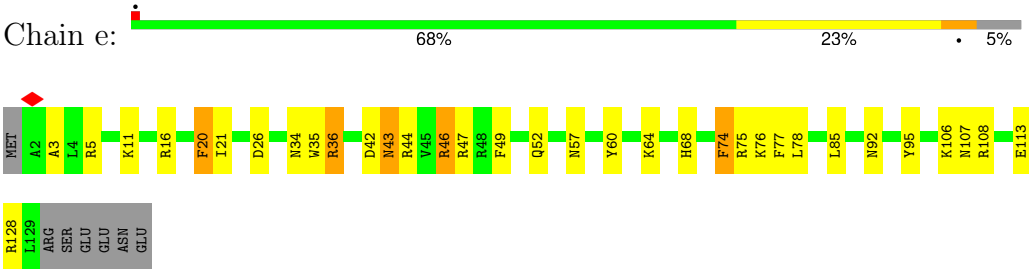
• Molecule 32: Ribosomal protein eL31

Chain d:



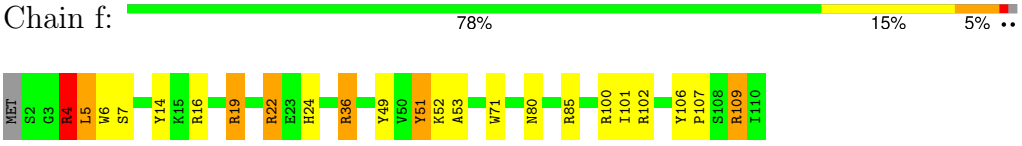
• Molecule 33: Ribosomal protein eL32

Chain e:



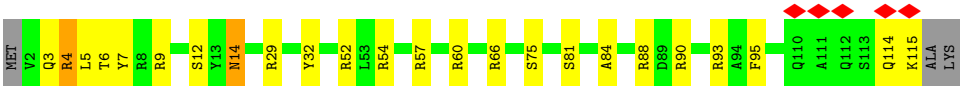
• Molecule 34: Ribosomal protein eL33

Chain f:



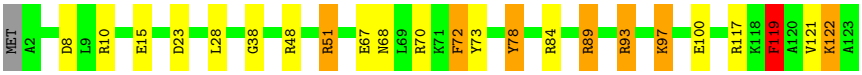
• Molecule 35: Ribosomal protein eL34

Chain g:



• Molecule 36: Ribosomal protein uL29

Chain h:



• Molecule 37: Ribosomal protein eL36

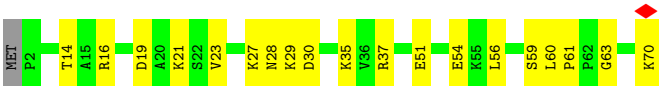
Chain i:

• Molecule 38: Ribosomal protein eL37

Chain j:

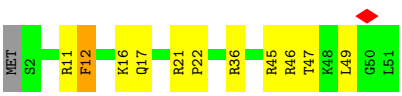
• Molecule 39: Ribosomal protein eL38

Chain k:



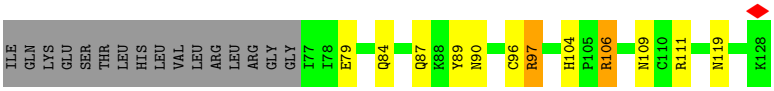
• Molecule 40: Ribosomal protein eL39

Chain l:



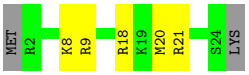
• Molecule 41: Ribosomal protein eL40

Chain m:



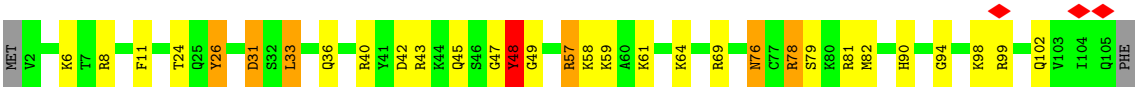
• Molecule 42: Ribosomal protein eL41

Chain n:



• Molecule 43: Ribosomal protein eL42

Chain o:

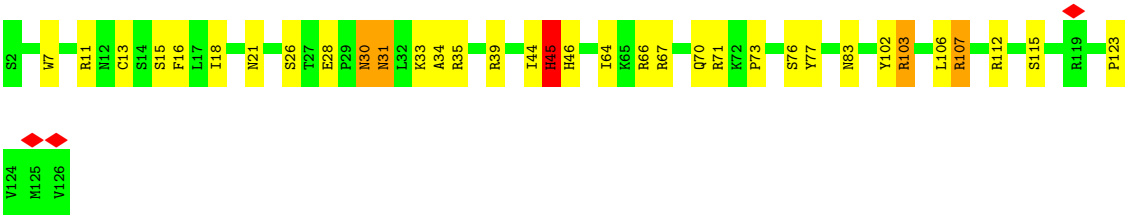


• Molecule 44: Ribosomal protein eL43

Chain p:

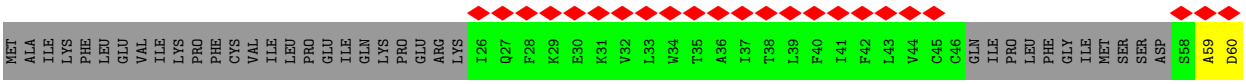
• Molecule 45: Ribosomal protein eL28

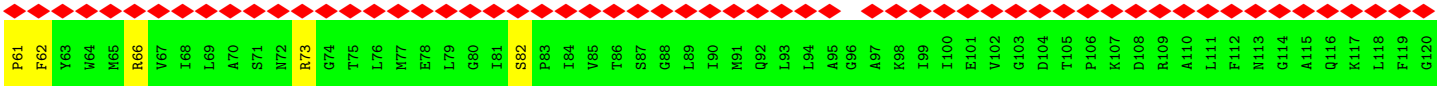
Chain r:

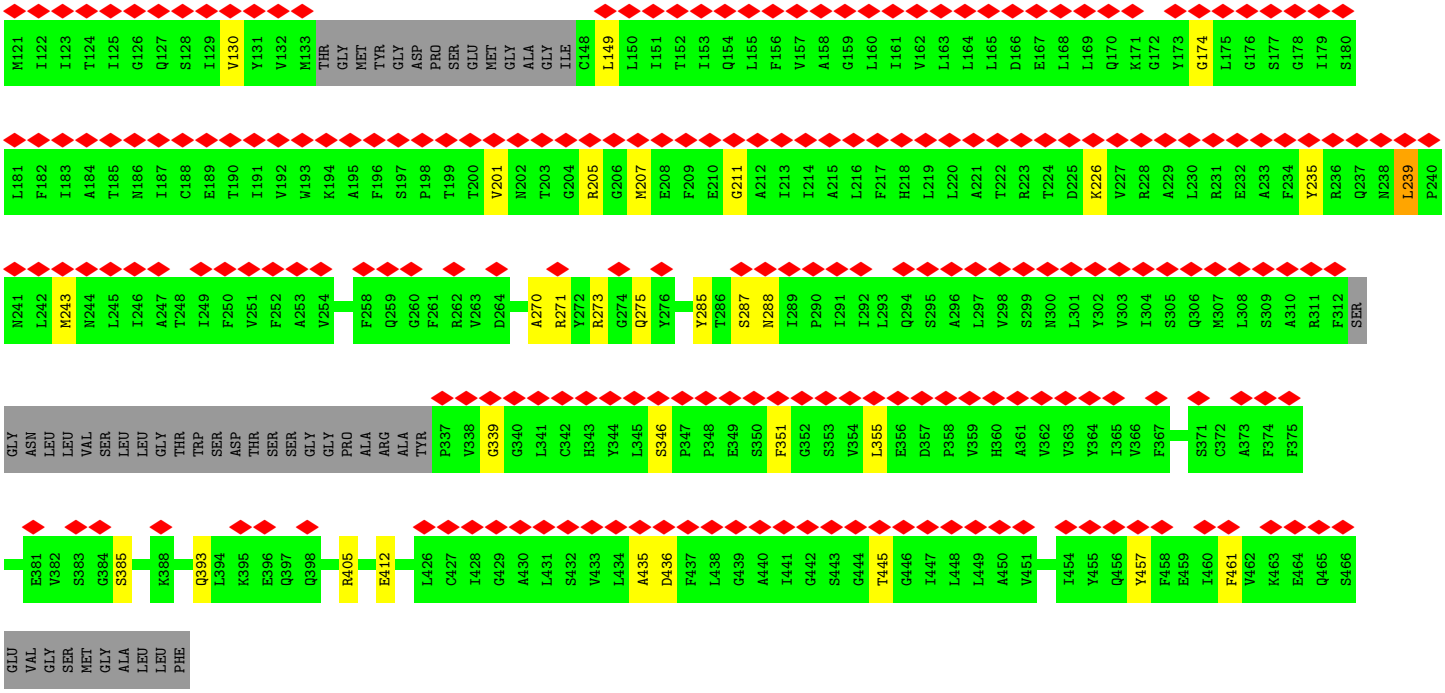


• Molecule 46: Sec61 alpha subunit

Chain 1:

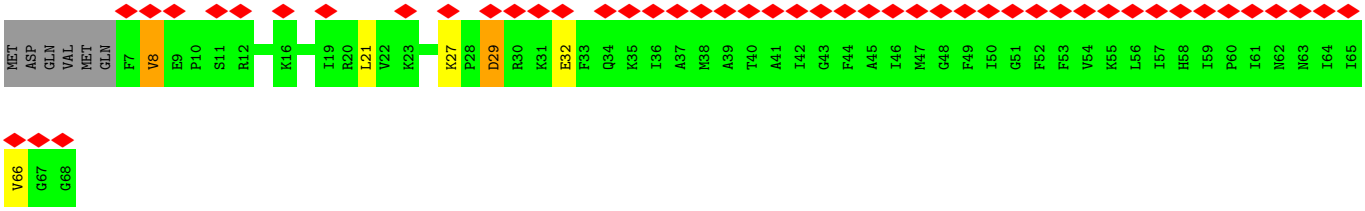






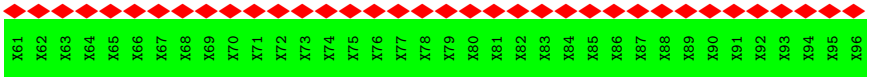
- Molecule 47: Sec61 gamma subunit

Chain 2:



- Molecule 48: Sec61 beta subunit

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80019	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.043	Depositor
Minimum map value	-0.599	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3399999, 1.3399999, 1.3399999	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	5	0.64	80/87792 (0.1%)	1.13	742/136945 (0.5%)
2	7	0.54	1/2858 (0.0%)	0.96	9/4455 (0.2%)
3	8	0.68	3/3701 (0.1%)	1.20	42/5766 (0.7%)
4	A	0.80	3/1906 (0.2%)	1.26	21/2556 (0.8%)
5	B	0.81	8/3214 (0.2%)	1.16	26/4308 (0.6%)
6	C	0.73	4/2973 (0.1%)	1.12	18/3990 (0.5%)
7	D	0.73	2/2426 (0.1%)	1.23	27/3252 (0.8%)
8	E	0.73	5/1941 (0.3%)	1.21	20/2601 (0.8%)
9	F	0.80	2/1905 (0.1%)	1.27	26/2539 (1.0%)
10	G	0.76	4/1966 (0.2%)	1.09	14/2645 (0.5%)
11	H	0.77	3/1537 (0.2%)	1.17	10/2066 (0.5%)
12	I	0.66	1/1753 (0.1%)	1.11	12/2343 (0.5%)
13	J	0.63	1/1382 (0.1%)	1.04	11/1849 (0.6%)
14	L	0.71	2/1734 (0.1%)	1.12	15/2318 (0.6%)
15	M	0.76	2/1152 (0.2%)	1.11	5/1539 (0.3%)
16	N	0.84	4/1746 (0.2%)	1.33	23/2338 (1.0%)
17	O	0.72	3/1684 (0.2%)	1.11	12/2251 (0.5%)
18	P	0.74	2/1268 (0.2%)	1.10	9/1701 (0.5%)
19	Q	0.69	0/1530	1.35	31/2041 (1.5%)
20	R	0.79	3/1524 (0.2%)	1.27	21/2013 (1.0%)
21	S	0.95	8/1493 (0.5%)	1.30	19/2002 (0.9%)
22	T	0.67	1/1326 (0.1%)	1.04	7/1770 (0.4%)
23	U	0.63	1/822 (0.1%)	1.03	2/1103 (0.2%)
24	V	0.89	4/993 (0.4%)	1.11	7/1332 (0.5%)
25	W	0.71	0/541	1.23	5/720 (0.7%)
26	X	0.64	0/993	1.09	10/1334 (0.7%)
27	Y	0.72	0/1132	1.24	19/1504 (1.3%)
28	Z	0.63	0/1130	1.11	8/1507 (0.5%)
29	a	0.93	6/1192 (0.5%)	1.37	17/1591 (1.1%)
30	b	0.88	2/620 (0.3%)	1.17	5/819 (0.6%)
31	c	0.70	0/742	1.14	5/996 (0.5%)
32	d	0.84	3/903 (0.3%)	1.37	16/1216 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.90	3/1071 (0.3%)	1.23	15/1429 (1.0%)
34	f	1.02	2/895 (0.2%)	1.34	17/1198 (1.4%)
35	g	0.65	0/916	1.08	5/1220 (0.4%)
36	h	0.63	0/1023	1.21	13/1350 (1.0%)
37	i	0.63	0/843	1.19	8/1115 (0.7%)
38	j	0.97	1/721 (0.1%)	1.43	11/953 (1.2%)
39	k	0.59	0/575	0.97	1/761 (0.1%)
40	l	0.68	0/454	1.07	3/599 (0.5%)
41	m	0.57	0/435	1.02	3/575 (0.5%)
42	n	0.48	0/223	1.02	0/284
43	o	0.64	0/864	1.27	9/1140 (0.8%)
44	p	0.64	1/718 (0.1%)	1.00	3/953 (0.3%)
45	r	0.68	0/1017	1.12	8/1365 (0.6%)
46	1	0.45	0/3114	0.63	0/4218
47	2	0.47	0/504	0.71	1/673 (0.1%)
All	All	0.68	165/151252 (0.1%)	1.14	1311/223243 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5	1	158
2	7	0	2
3	8	0	11
4	A	0	6
5	B	0	13
6	C	0	5
7	D	0	8
8	E	0	12
9	F	0	5
10	G	0	3
11	H	0	3
12	I	0	5
13	J	0	2
14	L	0	5
15	M	0	4
16	N	0	11
17	O	0	3
18	P	0	1
19	Q	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
20	R	0	6
21	S	0	11
22	T	0	2
23	U	0	2
24	V	0	3
25	W	0	1
26	X	0	1
27	Y	0	4
29	a	0	9
30	b	0	1
31	c	0	2
32	d	0	4
33	e	0	4
34	f	0	2
35	g	0	1
36	h	0	3
37	i	0	3
38	j	0	4
39	k	0	1
43	o	0	6
44	p	0	1
45	r	0	5
46	1	0	1
47	2	0	1
All	All	1	340

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1823	G	O3'-P	41.48	2.10	1.61
10	G	109	GLU	CD-OE2	16.17	1.43	1.25
11	H	66	GLU	CD-OE1	15.86	1.43	1.25
34	f	6	TRP	CB-CG	-15.77	1.21	1.50
30	b	16	TRP	CB-CG	-13.52	1.25	1.50
20	R	95	TRP	CB-CG	-12.10	1.28	1.50
24	V	97	TYR	CB-CG	-11.82	1.33	1.51
33	e	35	TRP	CB-CG	-10.24	1.31	1.50
10	G	54	PHE	CB-CG	-9.84	1.34	1.51
16	N	192	TRP	CB-CG	-9.32	1.33	1.50
15	M	6	PHE	CB-CG	-8.96	1.36	1.51
5	B	215	GLU	CD-OE1	8.87	1.35	1.25
24	V	97	TYR	CA-CB	8.62	1.73	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	278	TYR	CA-CB	8.50	1.72	1.53
29	a	109	TYR	CA-CB	8.37	1.72	1.53
1	5	4547	C	O3'-P	8.29	1.71	1.61
21	S	81	TRP	CA-CB	8.09	1.71	1.53
21	S	10	TYR	CB-CG	-8.09	1.39	1.51
1	5	45	U	O3'-P	-8.00	1.51	1.61
1	5	3652	A	O3'-P	7.96	1.70	1.61
8	E	278	TYR	CB-CG	-7.90	1.39	1.51
20	R	132	PHE	CB-CG	-7.86	1.38	1.51
29	a	84	GLU	CD-OE1	7.81	1.34	1.25
29	a	109	TYR	CB-CG	-7.64	1.40	1.51
34	f	6	TRP	CA-CB	7.36	1.70	1.53
1	5	4566	U	O3'-P	-7.28	1.52	1.61
1	5	2510	G	O3'-P	-7.20	1.52	1.61
1	5	2361	G	O3'-P	7.11	1.69	1.61
1	5	1851	G	O3'-P	-7.02	1.52	1.61
6	C	267	TRP	CB-CG	-6.99	1.37	1.50
21	S	81	TRP	CB-CG	-6.95	1.37	1.50
5	B	119	TYR	CB-CG	-6.94	1.41	1.51
1	5	1849	U	O3'-P	-6.90	1.52	1.61
1	5	1364	U	O3'-P	6.86	1.69	1.61
13	J	14	GLU	CD-OE1	6.85	1.33	1.25
38	j	49	TRP	CB-CG	-6.79	1.38	1.50
29	a	128	PHE	CB-CG	-6.79	1.39	1.51
1	5	4693	C	O3'-P	6.78	1.69	1.61
22	T	13	TYR	CB-CG	-6.77	1.41	1.51
1	5	2692	U	O3'-P	-6.71	1.53	1.61
1	5	514	U	O3'-P	6.70	1.69	1.61
32	d	25	TYR	CB-CG	-6.67	1.41	1.51
5	B	274	TYR	CA-CB	6.67	1.68	1.53
1	5	3692	A	O3'-P	6.66	1.69	1.61
1	5	964	A	O3'-P	6.64	1.69	1.61
1	5	2053	C	O3'-P	-6.63	1.53	1.61
1	5	1522	G	O3'-P	6.54	1.69	1.61
12	I	171	TRP	CB-CG	-6.54	1.38	1.50
21	S	33	PHE	CB-CG	-6.51	1.40	1.51
1	5	1912	G	O3'-P	-6.50	1.53	1.61
1	5	4375	C	O3'-P	-6.50	1.53	1.61
2	7	90	A	O3'-P	-6.47	1.53	1.61
1	5	2442	G	O3'-P	-6.42	1.53	1.61
6	C	111	TRP	CB-CG	-6.42	1.38	1.50
10	G	54	PHE	CA-CB	6.39	1.68	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	17	ASP	CG-OD2	6.37	1.40	1.25
17	O	194	GLU	CD-OE1	6.33	1.32	1.25
1	5	1669	A	O3'-P	-6.29	1.53	1.61
7	D	213	GLU	CG-CD	6.27	1.61	1.51
1	5	207	G	O3'-P	-6.26	1.53	1.61
8	E	101	ARG	CZ-NH2	6.26	1.41	1.33
21	S	10	TYR	CA-CB	6.24	1.67	1.53
17	O	106	ASP	CG-OD2	6.20	1.39	1.25
1	5	171	U	O3'-P	-6.19	1.53	1.61
11	H	61	TRP	CB-CG	-6.15	1.39	1.50
1	5	1756	U	C4-O4	-6.14	1.18	1.23
9	F	120	PHE	CB-CG	-6.09	1.41	1.51
1	5	1591	U	O3'-P	-6.09	1.53	1.61
1	5	2589	C	O3'-P	6.09	1.68	1.61
1	5	3901	A	O3'-P	-6.07	1.53	1.61
7	D	44	TYR	CA-CB	6.06	1.67	1.53
1	5	1636	U	O3'-P	-5.97	1.53	1.61
1	5	4464	A	O3'-P	5.97	1.68	1.61
23	U	99	TRP	CB-CG	-5.93	1.39	1.50
32	d	73	TRP	CB-CG	-5.93	1.39	1.50
1	5	2520	C	O3'-P	-5.90	1.54	1.61
1	5	1395	U	O3'-P	-5.90	1.54	1.61
21	S	152	PHE	CB-CG	-5.89	1.41	1.51
1	5	2811	G	O3'-P	5.88	1.68	1.61
18	P	139	TYR	CB-CG	-5.88	1.42	1.51
30	b	16	TRP	CA-CB	5.87	1.66	1.53
5	B	119	TYR	CA-CB	5.86	1.66	1.53
1	5	1357	C	O3'-P	5.80	1.68	1.61
5	B	274	TYR	CB-CG	-5.79	1.43	1.51
1	5	3635	A	O3'-P	5.78	1.68	1.61
18	P	139	TYR	CA-CB	5.76	1.66	1.53
44	p	18	TYR	CB-CG	-5.72	1.43	1.51
24	V	97	TYR	CD2-CE2	-5.71	1.30	1.39
1	5	147	A	O3'-P	-5.70	1.54	1.61
1	5	90	G	O3'-P	-5.70	1.54	1.61
14	L	173	GLU	CD-OE2	5.70	1.31	1.25
1	5	2394	G	O3'-P	-5.69	1.54	1.61
1	5	32	G	O3'-P	-5.68	1.54	1.61
5	B	235	TRP	CG-CD1	-5.68	1.28	1.36
1	5	2055	G	O3'-P	5.68	1.68	1.61
1	5	2325	C	O3'-P	5.67	1.68	1.61
1	5	2649	G	O3'-P	-5.65	1.54	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4239	A	O3'-P	5.65	1.68	1.61
32	d	25	TYR	CA-CB	5.65	1.66	1.53
1	5	2051	C	O3'-P	5.61	1.67	1.61
1	5	1627	G	O3'-P	5.60	1.67	1.61
1	5	53	C	O3'-P	5.60	1.67	1.61
1	5	2535	G	O3'-P	-5.58	1.54	1.61
16	N	119	TYR	CB-CG	-5.58	1.43	1.51
1	5	5001	U	O3'-P	-5.54	1.54	1.61
10	G	109	GLU	CG-CD	5.52	1.60	1.51
1	5	332	C	O3'-P	-5.50	1.54	1.61
1	5	4326	G	O3'-P	-5.47	1.54	1.61
29	a	79	TRP	CB-CG	-5.47	1.40	1.50
1	5	1282	G	O3'-P	-5.45	1.54	1.61
1	5	4276	G	O3'-P	5.45	1.67	1.61
1	5	3875	G	O3'-P	5.44	1.67	1.61
21	S	29	ARG	CG-CD	5.42	1.65	1.51
3	8	64	U	O3'-P	5.41	1.67	1.61
15	M	6	PHE	CA-CB	5.39	1.65	1.53
1	5	1381	U	O3'-P	-5.39	1.54	1.61
1	5	89	C	O3'-P	-5.38	1.54	1.61
17	O	106	ASP	CG-OD1	5.36	1.37	1.25
33	e	74	PHE	CB-CG	-5.35	1.42	1.51
1	5	372	A	O3'-P	-5.32	1.54	1.61
1	5	2043	A	O3'-P	-5.31	1.54	1.61
1	5	4977	A	O3'-P	-5.29	1.54	1.61
1	5	4548	A	O5'-C5'	5.27	1.52	1.44
24	V	98	PHE	CB-CG	-5.25	1.42	1.51
4	A	40	TYR	CA-CB	5.25	1.65	1.53
8	E	250	ASP	CG-OD2	5.25	1.37	1.25
4	A	211	PHE	CA-CB	5.24	1.65	1.53
1	5	2297	G	O3'-P	-5.23	1.54	1.61
1	5	2368	A	O3'-P	-5.23	1.54	1.61
11	H	66	GLU	CD-OE2	5.23	1.31	1.25
1	5	937	U	O3'-P	-5.22	1.54	1.61
20	R	132	PHE	CA-CB	5.22	1.65	1.53
1	5	943	A	O3'-P	-5.22	1.54	1.61
1	5	4237	C	O3'-P	-5.21	1.54	1.61
5	B	137	TRP	CB-CG	-5.20	1.40	1.50
1	5	1917	A	O3'-P	-5.20	1.54	1.61
8	E	97	ASN	CG-ND2	5.19	1.45	1.32
1	5	1457	G	O3'-P	-5.18	1.54	1.61
3	8	80	A	O3'-P	5.17	1.67	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2037	C	C2-O2	-5.16	1.19	1.24
16	N	130	PHE	CB-CG	-5.16	1.42	1.51
5	B	257	TRP	CE3-CZ3	-5.15	1.29	1.38
4	A	209	HIS	CA-CB	5.15	1.65	1.53
1	5	4275	G	O3'-P	5.14	1.67	1.61
1	5	381	U	O3'-P	-5.12	1.55	1.61
16	N	120	TRP	CE3-CZ3	-5.12	1.29	1.38
9	F	228	HIS	CA-CB	5.11	1.65	1.53
1	5	2406	G	O3'-P	5.10	1.67	1.61
1	5	1682	A	C6-N6	-5.10	1.29	1.33
1	5	2054	U	O3'-P	-5.08	1.55	1.61
1	5	1283	G	O3'-P	-5.08	1.55	1.61
21	S	152	PHE	CG-CD2	-5.07	1.31	1.38
1	5	97	G	O3'-P	5.07	1.67	1.61
1	5	4206	C	O3'-P	-5.07	1.55	1.61
3	8	73	U	O3'-P	5.07	1.67	1.61
1	5	1883	G	O3'-P	-5.06	1.55	1.61
1	5	2324	C	O3'-P	5.06	1.67	1.61
33	e	35	TRP	CG-CD1	-5.05	1.29	1.36
29	a	79	TRP	CA-CB	5.04	1.65	1.53
6	C	102	PHE	CG-CD2	-5.04	1.31	1.38
1	5	2667	C	O3'-P	-5.04	1.55	1.61
1	5	4489	G	O3'-P	5.03	1.67	1.61
6	C	35	ASP	CG-OD1	5.02	1.36	1.25
1	5	4334	U	O3'-P	-5.01	1.55	1.61
1	5	4497	U	O3'-P	5.01	1.67	1.61

All (1311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	8	60	G	N9-C1'-C2'	16.16	135.01	114.00
38	j	11	ARG	NE-CZ-NH2	-13.83	113.38	120.30
19	Q	37	ARG	NE-CZ-NH2	12.90	126.75	120.30
1	5	92	C	N1-C1'-C2'	-12.62	97.59	114.00
12	I	139	ARG	CG-CD-NE	12.29	137.61	111.80
1	5	1214	C	N1-C1'-C2'	11.93	129.51	114.00
1	5	1	C	N1-C1'-C2'	11.85	129.41	114.00
4	A	3	ARG	NE-CZ-NH1	11.74	126.17	120.30
32	d	44	ARG	NE-CZ-NH1	11.27	125.94	120.30
7	D	265	ARG	NE-CZ-NH1	11.20	125.90	120.30
36	h	93	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	5	4693	C	O4'-C1'-N1	-11.14	99.29	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	R	132	PHE	CB-CA-C	11.11	132.63	110.40
1	5	4275	G	N9-C1'-C2'	-11.10	99.58	114.00
1	5	4373	G	N9-C1'-C2'	11.06	128.37	114.00
29	a	61	TYR	CA-CB-CG	10.98	134.27	113.40
1	5	2361	G	N9-C1'-C2'	-10.96	99.76	114.00
1	5	4871	C	N1-C1'-C2'	10.89	128.16	114.00
1	5	1938	C	N1-C1'-C2'	10.85	128.10	114.00
15	M	6	PHE	CB-CG-CD2	-10.80	113.24	120.80
20	R	108	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	5	151	G	N9-C1'-C2'	-10.78	99.99	114.00
29	a	132	ARG	NE-CZ-NH1	10.71	125.65	120.30
16	N	192	TRP	CA-CB-CG	10.62	133.89	113.70
16	N	131	GLU	CA-CB-CG	10.57	136.65	113.40
27	Y	87	ARG	NE-CZ-NH2	10.53	125.57	120.30
1	5	4528	G	C2'-C3'-O3'	10.50	132.60	109.50
37	i	85	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	5	2513	A	N9-C1'-C2'	10.49	127.63	114.00
1	5	4163	U	C4'-C3'-O3'	10.45	133.91	113.00
3	8	34	U	C4'-C3'-O3'	-10.35	87.67	109.40
1	5	1211	G	C2'-C3'-O3'	10.34	132.25	109.50
29	a	109	TYR	CA-CB-CG	-10.24	93.95	113.40
1	5	62	A	N9-C1'-C2'	10.22	127.28	114.00
1	5	1329	G	C2'-C3'-O3'	10.19	131.92	109.50
43	o	78	ARG	NE-CZ-NH2	10.13	125.36	120.30
1	5	2436	U	N1-C1'-C2'	10.10	127.13	114.00
1	5	2586	G	N9-C1'-C2'	10.09	127.11	114.00
1	5	664	G	O4'-C1'-N9	10.07	116.26	108.20
1	5	1890	G	N9-C1'-C2'	-10.07	100.91	114.00
1	5	4518	A	O5'-P-OP2	-10.03	96.67	105.70
1	5	1358	G	C4'-C3'-O3'	10.02	133.04	113.00
1	5	2389	A	C2'-C3'-O3'	10.02	131.54	109.50
1	5	1887	G	N9-C1'-C2'	-9.99	101.00	112.00
32	d	25	TYR	CA-CB-CG	-9.99	94.41	113.40
10	G	54	PHE	CB-CG-CD1	-9.97	113.82	120.80
11	H	54	ARG	NE-CZ-NH1	9.94	125.27	120.30
8	E	278	TYR	CA-CB-CG	-9.94	94.52	113.40
1	5	1974	U	N1-C1'-C2'	9.91	126.88	114.00
1	5	1379	C	O4'-C1'-N1	9.89	116.11	108.20
1	5	1992	U	N1-C1'-C2'	9.86	126.82	114.00
20	R	132	PHE	CB-CG-CD1	-9.82	113.92	120.80
1	5	2666	U	N1-C1'-C2'	-9.78	101.25	112.00
1	5	4693	C	N1-C1'-C2'	9.77	126.69	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	W	44	ARG	NE-CZ-NH1	9.76	125.18	120.30
34	f	36	ARG	NE-CZ-NH1	9.75	125.17	120.30
3	8	14	U	N1-C1'-C2'	9.70	126.61	114.00
8	E	278	TYR	CB-CA-C	9.69	129.79	110.40
29	a	128	PHE	CB-CG-CD1	-9.69	114.01	120.80
1	5	2394	G	N9-C1'-C2'	-9.69	101.34	112.00
1	5	2046	G	O4'-C1'-N9	9.69	115.95	108.20
1	5	1398	A	N9-C1'-C2'	9.68	126.58	114.00
1	5	4750	G	N9-C1'-C2'	-9.67	101.37	112.00
1	5	4464	A	O4'-C1'-N9	-9.66	100.47	108.20
29	a	61	TYR	CB-CG-CD1	-9.63	115.22	121.00
28	Z	36	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	5	4677	U	N1-C1'-C2'	-9.59	101.45	112.00
1	5	514	U	N1-C1'-C2'	-9.56	101.48	112.00
14	L	34	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	5	4162	C	N1-C1'-C2'	9.56	126.42	114.00
1	5	1501	C	O4'-C1'-N1	9.54	115.83	108.20
1	5	5040	U	N1-C1'-C2'	9.54	126.40	114.00
1	5	172	C	O4'-C1'-N1	9.51	115.80	108.20
1	5	315	G	O4'-C1'-N9	9.48	115.78	108.20
1	5	1501	C	N1-C1'-C2'	9.45	126.29	114.00
11	H	31	ARG	NE-CZ-NH1	9.45	125.02	120.30
38	j	66	HIS	N-CA-CB	9.44	127.60	110.60
17	O	178	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	5	294	G	O4'-C1'-N9	9.43	115.74	108.20
1	5	2438	A	N9-C1'-C2'	-9.42	101.64	112.00
13	J	32	ARG	NE-CZ-NH2	-9.42	115.59	120.30
20	R	95	TRP	N-CA-CB	9.42	127.55	110.60
1	5	42	A	O4'-C1'-N9	9.40	115.72	108.20
7	D	54	ARG	CG-CD-NE	-9.39	92.08	111.80
12	I	171	TRP	CA-CB-CG	-9.35	95.94	113.70
1	5	4280	A	N9-C1'-C2'	-9.30	101.77	112.00
1	5	5059	C	C2'-C3'-O3'	9.24	129.83	109.50
1	5	1534	A	N9-C1'-C2'	9.21	125.98	114.00
16	N	49	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	5	280	G	O4'-C1'-N9	9.17	115.53	108.20
1	5	2406	G	N9-C1'-C2'	-9.15	101.93	112.00
27	Y	27	ARG	NE-CZ-NH2	9.15	124.87	120.30
1	5	4228	G	N9-C1'-C2'	-9.13	101.95	112.00
1	5	2553	A	N9-C1'-C2'	9.09	125.82	114.00
1	5	1474	C	C2'-C3'-O3'	9.09	129.49	109.50
5	B	100	ARG	NE-CZ-NH2	-9.09	115.76	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1685	G	N9-C1'-C2'	9.08	125.80	114.00
19	Q	91	ARG	NE-CZ-NH2	9.07	124.84	120.30
1	5	2658	G	N9-C1'-C2'	-9.05	102.05	112.00
29	a	79	TRP	CA-CB-CG	-9.03	96.55	113.70
6	C	78	ARG	NE-CZ-NH1	9.02	124.81	120.30
33	e	46	ARG	NE-CZ-NH1	8.99	124.80	120.30
37	i	4	ARG	NE-CZ-NH1	8.99	124.79	120.30
24	V	97	TYR	CB-CG-CD2	-8.95	115.63	121.00
27	Y	126	ARG	NE-CZ-NH1	8.95	124.77	120.30
6	C	267	TRP	CA-CB-CG	8.94	130.69	113.70
1	5	1882	U	O5'-P-OP1	-8.94	97.66	105.70
5	B	119	TYR	CB-CG-CD1	-8.94	115.64	121.00
3	8	94	G	O4'-C1'-N9	-8.93	101.05	108.20
1	5	4965	U	N1-C1'-C2'	-8.91	102.20	112.00
1	5	4385	A	N9-C1'-C2'	-8.91	102.20	112.00
32	d	85	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	5	125	C	C2'-C3'-O3'	8.89	129.06	109.50
1	5	4911	A	O4'-C1'-N9	8.87	115.29	108.20
32	d	25	TYR	CB-CA-C	8.84	128.07	110.40
22	T	13	TYR	CB-CG-CD2	-8.82	115.71	121.00
1	5	977	C	C2'-C3'-O3'	8.78	128.81	109.50
1	5	1815	G	N9-C1'-C2'	8.78	125.41	114.00
44	p	85	ARG	NE-CZ-NH1	8.78	124.69	120.30
10	G	62	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	5	1356	U	C2'-C3'-O3'	8.77	128.79	109.50
1	5	1998	A	N9-C1'-C2'	8.77	125.40	114.00
1	5	2268	A	N9-C1'-C2'	8.76	125.39	114.00
17	O	135	PHE	N-CA-C	8.76	134.65	111.00
1	5	1534	A	O4'-C1'-N9	-8.75	101.20	108.20
1	5	978	G	C2'-C3'-O3'	8.75	128.75	109.50
8	E	119	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	5	1668	A	N9-C1'-C2'	8.74	125.36	114.00
1	5	4976	U	O4'-C1'-N1	-8.73	101.22	108.20
1	5	1359	G	C2'-C3'-O3'	8.73	128.70	109.50
21	S	81	TRP	CB-CA-C	8.72	127.85	110.40
6	C	311	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	5	2517	A	N9-C1'-C2'	8.69	125.30	114.00
19	Q	58	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	5	31	U	N1-C1'-C2'	8.67	125.28	114.00
18	P	54	GLN	CA-CB-CG	8.67	132.48	113.40
1	5	2305	U	O4'-C1'-N1	-8.66	101.27	108.20
1	5	2446	C	N1-C1'-C2'	8.66	125.26	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	S	81	TRP	CA-CB-CG	-8.65	97.26	113.70
1	5	4234	A	N9-C1'-C2'	8.65	125.24	114.00
1	5	4404	U	N1-C1'-C2'	-8.65	102.49	112.00
2	7	56	G	N9-C1'-C2'	8.63	125.22	114.00
36	h	117	ARG	CG-CD-NE	-8.62	93.69	111.80
43	o	31	ASP	CB-CA-C	8.61	127.62	110.40
4	A	193	ARG	CG-CD-NE	-8.61	93.72	111.80
1	5	1637	A	N9-C1'-C2'	-8.58	102.56	112.00
1	5	352	G	N9-C1'-C2'	-8.57	102.57	112.00
28	Z	121	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	5	4221	C	N1-C1'-C2'	-8.56	102.58	112.00
1	5	1980	U	O4'-C1'-N1	8.56	115.05	108.20
1	5	2851	G	N9-C1'-C2'	-8.55	102.59	112.00
17	O	140	ARG	NE-CZ-NH2	8.50	124.55	120.30
1	5	4563	U	N1-C1'-C2'	8.49	125.04	114.00
1	5	1439	C	C4'-C3'-O3'	-8.48	91.58	109.40
1	5	1733	G	N9-C1'-C2'	-8.48	102.67	112.00
26	X	73	HIS	CB-CA-C	8.47	127.34	110.40
1	5	1296	G	O4'-C1'-N9	8.46	114.97	108.20
33	e	35	TRP	CA-CB-CG	-8.45	97.64	113.70
4	A	67	TYR	CA-CB-CG	8.44	129.43	113.40
1	5	4119	C	C2'-C3'-O3'	8.43	128.06	109.50
1	5	3790	U	N1-C1'-C2'	8.43	124.96	114.00
14	L	74	ARG	NE-CZ-NH1	8.41	124.50	120.30
9	F	120	PHE	CB-CA-C	8.40	127.20	110.40
3	8	85	U	C2'-C3'-O3'	8.40	127.98	109.50
1	5	1937	C	N1-C1'-C2'	8.39	124.90	114.00
36	h	78	TYR	CA-CB-CG	-8.39	97.46	113.40
21	S	29	ARG	CA-CB-CG	8.38	131.84	113.40
8	E	268	ARG	NE-CZ-NH1	8.35	124.48	120.30
7	D	268	ARG	NE-CZ-NH1	8.34	124.47	120.30
43	o	48	TYR	CB-CA-C	8.32	127.04	110.40
20	R	74	ARG	NE-CZ-NH1	-8.28	116.16	120.30
1	5	292	G	N9-C1'-C2'	8.28	124.77	114.00
36	h	78	TYR	CB-CA-C	8.28	126.95	110.40
1	5	958	G	C2'-C3'-O3'	8.27	127.69	109.50
3	8	70	G	N9-C1'-C2'	-8.24	102.94	112.00
21	S	29	ARG	CG-CD-NE	-8.24	94.50	111.80
10	G	53	ARG	NE-CZ-NH2	-8.22	116.19	120.30
21	S	10	TYR	CA-CB-CG	-8.20	97.81	113.40
20	R	132	PHE	N-CA-C	-8.20	88.86	111.00
1	5	3879	G	N9-C1'-C2'	-8.20	102.98	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	93	G	N9-C1'-C2'	8.19	124.65	114.00
1	5	2087	C	N1-C1'-C2'	-8.19	103.00	112.00
43	o	57	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	5	3653	A	N9-C1'-C2'	-8.17	103.01	112.00
1	5	4498	U	N1-C1'-C2'	-8.17	103.02	112.00
1	5	3938	G	N9-C1'-C2'	8.15	124.59	114.00
1	5	2465	C	N1-C1'-C2'	8.15	124.59	114.00
34	f	4	ARG	CA-CB-CG	8.14	131.30	113.40
1	5	2553	A	O4'-C1'-N9	8.12	114.70	108.20
30	b	44	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	5	2797	C	N1-C1'-C2'	-8.12	103.07	112.00
17	O	37	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	5	2246	C	C2'-C3'-O3'	8.10	127.33	109.50
1	5	3773	U	C4'-C3'-O3'	8.10	129.19	113.00
1	5	2806	A	N9-C1'-C2'	-8.09	103.10	112.00
3	8	34	U	C2'-C3'-O3'	8.08	127.28	109.50
9	F	58	HIS	CB-CA-C	-8.08	94.23	110.40
1	5	3735	G	C2'-C3'-O3'	8.08	127.28	109.50
1	5	4723	A	C4-N9-C1'	8.08	140.84	126.30
3	8	94	G	C2'-C3'-O3'	8.07	127.26	109.50
1	5	235	A	O4'-C1'-N9	8.07	114.66	108.20
1	5	1867	A	N9-C1'-C2'	8.07	124.50	114.00
1	5	3635	A	N9-C1'-C2'	-8.06	103.13	112.00
7	D	44	TYR	CB-CA-C	8.06	126.52	110.40
4	A	193	ARG	NE-CZ-NH2	-8.04	116.28	120.30
16	N	139	HIS	N-CA-CB	8.03	125.06	110.60
7	D	248	ARG	NE-CZ-NH2	-8.03	116.28	120.30
24	V	98	PHE	CB-CG-CD1	-8.02	115.18	120.80
1	5	3908	A	N9-C1'-C2'	8.02	124.42	114.00
1	5	2683	C	C2'-C3'-O3'	8.01	127.13	109.50
1	5	4600	G	N9-C1'-C2'	-8.01	103.19	112.00
1	5	3905	A	C2'-C3'-O3'	8.01	127.12	109.50
1	5	4497	U	N1-C1'-C2'	-8.00	103.20	112.00
16	N	143	ARG	CG-CD-NE	-7.99	95.02	111.80
1	5	4371	G	O4'-C1'-N9	7.99	114.59	108.20
34	f	85	ARG	NE-CZ-NH2	-7.99	116.31	120.30
3	8	34	U	C5'-C4'-O4'	7.97	118.67	109.10
34	f	22	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	5	4885	U	C2'-C3'-O3'	7.96	127.02	109.50
12	I	119	PHE	CB-CG-CD1	7.95	126.37	120.80
5	B	62	ARG	NE-CZ-NH1	7.95	124.28	120.30
15	M	119	ARG	NE-CZ-NH2	7.93	124.27	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Q	174	PHE	CB-CA-C	7.93	126.27	110.40
1	5	3692	A	C2'-C3'-O3'	7.93	126.95	109.50
1	5	2394	G	O4'-C1'-N9	7.91	114.53	108.20
17	O	110	PRO	C-N-CD	-7.91	103.20	120.60
1	5	4163	U	N1-C1'-C2'	-7.90	103.31	112.00
1	5	2263	A	C5'-C4'-O4'	7.89	118.57	109.10
27	Y	11	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	5	4723	A	C8-N9-C1'	-7.89	113.50	127.70
5	B	169	ARG	NE-CZ-NH1	7.89	124.24	120.30
18	P	3	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	5	315	G	C1'-O4'-C4'	-7.87	103.60	109.90
1	5	668	C	C2'-C3'-O3'	7.87	126.81	109.50
1	5	1805	A	N9-C1'-C2'	7.83	124.18	114.00
3	8	64	U	N1-C1'-C2'	7.82	124.16	114.00
1	5	716	C	C2'-C3'-O3'	7.81	126.68	109.50
1	5	353	A	N9-C1'-C2'	-7.81	103.41	112.00
1	5	157	U	O4'-C1'-N1	7.80	114.44	108.20
22	T	13	TYR	N-CA-CB	-7.80	96.56	110.60
1	5	962	C	N1-C1'-C2'	7.78	124.11	114.00
1	5	2263	A	O4'-C1'-N9	-7.76	101.99	108.20
1	5	964	A	C4'-C3'-O3'	7.76	128.51	113.00
1	5	4463	U	N1-C1'-C2'	-7.75	103.48	112.00
1	5	5066	U	N1-C1'-C2'	7.73	124.05	114.00
7	D	198	HIS	CB-CA-C	7.71	125.82	110.40
1	5	43	U	N1-C1'-C2'	-7.71	103.52	112.00
1	5	4282	A	N9-C1'-C2'	7.70	124.01	114.00
9	F	168	ARG	CG-CD-NE	-7.68	95.66	111.80
29	a	128	PHE	CB-CA-C	7.68	125.75	110.40
4	A	37	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	5	1522	G	N9-C1'-C2'	-7.65	103.58	112.00
1	5	292	G	O4'-C1'-N9	-7.65	102.08	108.20
1	5	4194	U	N1-C1'-C2'	-7.64	103.59	112.00
5	B	116	ARG	CG-CD-NE	7.64	127.85	111.80
34	f	4	ARG	CG-CD-NE	-7.64	95.75	111.80
4	A	211	PHE	CB-CA-C	7.64	125.67	110.40
1	5	1575	A	N9-C1'-C2'	7.62	123.91	114.00
1	5	4238	G	N9-C1'-C2'	-7.62	103.61	112.00
1	5	53	C	C2'-C3'-O3'	7.61	126.25	109.50
1	5	294	G	C1'-O4'-C4'	-7.61	103.81	109.90
1	5	2790	U	N1-C1'-C2'	7.61	123.89	114.00
1	5	4464	A	C5'-C4'-O4'	7.60	118.22	109.10
7	D	210	TYR	CA-CB-CG	-7.58	98.99	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	8	94	G	C5'-C4'-O4'	7.58	118.19	109.10
36	h	119	PHE	CB-CA-C	-7.57	95.25	110.40
1	5	158	A	N9-C1'-C2'	-7.57	103.67	112.00
9	F	36	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	5	1377	G	C2'-C3'-O3'	7.56	126.13	109.50
1	5	1916	G	N9-C1'-C2'	7.55	123.82	114.00
1	5	4548	A	O4'-C1'-N9	-7.55	102.16	108.20
3	8	38	U	O4'-C1'-N1	7.55	114.24	108.20
1	5	4583	C	N1-C1'-C2'	-7.55	103.70	112.00
1	5	354	U	N1-C1'-C2'	-7.54	103.71	112.00
12	I	4	ARG	CG-CD-NE	-7.54	95.97	111.80
1	5	1881	C	N1-C1'-C2'	7.54	123.80	114.00
3	8	104	A	O4'-C1'-N9	-7.53	102.17	108.20
1	5	4911	A	C1'-O4'-C4'	-7.53	103.87	109.90
1	5	4737	G	N9-C1'-C2'	7.53	123.78	114.00
8	E	179	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	5	5046	U	C2'-C3'-O3'	7.51	126.02	109.50
29	a	79	TRP	CB-CA-C	7.50	125.40	110.40
1	5	1382	G	N9-C1'-C2'	7.50	123.75	114.00
1	5	2588	C	C4'-C3'-O3'	7.49	127.99	113.00
1	5	1724	G	O4'-C4'-C3'	-7.49	96.51	104.00
9	F	228	HIS	N-CA-CB	7.49	124.08	110.60
1	5	3868	G	N9-C1'-C2'	-7.49	103.77	112.00
5	B	117	ARG	NE-CZ-NH2	-7.48	116.56	120.30
6	C	222	ARG	NE-CZ-NH1	7.48	124.04	120.30
12	I	171	TRP	N-CA-CB	7.48	124.06	110.60
1	5	2092	G	N9-C1'-C2'	7.47	123.71	114.00
37	i	28	ARG	CG-CD-NE	-7.47	96.11	111.80
1	5	4212	A	N9-C1'-C2'	7.47	123.71	114.00
1	5	157	U	N1-C1'-C2'	-7.46	103.79	112.00
1	5	4693	C	C5'-C4'-O4'	7.46	118.05	109.10
16	N	131	GLU	CB-CG-CD	-7.46	94.07	114.20
1	5	1378	C	N1-C1'-C2'	7.45	123.69	114.00
1	5	4322	G	N9-C1'-C2'	-7.44	103.81	112.00
19	Q	34	PHE	N-CA-CB	7.44	124.00	110.60
1	5	4535	A	C2'-C3'-O3'	7.44	125.87	109.50
3	8	73	U	N1-C1'-C2'	-7.43	103.83	112.00
1	5	2046	G	C1'-O4'-C4'	-7.43	103.96	109.90
1	5	4120	U	N1-C1'-C2'	-7.43	103.83	112.00
16	N	180	PHE	CB-CA-C	7.42	125.24	110.40
1	5	1521	C	N1-C1'-C2'	-7.42	103.84	112.00
29	a	34	ASN	CB-CA-C	7.42	125.23	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	35	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	5	1445	U	C2'-C3'-O3'	7.40	125.78	109.50
1	5	1266	G	C2'-C3'-O3'	7.40	125.77	109.50
10	G	235	ARG	NE-CZ-NH1	7.39	124.00	120.30
7	D	223	PHE	CB-CG-CD2	-7.38	115.63	120.80
1	5	3871	A	N9-C1'-C2'	7.38	123.59	114.00
1	5	1440	U	C2'-C3'-O3'	7.37	125.72	109.50
4	A	189	TYR	CA-CB-CG	7.36	127.38	113.40
1	5	394	G	N9-C1'-C2'	-7.36	103.91	112.00
7	D	210	TYR	N-CA-CB	7.36	123.84	110.60
1	5	979	C	C2'-C3'-O3'	7.35	125.67	109.50
1	5	1370	G	N9-C1'-C2'	7.35	123.56	114.00
1	5	2124	G	C2'-C3'-O3'	7.35	125.67	109.50
1	5	3938	G	O4'-C1'-N9	-7.35	102.32	108.20
1	5	4981	G	N9-C1'-C2'	-7.35	103.92	112.00
1	5	55	G	N9-C1'-C2'	-7.35	103.92	112.00
1	5	4464	A	N9-C1'-C2'	7.35	123.55	114.00
1	5	450	G	N9-C1'-C2'	-7.34	103.92	112.00
1	5	3843	C	N1-C1'-C2'	7.34	123.55	114.00
1	5	4251	A	N9-C1'-C2'	7.34	123.54	114.00
4	A	242	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	5	147	A	N9-C1'-C2'	7.33	123.53	114.00
1	5	974	C	C2'-C3'-O3'	7.33	125.63	109.50
1	5	5061	A	C2'-C3'-O3'	7.33	125.63	109.50
1	5	4531	U	N1-C1'-C2'	7.32	123.52	114.00
1	5	1601	A	N9-C1'-C2'	-7.32	103.95	112.00
1	5	1379	C	C1'-O4'-C4'	-7.31	104.05	109.90
1	5	2769	U	N1-C1'-C2'	-7.31	103.96	112.00
1	5	97	G	N9-C1'-C2'	-7.30	103.97	112.00
1	5	486	C	C2'-C3'-O3'	7.29	125.55	109.50
1	5	4084	G	C2'-C3'-O3'	7.28	125.51	109.50
1	5	406	C	C2'-C3'-O3'	7.27	125.50	109.50
1	5	4519	C	N1-C1'-C2'	-7.26	104.01	112.00
1	5	2280	G	N9-C1'-C2'	7.26	123.44	114.00
26	X	48	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	5	2848	G	N9-C1'-C2'	-7.25	104.02	112.00
1	5	2796	G	N9-C1'-C2'	7.25	123.42	114.00
1	5	1481	C	C2'-C3'-O3'	7.24	125.43	109.50
1	5	4966	A	N9-C1'-C2'	7.22	123.38	114.00
1	5	664	G	C1'-O4'-C4'	-7.21	104.13	109.90
38	j	71	TYR	CA-CB-CG	7.21	127.09	113.40
1	5	100	C	N1-C1'-C2'	-7.21	104.07	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	109	TYR	CB-CA-C	7.19	124.79	110.40
1	5	4279	A	N9-C1'-C2'	-7.19	104.09	112.00
36	h	51	ARG	NE-CZ-NH1	7.18	123.89	120.30
21	S	28	TYR	CB-CG-CD1	7.18	125.31	121.00
36	h	89	ARG	NE-CZ-NH1	7.17	123.89	120.30
38	j	11	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	5	2812	A	N9-C1'-C2'	7.17	123.32	114.00
1	5	2511	A	C4'-C3'-O3'	-7.17	94.34	109.40
1	5	1359	G	C4'-C3'-O3'	-7.17	94.34	109.40
1	5	1534	A	C5'-C4'-O4'	7.17	117.70	109.10
1	5	4750	G	C1'-O4'-C4'	-7.16	104.17	109.90
6	C	41	HIS	N-CA-CB	7.16	123.49	110.60
13	J	64	ARG	NE-CZ-NH2	7.15	123.88	120.30
26	X	48	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	5	4750	G	O4'-C1'-N9	7.14	113.91	108.20
3	8	34	U	O4'-C1'-N1	-7.14	102.49	108.20
37	i	39	PHE	N-CA-CB	7.13	123.43	110.60
1	5	350	C	N1-C1'-C2'	7.12	123.26	114.00
32	d	73	TRP	N-CA-CB	-7.12	97.79	110.60
1	5	29	G	N9-C1'-C2'	7.11	123.25	114.00
1	5	383	A	C1'-C2'-O2'	-7.11	89.26	110.60
29	a	62	HIS	N-CA-CB	7.11	123.40	110.60
1	5	1500	A	C4'-C3'-O3'	7.11	127.21	113.00
1	5	1946	G	N9-C1'-C2'	-7.10	104.19	112.00
1	5	2324	C	C2'-C3'-O3'	7.10	125.11	109.50
1	5	2038	U	N1-C1'-C2'	7.09	123.22	114.00
9	F	194	HIS	CB-CA-C	-7.09	96.22	110.40
1	5	4341	C	N1-C1'-C2'	-7.09	104.20	112.00
38	j	27	TYR	CA-CB-CG	-7.08	99.96	113.40
1	5	4500	U	O5'-P-OP1	-7.07	99.33	105.70
3	8	38	U	C1'-O4'-C4'	-7.07	104.24	109.90
1	5	2046	G	C2'-C3'-O3'	7.07	125.06	109.50
14	L	82	ARG	NE-CZ-NH2	-7.07	116.76	120.30
17	O	49	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	5	1355	G	N9-C1'-C2'	7.07	123.19	114.00
1	5	4519	C	O4'-C1'-N1	7.07	113.86	108.20
1	5	514	U	C2'-C3'-O3'	7.07	125.04	109.50
8	E	219	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	5	30	C	N1-C1'-C2'	7.06	123.18	114.00
1	5	4464	A	C2'-C3'-O3'	7.06	125.03	109.50
1	5	4510	A	O4'-C1'-N9	-7.05	102.56	108.20
1	5	291	U	N1-C1'-C2'	7.05	123.16	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	5	4589	A	O4'-C1'-N9	-7.04	102.57	108.20
3	8	94	G	N9-C1'-C2'	7.04	123.15	114.00
13	J	32	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	5	1479	G	N9-C1'-C2'	7.04	123.15	114.00
1	5	3817	A	N9-C1'-C2'	7.03	123.14	114.00
11	H	156	ASN	N-CA-CB	7.03	123.26	110.60
33	e	74	PHE	CB-CG-CD1	-7.03	115.88	120.80
1	5	669	C	O4'-C1'-N1	7.03	113.82	108.20
1	5	157	U	C1'-O4'-C4'	-7.02	104.28	109.90
1	5	1455	G	C2'-C3'-O3'	7.02	124.95	109.50
1	5	1625	G	N9-C1'-C2'	7.02	123.13	114.00
1	5	1552	G	N9-C1'-C2'	-7.02	104.28	112.00
1	5	2695	A	C2'-C3'-O3'	7.02	124.94	109.50
25	W	8	PHE	CB-CG-CD1	7.00	125.70	120.80
1	5	42	A	C1'-O4'-C4'	-7.00	104.30	109.90
1	5	235	A	N9-C1'-C2'	-7.00	104.31	112.00
1	5	209	U	O4'-C1'-N1	6.99	113.79	108.20
5	B	100	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	5	1676	C	C1'-C2'-O2'	-6.98	89.66	110.60
43	o	48	TYR	CA-CB-CG	-6.96	100.17	113.40
1	5	332	C	N1-C1'-C2'	6.96	123.05	114.00
9	F	197	TYR	CB-CA-C	-6.96	96.48	110.40
6	C	35	ASP	CB-CG-OD1	6.96	124.56	118.30
32	d	25	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	5	2589	C	C2'-C3'-O3'	6.94	124.81	113.70
1	5	2851	G	C2'-C3'-O3'	6.94	124.81	113.70
1	5	4265	U	N1-C1'-C2'	6.94	123.03	114.00
1	5	4531	U	O4'-C1'-N1	-6.94	102.65	108.20
1	5	4589	A	N9-C1'-C2'	6.94	123.03	114.00
24	V	97	TYR	N-CA-C	-6.94	92.25	111.00
1	5	4270	C	N1-C1'-C2'	-6.94	104.37	112.00
13	J	146	ARG	CG-CD-NE	-6.92	97.26	111.80
1	5	1815	G	O4'-C1'-N9	6.91	113.73	108.20
36	h	93	ARG	NE-CZ-NH2	-6.89	116.85	120.30
20	R	88	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	5	1832	C	C2'-C3'-O3'	6.89	124.72	113.70
1	5	54	G	N9-C1'-C2'	-6.88	104.43	112.00
1	5	5001	U	N1-C1'-C2'	6.88	122.94	114.00
1	5	943	A	N9-C1'-C2'	-6.87	104.44	112.00
11	H	156	ASN	N-CA-C	-6.87	92.44	111.00
1	5	1319	U	N1-C1'-C2'	-6.87	104.44	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	274	TYR	CA-CB-CG	-6.87	100.36	113.40
16	N	49	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	5	454	U	C2'-C3'-O3'	6.86	124.68	113.70
19	Q	37	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	5	1631	A	O4'-C1'-N9	-6.85	102.72	108.20
10	G	49	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	5	226	G	N9-C1'-C2'	-6.84	104.48	112.00
10	G	73	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	5	964	A	O4'-C1'-C2'	-6.83	98.97	105.80
34	f	4	ARG	N-CA-CB	6.83	122.90	110.60
19	Q	75	ARG	NE-CZ-NH1	6.83	123.72	120.30
34	f	85	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	5	4518	A	O5'-P-OP1	6.83	118.89	110.70
10	G	54	PHE	CB-CG-CD2	-6.83	116.02	120.80
1	5	5047	C	O5'-P-OP2	-6.82	99.56	105.70
9	F	219	ARG	NE-CZ-NH1	6.81	123.71	120.30
3	8	64	U	C2'-C3'-O3'	6.81	124.60	113.70
24	V	97	TYR	CA-CB-CG	-6.80	100.48	113.40
1	5	2271	C	N1-C1'-C2'	6.80	122.84	114.00
1	5	3611	A	N9-C1'-C2'	6.79	122.83	114.00
28	Z	65	ARG	CG-CD-NE	-6.79	97.55	111.80
1	5	3625	G	C2'-C3'-O3'	6.78	124.55	113.70
2	7	72	U	C2'-C3'-O3'	6.77	124.54	113.70
9	F	168	ARG	NE-CZ-NH2	-6.77	116.91	120.30
13	J	99	PHE	CB-CA-C	6.77	123.94	110.40
8	E	179	ARG	NE-CZ-NH2	-6.76	116.92	120.30
19	Q	33	ARG	CG-CD-NE	-6.76	97.60	111.80
8	E	101	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	5	2319	C	N1-C1'-C2'	6.75	122.78	114.00
20	R	74	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	5	1292	C	C2'-C3'-O3'	6.74	124.48	113.70
1	5	1	C	O4'-C1'-N1	6.74	113.59	108.20
1	5	2395	A	N9-C1'-C2'	-6.74	104.59	112.00
1	5	84	A	O4'-C1'-N9	-6.73	102.82	108.20
1	5	3875	G	N9-C1'-C2'	-6.72	104.61	112.00
8	E	278	TYR	N-CA-C	-6.72	92.86	111.00
19	Q	15	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	5	3901	A	O4'-C1'-N9	-6.72	102.83	108.20
1	5	2827	G	O4'-C1'-N9	-6.72	102.83	108.20
1	5	2675	G	N9-C1'-C2'	-6.71	104.62	112.00
1	5	1364	U	C2'-C3'-O3'	6.71	124.43	113.70
18	P	42	ARG	NE-CZ-NH1	6.70	123.65	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	73	TRP	CA-CB-CG	6.70	126.43	113.70
11	H	125	ARG	NE-CZ-NH1	6.69	123.65	120.30
28	Z	38	TYR	CB-CA-C	6.69	123.78	110.40
1	5	58	G	N9-C1'-C2'	6.69	122.69	114.00
1	5	2305	U	N1-C1'-C2'	6.69	122.69	114.00
1	5	4230	C	O5'-P-OP1	-6.69	99.68	105.70
1	5	4936	G	N9-C1'-C2'	-6.69	104.64	112.00
1	5	1631	A	N9-C1'-C2'	6.68	122.68	114.00
32	d	87	ARG	N-CA-C	-6.68	92.97	111.00
1	5	3882	C	N1-C1'-C2'	6.67	122.67	114.00
1	5	4280	A	C2'-C3'-O3'	6.67	124.37	113.70
1	5	4197	G	N9-C1'-C2'	-6.66	104.67	112.00
30	b	7	HIS	CB-CA-C	-6.64	97.13	110.40
1	5	4325	A	N9-C1'-C2'	6.63	122.62	114.00
1	5	314	G	N9-C1'-C2'	-6.62	104.72	112.00
1	5	336	A	O4'-C1'-N9	6.62	113.50	108.20
1	5	5022	U	C2'-C3'-O3'	6.62	124.29	113.70
34	f	109	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	5	3790	U	O4'-C1'-N1	-6.61	102.91	108.20
1	5	4518	A	C2'-C3'-O3'	-6.61	94.96	109.50
3	8	81	C	C1'-O4'-C4'	-6.61	104.61	109.90
1	5	4693	C	C2'-C3'-O3'	6.61	124.27	113.70
3	8	1	C	C5'-C4'-O4'	6.59	117.01	109.10
5	B	26	ARG	CG-CD-NE	-6.59	97.95	111.80
1	5	1650	A	O4'-C1'-N9	-6.58	102.93	108.20
1	5	514	U	C5'-C4'-O4'	6.57	116.99	109.10
1	5	3883	U	N1-C1'-C2'	6.57	122.55	114.00
1	5	2782	U	C4'-C3'-O3'	6.57	126.14	113.00
27	Y	81	TYR	CA-CB-CG	-6.57	100.93	113.40
1	5	1930	U	N1-C1'-C2'	6.56	122.53	114.00
18	P	23	ARG	NE-CZ-NH1	6.56	123.58	120.30
38	j	27	TYR	CB-CG-CD1	-6.56	117.06	121.00
1	5	927	G	C2'-C3'-O3'	6.56	124.19	113.70
1	5	432	U	N1-C1'-C2'	-6.55	104.80	112.00
16	N	150	TRP	CA-CB-CG	6.55	126.14	113.70
1	5	1215	C	O5'-P-OP2	-6.54	99.81	105.70
1	5	505	G	C2'-C3'-O3'	6.54	124.16	113.70
1	5	4336	A	N9-C1'-C2'	-6.54	104.81	112.00
1	5	187	U	C2'-C3'-O3'	6.54	124.16	113.70
1	5	964	A	N9-C1'-C2'	-6.54	104.81	112.00
1	5	4227	U	C2'-C3'-O3'	6.54	124.16	113.70
35	g	14	ASN	N-CA-CB	6.54	122.36	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1887	G	C2'-C3'-O3'	6.52	124.14	113.70
1	5	2075	G	C2'-C3'-O3'	6.52	124.13	113.70
1	5	384	A	N9-C1'-C2'	6.52	122.47	114.00
9	F	209	PHE	N-CA-CB	6.51	122.32	110.60
1	5	98	A	N9-C1'-C2'	-6.51	104.84	112.00
1	5	5043	A	N9-C1'-C2'	6.50	122.45	114.00
1	5	1379	C	N1-C1'-C2'	6.50	122.45	114.00
1	5	3827	G	N9-C1'-C2'	-6.50	104.86	112.00
1	5	1671	U	O4'-C1'-C2'	-6.49	99.31	105.80
18	P	25	HIS	CB-CA-C	6.49	123.39	110.40
1	5	119	G	O4'-C4'-C3'	-6.49	97.51	104.00
1	5	4338	G	N9-C1'-C2'	-6.48	104.87	112.00
10	G	223	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	5	209	U	C4'-C3'-O3'	6.48	125.96	113.00
1	5	307	A	N9-C1'-C2'	6.48	122.42	114.00
15	M	109	ARG	NE-CZ-NH2	6.48	123.54	120.30
17	O	37	ARG	NE-CZ-NH1	6.48	123.54	120.30
32	d	85	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	5	136	C	N1-C1'-C2'	-6.47	104.89	112.00
1	5	2118	G	C4'-C3'-O3'	6.46	125.92	113.00
1	5	4199	C	C4'-C3'-O3'	6.46	125.92	113.00
1	5	946	C	O4'-C1'-N1	6.46	113.37	108.20
3	8	64	U	C5'-C4'-O4'	6.45	116.84	109.10
6	C	143	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	5	1573	G	N9-C1'-C2'	6.44	122.38	114.00
1	5	2546	G	C4'-C3'-O3'	6.44	125.88	113.00
19	Q	181	ARG	CA-CB-CG	6.43	127.55	113.40
1	5	2665	U	C2'-C3'-O3'	6.42	123.98	113.70
1	5	4534	G	N9-C1'-C2'	-6.42	104.94	112.00
1	5	4976	U	N1-C1'-C2'	6.42	122.35	114.00
3	8	86	U	O4'-C1'-C2'	-6.42	99.38	105.80
1	5	1853	G	N9-C1'-C2'	-6.42	104.94	112.00
45	r	31	ASN	N-CA-CB	6.42	122.15	110.60
1	5	1572	U	N1-C1'-C2'	6.41	122.34	114.00
4	A	63	PHE	CB-CG-CD1	6.41	125.29	120.80
1	5	1724	G	C4'-C3'-O3'	-6.41	95.95	109.40
3	8	35	C	N1-C1'-C2'	6.41	122.33	114.00
1	5	1980	U	C1'-O4'-C4'	-6.41	104.78	109.90
1	5	4519	C	C2'-C3'-O3'	6.40	123.94	113.70
1	5	4076	G	N9-C1'-C2'	-6.40	104.96	112.00
22	T	13	TYR	CA-CB-CG	6.40	125.56	113.40
9	F	168	ARG	CB-CG-CD	6.40	128.24	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2088	A	C2'-C3'-O3'	6.39	123.93	113.70
1	5	2649	G	N9-C1'-C2'	6.39	122.30	114.00
1	5	1241	C	C2'-C3'-O3'	6.38	123.92	113.70
1	5	2581	A	N9-C1'-C2'	6.38	122.30	114.00
1	5	1642	A	C4'-C3'-O3'	-6.38	96.00	109.40
1	5	4911	A	O5'-P-OP2	-6.38	99.96	105.70
27	Y	81	TYR	CB-CA-C	6.38	123.16	110.40
1	5	4127	A	O4'-C1'-N9	6.38	113.30	108.20
7	D	293	ARG	NE-CZ-NH1	6.38	123.49	120.30
7	D	223	PHE	CB-CG-CD1	6.37	125.26	120.80
1	5	84	A	N9-C1'-C2'	6.36	122.27	114.00
1	5	3671	G	N9-C1'-C2'	6.35	122.25	114.00
1	5	336	A	C1'-O4'-C4'	-6.35	104.82	109.90
1	5	1272	C	O4'-C1'-N1	6.34	113.28	108.20
1	5	2511	A	O4'-C1'-N9	-6.34	103.12	108.20
1	5	2554	U	C2'-C3'-O3'	6.34	123.85	113.70
1	5	1615	C	C2'-C3'-O3'	6.34	123.84	113.70
10	G	235	ARG	CG-CD-NE	6.33	125.09	111.80
29	a	109	TYR	CB-CG-CD2	-6.33	117.20	121.00
27	Y	78	TYR	CB-CA-C	6.33	123.05	110.40
1	5	3901	A	C5'-C4'-O4'	6.31	116.68	109.10
1	5	2874	U	O4'-C1'-N1	-6.31	103.15	108.20
1	5	294	G	N9-C1'-C2'	6.31	122.20	114.00
1	5	3648	A	O4'-C1'-N9	6.30	113.24	108.20
3	8	104	A	N9-C1'-C2'	6.30	122.19	114.00
12	I	34	PHE	CB-CG-CD1	-6.30	116.39	120.80
1	5	3653	A	O5'-P-OP1	-6.30	100.03	105.70
25	W	55	TYR	CB-CG-CD1	6.30	124.78	121.00
1	5	1724	G	N9-C1'-C2'	6.29	122.18	114.00
1	5	4519	C	O4'-C4'-C3'	-6.29	97.71	104.00
33	e	5	ARG	NE-CZ-NH1	6.29	123.44	120.30
4	A	37	ARG	NE-CZ-NH1	6.29	123.44	120.30
9	F	136	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	5	1672	U	C2-N1-C1'	6.28	125.24	117.70
7	D	35	ARG	CG-CD-NE	6.28	124.99	111.80
1	5	2827	G	N9-C1'-C2'	6.28	122.16	114.00
9	F	36	ARG	NE-CZ-NH1	-6.28	117.16	120.30
7	D	145	TYR	CB-CA-C	6.28	122.95	110.40
18	P	139	TYR	CA-CB-CG	-6.27	101.48	113.40
1	5	2511	A	C2'-C3'-O3'	6.27	123.73	113.70
25	W	8	PHE	CB-CG-CD2	-6.27	116.41	120.80
1	5	417	G	O4'-C1'-N9	6.27	113.21	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	3880	G	N9-C1'-C2'	6.26	122.14	114.00
1	5	4519	C	C4'-C3'-C2'	-6.26	96.33	102.60
19	Q	33	ARG	NE-CZ-NH2	-6.26	117.17	120.30
21	S	83	ARG	CG-CD-NE	6.26	124.94	111.80
7	D	30	TYR	CB-CA-C	6.25	122.91	110.40
1	5	219	G	O5'-P-OP2	-6.25	100.08	105.70
3	8	62	A	C8-N9-C1'	6.25	138.94	127.70
1	5	1279	A	C2'-C3'-O3'	6.24	123.69	113.70
1	5	2403	A	N9-C1'-C2'	6.24	122.12	114.00
1	5	4718	G	N9-C1'-C2'	-6.24	105.14	112.00
1	5	1282	G	O5'-P-OP1	-6.24	100.09	105.70
1	5	220	C	C2'-C3'-O3'	6.23	123.67	113.70
14	L	192	PHE	N-CA-CB	6.23	121.81	110.60
1	5	1961	G	C2'-C3'-O3'	6.22	123.66	113.70
1	5	2673	G	O4'-C1'-C2'	-6.22	99.58	105.80
1	5	4677	U	C3'-C2'-C1'	6.22	106.47	101.50
1	5	4548	A	P-O5'-C5'	6.21	130.84	120.90
36	h	89	ARG	CG-CD-NE	6.21	124.84	111.80
1	5	5056	A	N9-C1'-C2'	6.21	122.07	114.00
20	R	107	ARG	NE-CZ-NH1	6.21	123.40	120.30
31	c	90	ARG	CA-CB-CG	6.21	127.06	113.40
1	5	99	A	N9-C1'-C2'	-6.21	105.17	112.00
1	5	2082	G	N9-C1'-C2'	6.21	122.07	114.00
6	C	80	ARG	NE-CZ-NH1	6.20	123.40	120.30
38	j	11	ARG	CG-CD-NE	-6.20	98.78	111.80
7	D	44	TYR	CA-CB-CG	-6.20	101.62	113.40
1	5	1934	A	N9-C1'-C2'	-6.19	105.19	112.00
3	8	81	C	O4'-C1'-N1	6.19	113.16	108.20
1	5	3791	C	O4'-C1'-N1	-6.19	103.25	108.20
10	G	54	PHE	CB-CA-C	6.19	122.78	110.40
1	5	747	A	C2'-C3'-O3'	6.19	123.60	113.70
1	5	3727	A	N9-C1'-C2'	6.18	122.04	114.00
5	B	137	TRP	CA-CB-CG	-6.18	101.96	113.70
1	5	2107	C	C2'-C3'-O3'	6.18	123.58	113.70
19	Q	4	ASP	CB-CA-C	6.18	122.75	110.40
1	5	5006	U	N1-C1'-C2'	-6.17	105.21	112.00
11	H	31	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	5	962	C	C4'-C3'-O3'	-6.17	96.44	109.40
1	5	2666	U	C4'-C3'-C2'	-6.17	96.43	102.60
16	N	96	ARG	NE-CZ-NH1	-6.17	117.22	120.30
29	a	61	TYR	CB-CG-CD2	6.17	124.70	121.00
1	5	1379	C	C5'-C4'-O4'	6.17	116.50	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2470	C	O4'-C1'-C2'	-6.17	99.63	105.80
6	C	35	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	5	409	G	N9-C1'-C2'	-6.16	105.22	112.00
35	g	90	ARG	CG-CD-NE	-6.16	98.86	111.80
1	5	4560	C	O4'-C1'-N1	-6.16	103.27	108.20
1	5	4579	U	C2-N1-C1'	6.16	125.09	117.70
17	O	117	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	5	514	U	C4'-C3'-C2'	-6.15	96.45	102.60
9	F	239	GLU	CA-CB-CG	6.15	126.93	113.40
20	R	9	ARG	NE-CZ-NH1	6.15	123.38	120.30
34	f	19	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	5	2854	G	C2'-C3'-O3'	6.15	123.53	113.70
1	5	4451	G	N9-C1'-C2'	6.14	121.99	114.00
1	5	4976	U	C5'-C4'-O4'	6.14	116.47	109.10
6	C	311	ARG	NE-CZ-NH1	6.14	123.37	120.30
31	c	39	ARG	CG-CD-NE	-6.14	98.90	111.80
9	F	168	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	5	1379	C	P-O5'-C5'	6.13	130.72	120.90
1	5	4239	A	C2'-C3'-O3'	6.13	123.52	113.70
1	5	2854	G	N9-C1'-C2'	-6.13	105.25	112.00
14	L	82	ARG	NE-CZ-NH1	6.13	123.36	120.30
32	d	87	ARG	CA-CB-CG	6.13	126.88	113.40
8	E	59	TYR	N-CA-C	-6.12	94.46	111.00
27	Y	15	ARG	NE-CZ-NH1	-6.12	117.24	120.30
3	8	62	A	C4-N9-C1'	-6.12	115.29	126.30
3	8	66	A	N9-C1'-C2'	6.12	121.95	114.00
1	5	4880	C	N1-C1'-C2'	6.12	121.95	114.00
1	5	219	G	O4'-C1'-C2'	-6.12	99.69	105.80
5	B	102	PHE	CB-CA-C	-6.11	98.18	110.40
43	o	78	ARG	NE-CZ-NH1	-6.11	117.25	120.30
9	F	98	ARG	NE-CZ-NH2	-6.11	117.25	120.30
45	r	45	HIS	CB-CA-C	-6.10	98.19	110.40
7	D	145	TYR	CA-CB-CG	-6.10	101.81	113.40
19	Q	58	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	5	1649	U	N1-C1'-C2'	6.09	121.92	114.00
1	5	4731	G	O4'-C1'-N9	6.09	113.07	108.20
1	5	4948	C	C2'-C3'-O3'	6.09	123.44	113.70
38	j	39	TYR	CB-CA-C	-6.09	98.22	110.40
1	5	1614	C	C2'-C3'-O3'	6.09	123.44	113.70
1	5	2119	C	O4'-C1'-N1	6.08	113.07	108.20
1	5	4876	U	N1-C1'-C2'	6.08	121.91	114.00
25	W	57	ARG	NE-CZ-NH1	6.08	123.34	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	87	ARG	CG-CD-NE	-6.07	99.04	111.80
1	5	1488	G	C2'-C3'-O3'	6.07	123.42	113.70
1	5	5040	U	C4'-C3'-O3'	-6.07	96.66	109.40
14	L	36	ARG	NE-CZ-NH1	6.07	123.33	120.30
4	A	83	HIS	N-CA-C	-6.06	94.64	111.00
19	Q	181	ARG	CG-CD-NE	-6.05	99.09	111.80
1	5	3843	C	O4'-C1'-N1	-6.05	103.36	108.20
1	5	235	A	C1'-O4'-C4'	-6.05	105.06	109.90
6	C	78	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	5	3738	G	N9-C1'-C2'	-6.04	105.36	112.00
1	5	1214	C	O4'-C1'-N1	-6.04	103.37	108.20
1	5	4986	G	N9-C1'-C2'	6.04	121.85	114.00
34	f	36	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	5	4270	C	C2'-C3'-O3'	6.03	123.35	113.70
1	5	4519	C	C1'-O4'-C4'	-6.03	105.07	109.90
29	a	132	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	5	4599	A	N9-C1'-C2'	6.02	121.83	114.00
37	i	85	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	5	4871	C	O4'-C1'-N1	-6.01	103.39	108.20
16	N	71	ARG	NE-CZ-NH1	6.01	123.31	120.30
27	Y	126	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	5	1210	C	N1-C1'-C2'	6.01	121.82	114.00
2	7	58	A	N9-C1'-C2'	-6.01	105.39	112.00
1	5	1658	G	N9-C1'-C2'	6.01	121.81	114.00
19	Q	166	TYR	CB-CG-CD1	6.01	124.61	121.00
6	C	312	ARG	CG-CD-NE	-6.01	99.19	111.80
8	E	157	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	5	52	G	C2'-C3'-O3'	6.00	123.30	113.70
1	5	3913	G	C2'-C3'-O3'	6.00	123.30	113.70
3	8	13	G	N9-C1'-C2'	6.00	121.80	114.00
36	h	84	ARG	CG-CD-NE	-6.00	99.20	111.80
1	5	67	C	N1-C1'-C2'	-6.00	105.40	112.00
1	5	3739	C	O4'-C1'-C2'	-6.00	99.80	105.80
3	8	64	U	C2-N1-C1'	6.00	124.89	117.70
1	5	4694	G	O5'-P-OP1	-5.99	100.31	105.70
31	c	56	ARG	NE-CZ-NH1	5.99	123.29	120.30
18	P	127	ARG	NE-CZ-NH2	-5.98	117.31	120.30
20	R	108	ARG	NE-CZ-NH2	-5.98	117.31	120.30
33	e	46	ARG	NE-CZ-NH2	-5.98	117.31	120.30
7	D	265	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	5	2744	A	N9-C1'-C2'	5.98	121.77	114.00
2	7	58	A	C2'-C3'-O3'	5.98	123.26	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	65	ARG	CG-CD-NE	-5.98	99.25	111.80
45	r	103	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	5	1697	G	O5'-P-OP2	5.97	117.86	110.70
43	o	40	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	5	669	C	C1'-O4'-C4'	-5.96	105.13	109.90
7	D	54	ARG	CB-CG-CD	5.96	127.08	111.60
1	5	1930	U	O4'-C1'-N1	-5.95	103.44	108.20
1	5	4979	A	N9-C1'-C2'	5.95	121.74	114.00
5	B	258	HIS	N-CA-C	5.95	127.07	111.00
1	5	4473	A	C4-N9-C1'	5.95	137.00	126.30
1	5	2307	A	N9-C1'-C2'	5.95	121.73	114.00
33	e	20	PHE	CB-CG-CD1	-5.94	116.64	120.80
1	5	4291	G	N9-C1'-C2'	5.94	121.72	114.00
1	5	1398	A	O5'-P-OP2	-5.94	100.35	105.70
1	5	1523	A	O5'-P-OP1	-5.94	100.36	105.70
1	5	231	U	C4'-C3'-O3'	-5.94	96.93	109.40
1	5	2515	G	N9-C1'-C2'	-5.94	105.47	112.00
1	5	4479	A	N9-C1'-C2'	-5.94	105.47	112.00
15	M	90	ARG	CG-CD-NE	-5.94	99.33	111.80
1	5	1495	G	N9-C1'-C2'	5.93	121.71	114.00
15	M	6	PHE	CB-CA-C	5.93	122.25	110.40
22	T	57	TYR	CA-CB-CG	5.93	124.66	113.40
31	c	56	ARG	CD-NE-CZ	5.92	131.90	123.60
1	5	2373	C	N1-C1'-C2'	5.92	121.69	114.00
1	5	2323	C	N1-C1'-C2'	-5.92	105.49	112.00
1	5	4670	C	O4'-C1'-N1	-5.91	103.47	108.20
1	5	936	C	C4'-C3'-O3'	5.91	124.82	113.00
1	5	2322	G	C2'-C3'-O3'	5.91	123.15	113.70
14	L	82	ARG	CG-CD-NE	-5.91	99.39	111.80
1	5	1992	U	O4'-C1'-N1	5.91	112.92	108.20
1	5	53	C	N1-C1'-C2'	-5.90	105.51	112.00
6	C	102	PHE	N-CA-CB	5.90	121.22	110.60
1	5	2642	A	N9-C1'-C2'	-5.90	105.51	112.00
1	5	4449	A	N9-C1'-C2'	-5.90	105.51	112.00
1	5	40	G	N9-C1'-C2'	5.89	121.66	114.00
1	5	3774	A	N9-C1'-C2'	5.89	121.66	114.00
32	d	78	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	5	2305	U	C5'-C4'-O4'	5.88	116.16	109.10
1	5	4510	A	N9-C1'-C2'	5.88	121.65	114.00
1	5	1894	C	N1-C1'-C2'	5.88	121.65	114.00
8	E	275	ASN	N-CA-CB	5.88	121.19	110.60
1	5	2070	U	N1-C1'-C2'	5.88	121.64	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1324	A	N9-C1'-C2'	5.88	121.64	114.00
1	5	4201	G	N9-C1'-C2'	5.87	121.63	114.00
1	5	4763	U	O4'-C1'-N1	5.87	112.90	108.20
1	5	2305	U	O4'-C4'-C3'	-5.87	98.13	104.00
1	5	4215	C	O4'-C1'-C2'	-5.86	99.94	105.80
12	I	94	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	5	33	A	N9-C1'-C2'	5.86	121.62	114.00
1	5	1487	G	C2'-C3'-O3'	5.85	123.07	113.70
14	L	34	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	5	4199	C	O4'-C1'-C2'	-5.85	99.95	105.80
1	5	2268	A	O4'-C1'-N9	-5.84	103.53	108.20
11	H	54	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	5	4481	U	C5'-C4'-O4'	5.84	116.10	109.10
1	5	934	C	O4'-C1'-N1	-5.83	103.53	108.20
1	5	4548	A	C5'-C4'-O4'	5.83	116.09	109.10
1	5	4074	C	N1-C1'-C2'	5.83	121.57	114.00
3	8	81	C	C5'-C4'-C3'	5.82	125.31	116.00
1	5	2586	G	O4'-C1'-N9	5.82	112.86	108.20
21	S	84	TYR	CB-CG-CD1	5.82	124.49	121.00
33	e	60	TYR	CB-CA-C	5.81	122.03	110.40
1	5	2448	G	N9-C1'-C2'	5.81	121.56	114.00
1	5	1650	A	C4-N9-C1'	-5.81	115.84	126.30
27	Y	121	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	5	657	C	C2'-C3'-O3'	5.81	122.99	113.70
1	5	85	G	N9-C1'-C2'	-5.80	105.62	112.00
1	5	1341	U	N1-C1'-C2'	5.80	121.54	114.00
1	5	920	C	C5'-C4'-O4'	5.80	116.06	109.10
3	8	34	U	C3'-C2'-C1'	5.80	106.14	101.50
1	5	72	C	C1'-O4'-C4'	-5.79	105.26	109.90
1	5	4463	U	O4'-C1'-N1	5.79	112.84	108.20
1	5	2553	A	C1'-O4'-C4'	-5.78	105.27	109.90
5	B	117	ARG	CG-CD-NE	-5.78	99.66	111.80
12	I	119	PHE	CB-CG-CD2	-5.78	116.75	120.80
1	5	1815	G	C1'-O4'-C4'	-5.78	105.28	109.90
1	5	197	A	N9-C1'-C2'	5.77	121.51	114.00
36	h	119	PHE	CB-CG-CD2	-5.77	116.76	120.80
44	p	14	TYR	CB-CA-C	5.77	121.94	110.40
1	5	4481	U	N1-C1'-C2'	5.77	121.50	114.00
1	5	4473	A	C8-N9-C1'	-5.76	117.33	127.70
34	f	6	TRP	N-CA-C	-5.76	95.44	111.00
1	5	2807	A	C2'-C3'-O3'	5.76	122.92	113.70
3	8	115	G	C2'-C3'-O3'	5.76	122.91	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Q	32	TYR	CA-CB-CG	5.76	124.34	113.40
16	N	30	TYR	N-CA-CB	-5.75	100.24	110.60
1	5	1506	G	N9-C1'-C2'	-5.75	105.68	112.00
21	S	97	TYR	CA-CB-CG	-5.75	102.48	113.40
1	5	292	G	C4-N9-C1'	-5.74	119.03	126.50
1	5	2769	U	O4'-C1'-N1	5.74	112.80	108.20
1	5	3691	G	N9-C1'-C2'	5.74	121.47	114.00
1	5	3686	G	N9-C1'-C2'	-5.74	105.69	112.00
3	8	135	C	N1-C1'-C2'	5.74	121.46	114.00
1	5	85	G	O4'-C1'-C2'	-5.73	100.07	105.80
1	5	88	A	N9-C1'-C2'	5.73	121.45	114.00
1	5	1398	A	O5'-P-OP1	5.73	117.58	110.70
8	E	268	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	5	4125	C	C4'-C3'-O3'	-5.72	97.38	109.40
4	A	147	ARG	NE-CZ-NH1	5.72	123.16	120.30
4	A	63	PHE	CB-CG-CD2	-5.72	116.80	120.80
1	5	236	G	N9-C1'-C2'	5.72	121.43	114.00
1	5	1398	A	O4'-C1'-N9	5.71	112.77	108.20
1	5	4385	A	C2'-C3'-O3'	-5.71	96.93	109.50
3	8	79	G	N9-C1'-C2'	5.71	121.43	114.00
27	Y	18	HIS	N-CA-CB	5.71	120.89	110.60
1	5	1285	U	O4'-C1'-N1	5.71	112.77	108.20
4	A	34	PHE	N-CA-CB	5.71	120.87	110.60
1	5	1264	C	C2'-C3'-O3'	5.70	122.83	113.70
1	5	2118	G	O4'-C4'-C3'	-5.70	98.30	104.00
1	5	2119	C	C1'-O4'-C4'	-5.70	105.34	109.90
1	5	2643	G	C2'-C3'-O3'	5.70	122.82	113.70
9	F	100	ILE	CG1-CB-CG2	5.70	123.94	111.40
1	5	2360	A	N9-C1'-C2'	5.70	121.41	114.00
9	F	136	ARG	CG-CD-NE	-5.70	99.83	111.80
1	5	1438	U	C2'-C3'-O3'	5.69	122.81	113.70
19	Q	68	ARG	NE-CZ-NH2	-5.69	117.45	120.30
8	E	278	TYR	CB-CG-CD1	-5.69	117.58	121.00
6	C	200	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	5	703	G	C1'-O4'-C4'	-5.68	105.35	109.90
20	R	97	ARG	CG-CD-NE	-5.68	99.86	111.80
1	5	111	C	N1-C1'-C2'	-5.68	105.75	112.00
1	5	2282	A	N9-C1'-C2'	5.68	121.39	114.00
1	5	1696	C	C2'-C3'-O3'	5.68	122.79	113.70
27	Y	61	HIS	N-CA-CB	5.68	120.82	110.60
1	5	2405	G	N9-C1'-C2'	-5.68	105.76	112.00
4	A	37	ARG	CG-CD-NE	-5.68	99.88	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	370	U	N1-C1'-C2'	5.67	121.38	114.00
1	5	1849	U	O5'-P-OP1	5.67	117.51	110.70
7	D	35	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	5	84	A	C4-N9-C1'	-5.67	116.09	126.30
30	b	17	HIS	CB-CA-C	-5.67	99.06	110.40
38	j	27	TYR	N-CA-CB	5.67	120.80	110.60
6	C	350	ARG	NE-CZ-NH2	-5.66	117.47	120.30
26	X	137	TYR	CB-CG-CD1	5.66	124.40	121.00
8	E	101	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	5	100	C	C5'-C4'-O4'	5.65	115.88	109.10
1	5	1876	U	C2'-C3'-O3'	5.65	122.74	113.70
1	5	4114	C	N1-C1'-C2'	5.65	121.34	114.00
2	7	7	G	C5'-C4'-O4'	5.65	115.88	109.10
21	S	10	TYR	CB-CG-CD1	-5.65	117.61	121.00
33	e	75	ARG	CG-CD-NE	-5.65	99.94	111.80
11	H	180	TYR	CA-CB-CG	5.65	124.13	113.40
1	5	1494	U	N1-C1'-C2'	5.64	121.34	114.00
1	5	3776	G	N9-C1'-C2'	-5.64	105.79	112.00
1	5	1281	G	C5'-C4'-O4'	5.64	115.87	109.10
1	5	5062	G	P-O5'-C5'	5.64	129.93	120.90
40	l	12	PHE	CB-CG-CD2	-5.64	116.85	120.80
19	Q	176	ARG	CG-CD-NE	-5.64	99.95	111.80
1	5	1642	A	P-O3'-C3'	5.64	126.47	119.70
1	5	1639	U	N1-C1'-C2'	5.64	121.33	114.00
1	5	4966	A	C8-N9-C1'	-5.63	117.56	127.70
1	5	2383	C	N1-C1'-C2'	5.63	121.32	114.00
1	5	490	C	N1-C1'-C2'	5.63	121.32	114.00
5	B	169	ARG	CG-CD-NE	5.63	123.62	111.80
1	5	514	U	C4'-C3'-O3'	5.63	124.25	113.00
6	C	311	ARG	CG-CD-NE	-5.62	99.99	111.80
21	S	94	TYR	CA-CB-CG	-5.62	102.72	113.40
1	5	4753	U	C2'-C3'-O3'	5.62	122.68	113.70
38	j	66	HIS	CA-CB-CG	-5.61	104.06	113.60
1	5	85	G	O4'-C1'-N9	5.61	112.69	108.20
1	5	2665	U	N1-C1'-C2'	-5.61	105.83	112.00
1	5	2686	G	N9-C1'-C2'	-5.61	105.83	112.00
1	5	3773	U	N1-C1'-C2'	-5.61	105.83	112.00
28	Z	121	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	5	2077	C	N1-C1'-C2'	-5.60	105.83	112.00
1	5	4950	U	N1-C1'-C2'	5.60	121.28	114.00
5	B	169	ARG	NE-CZ-NH2	-5.60	117.50	120.30
5	B	246	ARG	NE-CZ-NH1	5.60	123.10	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	57	TRP	CA-CB-CG	-5.60	103.06	113.70
1	5	1539	G	C2'-C3'-O3'	5.60	122.66	113.70
1	5	1295	C	N1-C1'-C2'	5.60	121.28	114.00
10	G	235	ARG	NE-CZ-NH2	-5.60	117.50	120.30
20	R	110	ARG	NE-CZ-NH1	5.60	123.10	120.30
14	L	7	GLY	N-CA-C	-5.60	99.11	113.10
1	5	1932	A	N9-C1'-C2'	5.59	121.27	114.00
1	5	118	C	C2'-C3'-O3'	5.59	122.65	113.70
1	5	2857	A	C1'-C2'-O2'	-5.59	93.82	110.60
3	8	39	G	N9-C1'-C2'	-5.59	105.85	112.00
45	r	21	ASN	CB-CA-C	5.59	121.58	110.40
1	5	2487	G	C2'-C3'-O3'	5.59	122.64	113.70
1	5	3773	U	C4'-C3'-C2'	-5.59	97.01	102.60
1	5	2088	A	N9-C1'-C2'	-5.58	105.86	112.00
12	I	213	HIS	CB-CA-C	5.58	121.56	110.40
23	U	101	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	5	3663	A	O4'-C1'-N9	-5.58	103.74	108.20
19	Q	32	TYR	CB-CG-CD2	-5.58	117.65	121.00
35	g	9	ARG	CG-CD-NE	-5.58	100.08	111.80
1	5	4693	C	O4'-C4'-C3'	-5.58	98.42	104.00
1	5	1614	C	N1-C1'-C2'	-5.58	105.87	112.00
11	H	115	ARG	CG-CD-NE	-5.57	100.10	111.80
14	L	6	ASN	N-CA-CB	5.57	120.63	110.60
1	5	977	C	C4'-C3'-C2'	-5.57	97.03	102.60
16	N	182	HIS	N-CA-CB	5.57	120.63	110.60
19	Q	178	ARG	CG-CD-NE	-5.57	100.11	111.80
1	5	1521	C	C2'-C3'-O3'	5.57	122.61	113.70
7	D	210	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	5	2474	G	C2'-C3'-O3'	5.56	122.60	113.70
1	5	1632	A	O4'-C1'-N9	5.56	112.65	108.20
1	5	4723	A	C5'-C4'-O4'	5.56	115.77	109.10
2	7	75	G	O4'-C1'-N9	5.56	112.64	108.20
9	F	72	ARG	NE-CZ-NH2	-5.55	117.52	120.30
28	Z	28	ASN	N-CA-C	-5.55	96.01	111.00
1	5	956	A	N9-C1'-C2'	-5.55	105.90	112.00
1	5	1631	A	C5'-C4'-O4'	5.55	115.76	109.10
1	5	1534	A	P-O5'-C5'	5.54	129.77	120.90
1	5	4326	G	N9-C1'-C2'	5.54	121.21	114.00
1	5	1398	A	C2'-C3'-O3'	5.54	122.57	113.70
1	5	4767	C	C2'-C3'-O3'	5.54	122.57	113.70
19	Q	104	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	5	2396	A	N9-C1'-C2'	5.54	121.20	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2468	U	C4'-C3'-O3'	5.54	124.08	113.00
1	5	1672	U	C6-N1-C1'	-5.54	113.45	121.20
1	5	1827	C	N1-C1'-C2'	5.53	121.19	114.00
1	5	1734	G	N9-C1'-C2'	-5.53	105.92	112.00
44	p	18	TYR	CA-CB-CG	5.53	123.91	113.40
1	5	3735	G	C4'-C3'-O3'	-5.53	97.79	109.40
14	L	163	ARG	NE-CZ-NH1	5.53	123.06	120.30
29	a	61	TYR	N-CA-C	-5.53	96.08	111.00
1	5	1359	G	N9-C1'-C2'	5.52	121.18	114.00
4	A	211	PHE	CB-CG-CD2	-5.52	116.93	120.80
1	5	687	U	N1-C1'-C2'	-5.52	105.93	112.00
1	5	1501	C	C1'-O4'-C4'	-5.52	105.48	109.90
1	5	2754	G	N9-C1'-C2'	-5.52	105.93	112.00
21	S	152	PHE	CB-CG-CD2	-5.52	116.94	120.80
33	e	35	TRP	CB-CG-CD1	-5.52	119.82	127.00
1	5	2398	U	C2'-C3'-O3'	5.52	122.53	113.70
1	5	3886	G	N9-C1'-C2'	-5.52	105.93	112.00
43	o	26	TYR	CB-CG-CD1	5.52	124.31	121.00
1	5	2450	G	N9-C1'-C2'	-5.51	105.94	112.00
1	5	2673	G	C1'-O4'-C4'	-5.51	105.49	109.90
1	5	2360	A	O4'-C1'-N9	-5.51	103.79	108.20
1	5	4076	G	C1'-O4'-C4'	-5.51	105.49	109.90
45	r	45	HIS	N-CA-CB	-5.51	100.68	110.60
1	5	4944	C	N1-C1'-C2'	5.51	121.16	114.00
19	Q	184	ARG	CB-CG-CD	5.51	125.93	111.60
23	U	90	TYR	CB-CA-C	-5.51	99.38	110.40
1	5	4731	G	N9-C1'-C2'	5.50	121.16	114.00
1	5	3667	C	C2'-C3'-O3'	5.50	122.50	113.70
1	5	977	C	C5'-C4'-O4'	5.50	115.70	109.10
1	5	1282	G	O5'-P-OP2	5.50	117.30	110.70
1	5	4909	A	C1'-O4'-C4'	-5.50	105.50	109.90
1	5	2385	U	N1-C1'-C2'	5.49	121.14	114.00
9	F	98	ARG	NE-CZ-NH1	5.49	123.05	120.30
19	Q	75	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	5	4076	G	O4'-C1'-N9	5.49	112.59	108.20
1	5	4975	G	O4'-C1'-N9	5.49	112.59	108.20
33	e	36	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	5	1626	G	N9-C1'-C2'	-5.48	105.97	112.00
1	5	3912	U	C1'-C2'-O2'	-5.48	94.15	110.60
1	5	2858	A	N9-C1'-C2'	5.48	121.13	114.00
1	5	3906	A	N9-C1'-C2'	-5.48	105.97	112.00
31	c	78	ASN	N-CA-CB	5.48	120.47	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	278	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	5	1211	G	N9-C1'-C2'	-5.47	105.98	112.00
8	E	153	HIS	N-CA-CB	-5.47	100.75	110.60
1	5	4978	G	N9-C1'-C2'	5.47	121.11	114.00
1	5	2583	C	C2'-C3'-O3'	5.47	122.45	113.70
45	r	103	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	5	210	C	N1-C1'-C2'	5.47	121.11	114.00
1	5	3634	G	C2'-C3'-O3'	5.47	122.45	113.70
1	5	2056	G	N9-C1'-C2'	-5.46	105.99	112.00
1	5	398	A	N9-C1'-C2'	5.46	121.10	114.00
1	5	3905	A	N9-C1'-C2'	-5.46	105.99	112.00
1	5	4873	G	N9-C1'-C2'	5.46	121.10	114.00
40	l	45	ARG	CB-CG-CD	5.46	125.80	111.60
1	5	2852	U	O4'-C1'-C2'	-5.46	100.34	105.80
1	5	421	C	C2'-C3'-O3'	5.45	122.42	113.70
1	5	4713	G	C2'-C3'-O3'	5.45	122.42	113.70
33	e	43	ASN	CB-CA-C	5.45	121.30	110.40
1	5	3898	G	C2'-C3'-O3'	5.45	122.42	113.70
1	5	372	A	N9-C1'-C2'	5.45	121.08	114.00
19	Q	26	ARG	NE-CZ-NH1	5.44	123.02	120.30
8	E	129	PHE	CB-CG-CD1	5.44	124.61	120.80
20	R	108	ARG	CD-NE-CZ	5.44	131.22	123.60
1	5	3875	G	C2'-C3'-O3'	5.44	122.40	113.70
34	f	6	TRP	CB-CA-C	5.44	121.28	110.40
1	5	2117	G	O4'-C4'-C3'	-5.44	98.56	104.00
4	A	16	PHE	CB-CA-C	5.43	121.27	110.40
13	J	54	ARG	NE-CZ-NH1	5.43	123.02	120.30
26	X	117	TYR	CB-CA-C	5.43	121.27	110.40
1	5	693	C	C2'-C3'-O3'	5.43	122.39	113.70
24	V	14	PHE	CB-CG-CD2	-5.43	117.00	120.80
33	e	47	ARG	NE-CZ-NH2	-5.43	117.58	120.30
10	G	49	ARG	CG-CD-NE	-5.43	100.40	111.80
1	5	1365	C	C4'-C3'-O3'	5.42	123.85	113.00
1	5	1724	G	C8-N9-C1'	-5.42	119.95	127.00
1	5	4481	U	C2-N1-C1'	5.42	124.21	117.70
37	i	26	HIS	N-CA-CB	5.42	120.36	110.60
1	5	2268	A	C2'-C3'-O3'	5.42	122.37	113.70
1	5	2054	U	C1'-O4'-C4'	-5.42	105.57	109.90
1	5	2325	C	O4'-C1'-C2'	-5.42	100.38	105.80
21	S	171	ARG	CG-CD-NE	5.42	123.17	111.80
1	5	4915	G	C2'-C3'-O3'	5.41	122.36	113.70
5	B	119	TYR	CB-CA-C	5.41	121.22	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	280	G	C1'-O4'-C4'	-5.41	105.57	109.90
1	5	4745	G	N9-C1'-C2'	5.41	121.03	114.00
1	5	4909	A	O4'-C1'-N9	5.41	112.53	108.20
13	J	32	ARG	CG-CD-NE	-5.41	100.45	111.80
17	O	128	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	5	4579	U	C6-N1-C1'	-5.40	113.64	121.20
1	5	293	G	C2'-C3'-O3'	5.40	122.34	113.70
37	i	29	ARG	NE-CZ-NH1	5.40	123.00	120.30
18	P	42	ARG	CG-CD-NE	5.40	123.14	111.80
21	S	28	TYR	CA-CB-CG	5.40	123.65	113.40
1	5	1975	G	O4'-C1'-N9	-5.39	103.88	108.20
1	5	1464	C	N1-C1'-C2'	-5.39	106.07	112.00
1	5	3625	G	C4'-C3'-O3'	-5.39	98.08	109.40
1	5	2272	C	C1'-C2'-O2'	-5.39	94.43	110.60
30	b	6	ASN	CB-CA-C	5.39	121.18	110.40
1	5	1852	U	N1-C1'-C2'	-5.39	106.07	112.00
1	5	3648	A	C1'-O4'-C4'	-5.39	105.59	109.90
1	5	4280	A	C4'-C3'-C2'	-5.39	97.21	102.60
1	5	4975	G	N9-C1'-C2'	-5.38	106.08	112.00
1	5	1588	U	N1-C1'-C2'	5.38	121.00	114.00
5	B	117	ARG	NE-CZ-NH1	5.38	122.99	120.30
33	e	36	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	5	2014	C	C2'-C3'-O3'	5.38	122.31	113.70
3	8	68	G	N9-C1'-C2'	5.38	120.99	114.00
16	N	114	ARG	NE-CZ-NH2	-5.37	117.61	120.30
4	A	19	HIS	N-CA-CB	-5.37	100.94	110.60
1	5	1667	G	C2'-C3'-O3'	5.37	122.29	113.70
21	S	81	TRP	N-CA-C	-5.37	96.51	111.00
1	5	82	U	N1-C1'-C2'	-5.37	106.10	112.00
8	E	236	TYR	CA-CB-CG	-5.36	103.21	113.40
16	N	192	TRP	N-CA-CB	-5.36	100.95	110.60
20	R	60	ARG	NE-CZ-NH1	5.36	122.98	120.30
7	D	66	TYR	CB-CG-CD1	5.36	124.22	121.00
26	X	129	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	5	3626	G	N9-C1'-C2'	-5.36	106.11	112.00
2	7	59	G	N9-C1'-C2'	-5.36	106.11	112.00
12	I	139	ARG	CB-CG-CD	-5.35	97.69	111.60
1	5	215	C	C4'-C3'-O3'	-5.35	98.17	109.40
1	5	1390	G	N9-C1'-C2'	-5.35	106.12	112.00
18	P	30	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	5	911	U	C2'-C3'-O3'	5.34	122.25	113.70
1	5	2348	G	O4'-C1'-N9	-5.34	103.93	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	3590	G	C2'-C3'-O3'	5.34	122.25	113.70
8	E	212	TYR	CA-CB-CG	5.34	123.55	113.40
11	H	115	ARG	CA-CB-CG	5.34	125.15	113.40
7	D	20	PHE	CB-CA-C	5.34	121.08	110.40
41	m	106	ARG	NE-CZ-NH1	5.34	122.97	120.30
12	I	98	ARG	NE-CZ-NH2	5.34	122.97	120.30
24	V	97	TYR	CB-CA-C	5.34	121.08	110.40
1	5	1272	C	O4'-C1'-C2'	-5.33	100.47	105.80
36	h	70	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	5	703	G	N9-C1'-C2'	-5.33	106.14	112.00
26	X	79	PHE	CB-CG-CD1	5.33	124.53	120.80
1	5	4883	C	O4'-C1'-N1	5.32	112.46	108.20
1	5	416	U	N1-C1'-C2'	5.32	120.91	114.00
22	T	140	PHE	CB-CA-C	-5.31	99.78	110.40
16	N	192	TRP	CB-CG-CD1	-5.31	120.10	127.00
19	Q	168	ARG	NE-CZ-NH1	5.31	122.95	120.30
36	h	72	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	5	3753	G	C2'-C3'-O3'	5.31	122.19	113.70
19	Q	174	PHE	CB-CG-CD1	-5.31	117.09	120.80
1	5	1632	A	N9-C1'-C2'	-5.30	106.17	112.00
1	5	4497	U	C2'-C3'-O3'	5.30	122.19	113.70
1	5	212	A	N9-C1'-C2'	5.30	120.89	114.00
5	B	62	ARG	NE-CZ-NH2	-5.30	117.65	120.30
9	F	228	HIS	CA-CB-CG	-5.30	104.59	113.60
1	5	4302	U	N1-C1'-C2'	-5.30	106.17	112.00
9	F	136	ARG	CA-CB-CG	5.30	125.06	113.40
32	d	44	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	5	3726	A	N9-C1'-C2'	5.29	120.88	114.00
1	5	3692	A	N9-C1'-C2'	-5.29	106.18	112.00
3	8	34	U	C2-N1-C1'	-5.29	111.35	117.70
40	l	45	ARG	CG-CD-NE	-5.29	100.68	111.80
1	5	1961	G	C4'-C3'-C2'	-5.29	97.31	102.60
5	B	246	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	5	4528	G	O4'-C1'-C2'	-5.29	100.51	105.80
14	L	198	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	5	2056	G	P-O5'-C5'	-5.28	112.45	120.90
1	5	2817	C	C2'-C3'-O3'	5.28	122.16	113.70
16	N	143	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	5	3739	C	C2'-C3'-O3'	5.28	122.14	113.70
27	Y	45	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	5	1390	G	C2'-C3'-O3'	5.27	122.14	113.70
26	X	137	TYR	CA-CB-CG	5.27	123.42	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4228	G	O4'-C1'-N9	5.27	112.42	108.20
1	5	1211	G	C4'-C3'-C2'	-5.27	97.33	102.60
6	C	110	ARG	NE-CZ-NH1	5.26	122.93	120.30
37	i	39	PHE	CB-CG-CD1	-5.26	117.11	120.80
19	Q	75	ARG	CG-CD-NE	5.26	122.84	111.80
27	Y	87	ARG	CD-NE-CZ	5.26	130.96	123.60
1	5	3666	C	N1-C1'-C2'	-5.25	106.22	112.00
1	5	2263	A	C2'-C3'-O3'	5.25	122.10	113.70
1	5	194	C	N1-C1'-C2'	-5.25	106.22	112.00
45	r	77	TYR	CB-CG-CD2	-5.25	117.85	121.00
5	B	119	TYR	CA-CB-CG	-5.25	103.43	113.40
34	f	19	ARG	CG-CD-NE	-5.25	100.78	111.80
24	V	128	LEU	CA-CB-CG	5.24	127.36	115.30
1	5	2262	G	N9-C1'-C2'	5.24	120.81	114.00
1	5	2753	G	C2'-C3'-O3'	5.24	122.08	113.70
1	5	4463	U	O4'-C1'-C2'	-5.24	100.56	105.80
30	b	45	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	5	4736	C	N1-C1'-C2'	5.24	120.81	114.00
1	5	1484	G	O4'-C4'-C3'	-5.23	98.77	104.00
4	A	89	TYR	CB-CA-C	5.23	120.86	110.40
1	5	216	C	C2'-C3'-O3'	5.23	122.06	113.70
1	5	931	C	N1-C1'-C2'	5.23	120.80	114.00
41	m	97	ARG	NE-CZ-NH2	5.23	122.91	120.30
1	5	2467	U	N1-C1'-C2'	-5.23	106.25	112.00
1	5	4966	A	C4-N9-C1'	5.22	135.70	126.30
5	B	25	HIS	CB-CA-C	5.22	120.84	110.40
1	5	2597	G	N9-C1'-C2'	5.22	120.79	114.00
17	O	178	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	5	2325	C	C2'-C3'-O3'	5.21	122.04	113.70
34	f	19	ARG	CA-CB-CG	5.21	124.87	113.40
35	g	14	ASN	N-CA-C	-5.21	96.93	111.00
1	5	2529	A	O4'-C1'-N9	5.21	112.36	108.20
1	5	1	C	C3'-C2'-C1'	-5.20	97.34	101.50
1	5	267	G	C2'-C3'-O3'	5.20	122.03	113.70
9	F	58	HIS	N-CA-CB	5.20	119.97	110.60
1	5	223	G	N9-C1'-C2'	-5.20	106.28	112.00
1	5	1886	G	N9-C1'-C2'	-5.20	106.28	112.00
1	5	2310	C	C2'-C3'-O3'	5.20	122.02	113.70
1	5	2443	G	N9-C1'-C2'	5.20	120.76	114.00
34	f	102	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	5	63	G	N9-C1'-C2'	5.19	120.75	114.00
1	5	664	G	C4'-C3'-O3'	5.19	123.38	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4328	G	N9-C1'-C2'	-5.19	106.29	112.00
13	J	147	ARG	NE-CZ-NH1	5.19	122.89	120.30
34	f	51	TYR	CA-CB-CG	5.19	123.26	113.40
9	F	136	ARG	NE-CZ-NH1	5.19	122.89	120.30
13	J	147	ARG	NE-CZ-NH2	-5.19	117.71	120.30
21	S	77	ASN	CB-CA-C	5.18	120.77	110.40
1	5	1698	C	O5'-P-OP1	-5.18	101.03	105.70
32	d	24	GLU	CA-CB-CG	5.18	124.80	113.40
1	5	172	C	O4'-C1'-C2'	-5.18	100.62	105.80
1	5	1394	G	N9-C1'-C2'	5.18	120.73	114.00
1	5	1642	A	C5'-C4'-O4'	5.18	115.31	109.10
1	5	2044	U	C3'-C2'-C1'	5.18	105.64	101.50
5	B	274	TYR	CB-CG-CD1	-5.18	117.89	121.00
20	R	108	ARG	CG-CD-NE	5.18	122.68	111.80
39	k	16	ARG	NE-CZ-NH1	5.18	122.89	120.30
6	C	143	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	5	4543	G	N9-C1'-C2'	5.18	120.73	114.00
1	5	961	G	C4'-C3'-O3'	5.17	123.34	113.00
7	D	268	ARG	CG-CD-NE	5.17	122.66	111.80
20	R	124	TYR	CA-CB-CG	5.17	123.23	113.40
1	5	2879	A	N9-C1'-C2'	5.17	120.72	114.00
38	j	76	HIS	CB-CA-C	5.17	120.74	110.40
1	5	272	U	N1-C1'-C2'	5.17	120.72	114.00
1	5	4165	C	C2'-C3'-O3'	5.17	121.97	113.70
21	S	29	ARG	CB-CA-C	5.17	120.73	110.40
41	m	97	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	5	1850	A	N9-C1'-C2'	5.17	120.72	114.00
1	5	2323	C	C2'-C3'-O3'	5.16	121.96	113.70
16	N	59	TYR	CA-CB-CG	5.16	123.21	113.40
1	5	2538	U	O5'-P-OP1	-5.16	101.06	105.70
1	5	2256	C	N1-C1'-C2'	5.16	120.70	114.00
1	5	4436	U	N1-C1'-C2'	-5.16	106.33	112.00
14	L	99	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	5	268	G	C2'-C3'-O3'	5.15	121.95	113.70
1	5	405	U	C2'-C3'-O3'	5.15	121.94	113.70
3	8	1	C	C5'-C4'-C3'	5.15	124.24	116.00
28	Z	36	ARG	NE-CZ-NH2	-5.15	117.72	120.30
16	N	63	ARG	NE-CZ-NH2	-5.15	117.73	120.30
19	Q	68	ARG	CG-CD-NE	-5.15	100.99	111.80
34	f	6	TRP	CA-CB-CG	-5.15	103.92	113.70
1	5	2075	G	N9-C1'-C2'	-5.14	106.34	112.00
2	7	6	C	C2'-C3'-O3'	5.14	121.93	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Y	87	ARG	NE-CZ-NH1	-5.14	117.73	120.30
22	T	8	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	8	46	G	N9-C1'-C2'	5.14	120.68	114.00
7	D	130	TYR	CA-CB-CG	-5.14	103.64	113.40
16	N	130	PHE	CB-CA-C	5.14	120.68	110.40
26	X	137	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	5	4163	U	C4'-C3'-C2'	-5.14	97.46	102.60
1	5	658	C	C2'-C3'-O3'	5.13	121.92	113.70
21	S	28	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	5	2785	C	N1-C1'-C2'	5.13	120.67	114.00
9	F	72	ARG	NE-CZ-NH1	5.13	122.86	120.30
33	e	47	ARG	N-CA-C	-5.13	97.15	111.00
20	R	103	ARG	NE-CZ-NH1	5.13	122.86	120.30
35	g	4	ARG	NE-CZ-NH2	-5.13	117.74	120.30
2	7	65	G	C2'-C3'-O3'	5.13	121.90	113.70
14	L	99	ASP	N-CA-C	-5.13	97.16	111.00
1	5	703	G	O4'-C1'-N9	5.12	112.30	108.20
1	5	1577	G	N9-C1'-C2'	-5.12	106.37	112.00
3	8	125	C	O4'-C1'-N1	-5.12	104.11	108.20
21	S	10	TYR	CB-CA-C	5.12	120.64	110.40
1	5	1615	C	N1-C1'-C2'	-5.12	106.37	112.00
9	F	197	TYR	N-CA-CB	5.12	119.81	110.60
1	5	3870	C	N1-C1'-C2'	5.11	120.64	114.00
16	N	65	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	5	3880	G	C1'-C2'-O2'	-5.11	95.28	110.60
1	5	107	G	N9-C1'-C2'	-5.10	106.39	112.00
1	5	4975	G	C1'-O4'-C4'	-5.10	105.82	109.90
4	A	209	HIS	CA-CB-CG	-5.10	104.94	113.60
10	G	53	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	5	2361	G	P-O3'-C3'	5.09	125.81	119.70
1	5	3667	C	N1-C1'-C2'	-5.09	106.40	112.00
27	Y	126	ARG	CD-NE-CZ	5.09	130.73	123.60
1	5	2614	C	N1-C1'-C2'	-5.09	106.40	112.00
7	D	248	ARG	NE-CZ-NH1	5.09	122.85	120.30
20	R	9	ARG	CG-CD-NE	5.09	122.49	111.80
28	Z	36	ARG	CG-CD-NE	5.09	122.49	111.80
1	5	3804	G	N9-C1'-C2'	-5.09	106.40	112.00
1	5	218	A	N9-C1'-C2'	-5.09	106.41	112.00
1	5	297	U	N1-C1'-C2'	-5.09	106.40	112.00
3	8	104	A	P-O5'-C5'	5.09	129.04	120.90
1	5	1359	G	O4'-C4'-C3'	-5.08	98.92	104.00
1	5	4276	G	N9-C1'-C2'	-5.08	106.41	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	85	ARG	CG-CD-NE	5.08	122.47	111.80
1	5	2117	G	C1'-O4'-C4'	-5.08	105.84	109.90
1	5	3666	C	C2'-C3'-O3'	5.08	121.82	113.70
13	J	170	HIS	CB-CA-C	5.08	120.56	110.40
27	Y	87	ARG	CG-CD-NE	5.08	122.46	111.80
45	r	77	TYR	N-CA-CB	-5.07	101.47	110.60
1	5	648	G	C2'-C3'-O3'	5.07	121.81	113.70
1	5	1361	G	C2'-C3'-O3'	5.07	121.81	113.70
1	5	3863	C	N1-C1'-C2'	5.07	120.59	114.00
32	d	87	ARG	N-CA-CB	5.07	119.72	110.60
1	5	1398	A	C3'-C2'-C1'	-5.07	97.45	101.50
1	5	1887	G	C4'-C3'-C2'	-5.07	97.53	102.60
17	O	140	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	5	4670	C	P-O5'-C5'	5.07	129.00	120.90
16	N	143	ARG	CB-CG-CD	5.07	124.77	111.60
19	Q	33	ARG	CB-CG-CD	5.07	124.77	111.60
1	5	2459	G	N9-C1'-C2'	-5.06	106.43	112.00
20	R	117	ARG	CB-CA-C	5.06	120.53	110.40
5	B	257	TRP	N-CA-CB	5.06	119.71	110.60
17	O	117	ARG	NE-CZ-NH2	-5.06	117.77	120.30
27	Y	126	ARG	CG-CD-NE	5.06	122.43	111.80
1	5	4498	U	C1'-C2'-O2'	5.06	125.77	110.60
1	5	54	G	C2'-C3'-O3'	5.05	121.79	113.70
1	5	1268	G	N9-C1'-C2'	5.05	120.57	114.00
1	5	1896	A	N9-C1'-C2'	-5.05	106.44	112.00
1	5	3627	G	C2'-C3'-O3'	5.05	121.79	113.70
27	Y	74	TYR	N-CA-CB	5.05	119.70	110.60
29	a	6	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	5	2787	A	N9-C1'-C2'	-5.05	106.44	112.00
1	5	4936	G	C4'-C3'-O3'	5.05	123.11	113.00
1	5	1216	C	C2'-C3'-O3'	5.05	121.78	113.70
1	5	1672	U	N1-C1'-C2'	5.05	120.57	114.00
1	5	2054	U	N1-C1'-C2'	5.05	120.57	114.00
19	Q	38	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	5	20	U	N1-C1'-C2'	-5.05	106.45	112.00
1	5	352	G	C3'-C2'-C1'	5.05	105.54	101.50
47	2	29	ASP	O-C-N	-5.05	114.62	122.70
1	5	74	G	N9-C1'-C2'	5.05	120.56	114.00
1	5	88	A	C1'-C2'-O2'	-5.05	95.46	110.60
1	5	1963	C	C2'-C3'-O3'	5.04	121.77	113.70
1	5	1067	G	C2'-C3'-O3'	5.04	121.76	113.70
1	5	1281	G	C3'-C2'-C1'	5.04	105.53	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1358	G	O4'-C1'-C2'	-5.04	100.76	105.80
1	5	336	A	N9-C1'-C2'	-5.04	106.46	112.00
1	5	1895	G	N9-C1'-C2'	5.04	120.55	114.00
1	5	4270	C	C5'-C4'-O4'	5.04	115.14	109.10
1	5	1440	U	C4'-C3'-C2'	-5.03	97.57	102.60
22	T	19	PHE	CB-CA-C	-5.03	100.34	110.40
1	5	1947	U	C4'-C3'-O3'	5.03	123.06	113.00
1	5	2275	G	C2'-C3'-O3'	5.03	121.75	113.70
1	5	1591	U	N1-C1'-C2'	5.03	120.53	114.00
1	5	4398	C	C2'-C3'-O3'	5.03	121.75	113.70
14	L	103	ARG	CA-CB-CG	5.03	124.46	113.40
20	R	124	TYR	CB-CG-CD1	5.03	124.02	121.00
5	B	161	ARG	NE-CZ-NH1	5.03	122.81	120.30
12	I	181	PHE	CB-CG-CD1	5.03	124.32	120.80
43	o	78	ARG	CD-NE-CZ	5.03	130.64	123.60
1	5	4404	U	C3'-C2'-C1'	5.02	105.52	101.50
26	X	56	ARG	CG-CD-NE	-5.02	101.25	111.80
1	5	1953	U	N1-C1'-C2'	5.02	120.53	114.00
1	5	2533	C	N1-C1'-C2'	5.02	120.53	114.00
1	5	4373	G	C3'-C2'-C1'	-5.02	97.48	101.50
1	5	4563	U	C2-N1-C1'	5.02	123.72	117.70
33	e	44	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	5	1272	C	C5'-C4'-O4'	5.01	115.12	109.10
1	5	2827	G	O4'-C4'-C3'	-5.01	98.99	104.00
1	5	1479	G	C1'-C2'-O2'	-5.01	95.56	110.60
1	5	1864	G	C2'-C3'-O3'	5.01	121.72	113.70
1	5	4454	G	C2'-C3'-O3'	5.01	121.72	113.70
1	5	4937	C	N1-C1'-C2'	5.01	120.52	114.00
19	Q	33	ARG	N-CA-CB	5.01	119.61	110.60
1	5	514	U	O4'-C4'-C3'	-5.01	98.99	104.00
1	5	2116	C	C2'-C3'-O3'	5.01	121.71	113.70
1	5	3908	A	C3'-C2'-C1'	-5.01	97.49	101.50
1	5	52	G	N9-C1'-C2'	-5.00	106.50	112.00
1	5	4224	A	N9-C1'-C2'	-5.00	106.50	112.00
1	5	1296	G	C1'-O4'-C4'	-5.00	105.90	109.90
5	B	122	TRP	CA-CB-CG	5.00	123.20	113.70
7	D	119	TYR	CB-CA-C	5.00	120.41	110.40
13	J	146	ARG	NE-CZ-NH1	-5.00	117.80	120.30
16	N	6	TYR	CA-CB-CG	-5.00	103.90	113.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	5	1992	U	C1'

All (340) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	1	405	ARG	Sidechain
47	2	29	ASP	Peptide
1	5	100	C	Sidechain
1	5	103	G	Sidechain
1	5	1167	C	Sidechain
1	5	120	A	Sidechain
1	5	1214	C	Sidechain
1	5	1281	G	Sidechain
1	5	1319	U	Sidechain
1	5	1324	A	Sidechain
1	5	1355	G	Sidechain
1	5	1398	A	Sidechain
1	5	147	A	Sidechain
1	5	1501	C	Sidechain
1	5	151	G	Sidechain
1	5	1522	G	Sidechain
1	5	1534	A	Sidechain
1	5	1539	G	Sidechain
1	5	157	U	Sidechain
1	5	1625	G	Sidechain
1	5	1627	G	Sidechain
1	5	1631	A	Sidechain
1	5	1658	G	Sidechain
1	5	1668	A	Sidechain
1	5	1671	U	Sidechain
1	5	1676	C	Sidechain
1	5	172	C	Sidechain
1	5	1733	G	Sidechain
1	5	1887	G	Sidechain
1	5	1894	C	Sidechain
1	5	1938	C	Sidechain
1	5	2035	C	Sidechain
1	5	2037	C	Sidechain
1	5	2046	G	Sidechain
1	5	2056	G	Sidechain
1	5	2077	C	Sidechain
1	5	2082	G	Sidechain
1	5	2087	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	5	22	G	Sidechain
1	5	2263	A	Sidechain
1	5	2268	A	Sidechain
1	5	2271	C	Sidechain
1	5	2305	U	Sidechain
1	5	2325	C	Sidechain
1	5	235	A	Sidechain
1	5	2360	A	Sidechain
1	5	2361	G	Sidechain
1	5	2394	G	Sidechain
1	5	2403	A	Sidechain
1	5	2406	G	Sidechain
1	5	2436	U	Sidechain
1	5	2438	A	Sidechain
1	5	2446	C	Sidechain
1	5	2450	G	Sidechain
1	5	2465	C	Sidechain
1	5	2511	A	Sidechain
1	5	2513	A	Sidechain
1	5	2515	G	Sidechain
1	5	2517	A	Sidechain
1	5	2553	A	Sidechain
1	5	2581	A	Sidechain
1	5	2649	G	Sidechain
1	5	2666	U	Sidechain
1	5	2675	G	Sidechain
1	5	2769	U	Sidechain
1	5	2796	G	Sidechain
1	5	280	G	Sidechain
1	5	2812	A	Sidechain
1	5	2827	G	Sidechain
1	5	2851	G	Sidechain
1	5	2858	A	Sidechain
1	5	291	U	Sidechain
1	5	292	G	Sidechain
1	5	293	G	Sidechain
1	5	294	G	Sidechain
1	5	31	U	Sidechain
1	5	315	G	Sidechain
1	5	332	C	Sidechain
1	5	336	A	Sidechain
1	5	352	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	5	354	U	Sidechain
1	5	3621	A	Sidechain
1	5	3635	A	Sidechain
1	5	3648	A	Sidechain
1	5	3653	A	Sidechain
1	5	3692	A	Sidechain
1	5	3726	A	Sidechain
1	5	3774	A	Sidechain
1	5	3790	U	Sidechain
1	5	3791	C	Sidechain
1	5	383	A	Sidechain
1	5	384	A	Sidechain
1	5	3843	C	Sidechain
1	5	3844	U	Sidechain
1	5	3871	A	Sidechain
1	5	3880	G	Sidechain
1	5	3881	G	Sidechain
1	5	3901	A	Sidechain
1	5	3938	G	Sidechain
1	5	405	U	Sidechain
1	5	4076	G	Sidechain
1	5	4162	C	Sidechain
1	5	417	G	Sidechain
1	5	42	A	Sidechain
1	5	4228	G	Sidechain
1	5	4229	U	Sidechain
1	5	4234	A	Sidechain
1	5	4239	A	Sidechain
1	5	4270	C	Sidechain
1	5	4275	G	Sidechain
1	5	4280	A	Sidechain
1	5	4282	A	Sidechain
1	5	43	U	Sidechain
1	5	4330	G	Sidechain
1	5	4341	C	Sidechain
1	5	4371	G	Sidechain
1	5	4373	G	Sidechain
1	5	4385	A	Sidechain
1	5	4463	U	Sidechain
1	5	4464	A	Sidechain
1	5	4497	U	Sidechain
1	5	4498	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	5	4510	A	Sidechain
1	5	4519	C	Sidechain
1	5	4528	G	Sidechain
1	5	4531	U	Sidechain
1	5	4548	A	Sidechain
1	5	4563	U	Sidechain
1	5	4564	A	Sidechain
1	5	4589	A	Sidechain
1	5	4600	G	Sidechain
1	5	4670	C	Sidechain
1	5	4677	U	Sidechain
1	5	4693	C	Sidechain
1	5	4763	U	Sidechain
1	5	4871	C	Sidechain
1	5	4911	A	Sidechain
1	5	4965	U	Sidechain
1	5	4966	A	Sidechain
1	5	4976	U	Sidechain
1	5	4981	G	Sidechain
1	5	5006	U	Sidechain
1	5	5040	U	Sidechain
1	5	5043	A	Sidechain
1	5	5050	C	Sidechain
1	5	5066	U	Sidechain
1	5	514	U	Sidechain
1	5	53	C	Sidechain
1	5	54	G	Sidechain
1	5	62	A	Sidechain
1	5	664	G	Sidechain
1	5	84	A	Sidechain
1	5	85	G	Sidechain
1	5	89	C	Sidechain
1	5	92	C	Sidechain
1	5	93	G	Sidechain
1	5	94	A	Sidechain
1	5	964	A	Sidechain
1	5	97	G	Sidechain
1	5	99	A	Sidechain
2	7	42	A	Sidechain
2	7	56	G	Sidechain
3	8	104	A	Sidechain
3	8	14	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	8	34	U	Sidechain
3	8	35	C	Sidechain
3	8	38	U	Sidechain
3	8	39	G	Sidechain
3	8	60	G	Sidechain
3	8	65	A	Sidechain
3	8	73	U	Sidechain
3	8	9	A	Sidechain
3	8	94	G	Sidechain
4	A	18	ALA	Peptide
4	A	194	ASN	Peptide
4	A	196	TRP	Peptide
4	A	209	HIS	Sidechain
4	A	211	PHE	Sidechain
4	A	215	ASN	Peptide
5	B	100	ARG	Sidechain
5	B	102	PHE	Peptide
5	B	117	ARG	Sidechain
5	B	119	TYR	Sidechain
5	B	142	GLY	Peptide
5	B	15	GLY	Peptide
5	B	16	PHE	Peptide
5	B	179	HIS	Sidechain
5	B	274	TYR	Sidechain
5	B	322	HIS	Peptide
5	B	379	PHE	Peptide
5	B	387	ALA	Peptide
5	B	388	PHE	Peptide
6	C	102	PHE	Sidechain
6	C	113	ARG	Peptide
6	C	264	TYR	Peptide
6	C	309	ILE	Peptide
6	C	41	HIS	Sidechain
7	D	129	GLU	Peptide
7	D	190	PHE	Peptide
7	D	198	HIS	Sidechain
7	D	20	PHE	Peptide
7	D	261	VAL	Peptide
7	D	266	TRP	Peptide
7	D	30	TYR	Peptide
7	D	44	TYR	Sidechain
8	E	102	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	E	103	VAL	Peptide
8	E	111	TYR	Peptide
8	E	123	SER	Peptide
8	E	152	ARG	Peptide
8	E	177	LEU	Peptide
8	E	216	LYS	Peptide
8	E	224	GLN	Peptide
8	E	230	ASP	Peptide
8	E	235	LYS	Peptide
8	E	278	TYR	Sidechain
8	E	41	SER	Peptide
9	F	127	LEU	Peptide
9	F	197	TYR	Peptide
9	F	228	HIS	Sidechain
9	F	81	GLY	Peptide
9	F	82	ASN	Peptide
10	G	101	LYS	Peptide
10	G	261	LEU	Peptide
10	G	54	PHE	Sidechain
11	H	156	ASN	Sidechain,Peptide
11	H	50	LYS	Peptide
12	I	113	THR	Peptide
12	I	139	ARG	Sidechain
12	I	158	LYS	Peptide
12	I	77	VAL	Peptide
12	I	93	PRO	Peptide
13	J	87	LEU	Peptide
13	J	99	PHE	Sidechain
14	L	146	LEU	Peptide
14	L	147	ALA	Peptide
14	L	192	PHE	Sidechain
14	L	62	PRO	Peptide
14	L	66	TYR	Peptide
15	M	6	PHE	Sidechain
15	M	65	PRO	Peptide
15	M	79	LYS	Peptide
15	M	94	LYS	Peptide
16	N	119	TYR	Sidechain
16	N	130	PHE	Sidechain
16	N	131	GLU	Sidechain
16	N	138	PHE	Peptide
16	N	139	HIS	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
16	N	180	PHE	Sidechain
16	N	184	ILE	Peptide
16	N	202	ARG	Peptide
16	N	37	HIS	Sidechain
16	N	90	ASN	Peptide
16	N	94	PHE	Sidechain
17	O	110	PRO	Peptide
17	O	117	ARG	Peptide
17	O	135	PHE	Sidechain
18	P	139	TYR	Sidechain
19	Q	161	SER	Peptide
19	Q	162	HIS	Peptide
19	Q	174	PHE	Sidechain
19	Q	32	TYR	Peptide
19	Q	34	PHE	Sidechain
20	R	118	HIS	Sidechain
20	R	132	PHE	Sidechain
20	R	174	GLU	Peptide
20	R	19	LYS	Peptide
20	R	57	VAL	Peptide
20	R	94	THR	Peptide
21	S	10	TYR	Sidechain
21	S	145	PHE	Sidechain,Peptide
21	S	152	PHE	Peptide
21	S	154	LEU	Peptide
21	S	159	LEU	Peptide
21	S	164	LYS	Peptide
21	S	32	ILE	Peptide
21	S	33	PHE	Peptide
21	S	68	PHE	Peptide
21	S	90	THR	Peptide
22	T	140	PHE	Sidechain
22	T	142	ARG	Peptide
23	U	110	TYR	Peptide
23	U	55	ASN	Peptide
24	V	108	ASN	Peptide
24	V	97	TYR	Sidechain
24	V	98	PHE	Sidechain
25	W	27	LYS	Peptide
26	X	73	HIS	Sidechain
27	Y	18	HIS	Sidechain
27	Y	61	HIS	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
27	Y	62	TYR	Peptide
27	Y	81	TYR	Sidechain
29	a	109	TYR	Sidechain
29	a	128	PHE	Sidechain
29	a	34	ASN	Sidechain
29	a	39	HIS	Peptide
29	a	60	HIS	Sidechain
29	a	61	TYR	Sidechain,Peptide
29	a	62	HIS	Sidechain
29	a	91	ALA	Peptide
30	b	6	ASN	Sidechain
31	c	77	ASN	Peptide
31	c	78	ASN	Sidechain
32	d	103	TYR	Peptide
32	d	108	TYR	Peptide
32	d	25	TYR	Sidechain
32	d	72	VAL	Peptide
33	e	20	PHE	Sidechain
33	e	3	ALA	Peptide
33	e	74	PHE	Sidechain
33	e	76	LYS	Peptide
34	f	100	ARG	Peptide
34	f	53	ALA	Peptide
35	g	6	THR	Peptide
36	h	121	VAL	Peptide
36	h	78	TYR	Sidechain
36	h	97	LYS	Peptide
37	i	26	HIS	Sidechain
37	i	39	PHE	Sidechain
37	i	49	GLY	Peptide
38	j	46	LYS	Peptide
38	j	48	ASN	Peptide
38	j	66	HIS	Sidechain
38	j	8	PHE	Sidechain
39	k	28	ASN	Peptide
43	o	31	ASP	Sidechain,Peptide
43	o	43	ARG	Peptide
43	o	47	GLY	Peptide
43	o	48	TYR	Sidechain
43	o	76	ASN	Peptide
44	p	17	ARG	Peptide
45	r	30	ASN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
45	r	31	ASN	Sidechain
45	r	45	HIS	Sidechain
45	r	70	GLN	Peptide
45	r	76	SER	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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
4	A	242/257 (94%)	203 (84%)	30 (12%)	9 (4%)	2 16
5	B	392/394 (100%)	319 (81%)	40 (10%)	33 (8%)	0 4
6	C	365/367 (100%)	304 (83%)	46 (13%)	15 (4%)	2 15
7	D	290/297 (98%)	235 (81%)	33 (11%)	22 (8%)	1 5
8	E	232/236 (98%)	150 (65%)	51 (22%)	31 (13%)	0 1
9	F	223/225 (99%)	190 (85%)	23 (10%)	10 (4%)	2 13
10	G	239/266 (90%)	200 (84%)	32 (13%)	7 (3%)	3 19
11	H	188/192 (98%)	164 (87%)	20 (11%)	4 (2%)	5 24
12	I	211/213 (99%)	168 (80%)	30 (14%)	13 (6%)	1 8
13	J	168/178 (94%)	137 (82%)	23 (14%)	8 (5%)	2 12
14	L	208/211 (99%)	172 (83%)	25 (12%)	11 (5%)	1 10
15	M	136/213 (64%)	118 (87%)	16 (12%)	2 (2%)	8 30
16	N	201/204 (98%)	172 (86%)	23 (11%)	6 (3%)	3 19
17	O	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	8 30
18	P	151/153 (99%)	140 (93%)	9 (6%)	2 (1%)	10 33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	Q	185/188 (98%)	160 (86%)	20 (11%)	5 (3%)	4 21
20	R	178/196 (91%)	153 (86%)	21 (12%)	4 (2%)	5 24
21	S	173/224 (77%)	146 (84%)	24 (14%)	3 (2%)	7 28
22	T	157/160 (98%)	128 (82%)	26 (17%)	3 (2%)	6 26
23	U	97/128 (76%)	74 (76%)	21 (22%)	2 (2%)	5 24
24	V	129/140 (92%)	112 (87%)	14 (11%)	3 (2%)	5 23
25	W	61/157 (39%)	57 (93%)	3 (5%)	1 (2%)	8 29
26	X	117/156 (75%)	108 (92%)	7 (6%)	2 (2%)	7 28
27	Y	132/145 (91%)	112 (85%)	14 (11%)	6 (4%)	2 13
28	Z	133/136 (98%)	113 (85%)	15 (11%)	5 (4%)	2 15
29	a	145/148 (98%)	111 (77%)	26 (18%)	8 (6%)	1 10
30	b	73/160 (46%)	58 (80%)	11 (15%)	4 (6%)	1 10
31	c	92/115 (80%)	78 (85%)	10 (11%)	4 (4%)	2 14
32	d	105/125 (84%)	85 (81%)	16 (15%)	4 (4%)	2 15
33	e	126/135 (93%)	110 (87%)	15 (12%)	1 (1%)	16 44
34	f	107/110 (97%)	95 (89%)	7 (6%)	5 (5%)	2 12
35	g	112/117 (96%)	103 (92%)	7 (6%)	2 (2%)	7 27
36	h	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	4 22
37	i	100/105 (95%)	91 (91%)	7 (7%)	2 (2%)	6 25
38	j	84/86 (98%)	67 (80%)	13 (16%)	4 (5%)	2 12
39	k	67/70 (96%)	55 (82%)	7 (10%)	5 (8%)	1 5
40	l	48/51 (94%)	42 (88%)	4 (8%)	2 (4%)	2 14
41	m	50/128 (39%)	44 (88%)	6 (12%)	0	100 100
42	n	21/25 (84%)	21 (100%)	0	0	100 100
43	o	102/106 (96%)	85 (83%)	11 (11%)	6 (6%)	1 8
44	p	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	12 37
45	r	123/125 (98%)	97 (79%)	20 (16%)	6 (5%)	2 11
46	1	384/476 (81%)	325 (85%)	42 (11%)	17 (4%)	2 13
47	2	60/68 (88%)	51 (85%)	6 (10%)	3 (5%)	1 11
All	All	6815/7601 (90%)	5717 (84%)	811 (12%)	287 (4%)	4 14

All (287) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	19	HIS
4	A	197	PRO
5	B	16	PHE
5	B	40	PRO
5	B	108	GLU
5	B	109	HIS
5	B	111	SER
5	B	120	LYS
5	B	138	GLN
5	B	143	ALA
5	B	169	ARG
5	B	191	ALA
5	B	196	TRP
5	B	388	PHE
5	B	389	MET
6	C	69	THR
6	C	99	GLY
6	C	309	ILE
6	C	318	PRO
6	C	319	LEU
7	D	19	LYS
7	D	212	ILE
7	D	262	LYS
7	D	285	ALA
8	E	55	ARG
8	E	59	TYR
8	E	96	LYS
8	E	131	LYS
8	E	175	LEU
8	E	221	PRO
8	E	230	ASP
8	E	280	HIS
9	F	72	ARG
9	F	128	ASN
9	F	236	GLY
10	G	128	VAL
11	H	60	TRP
12	I	78	LYS
12	I	79	SER
12	I	178	ALA
12	I	179	ASP
12	I	187	LYS
13	J	91	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	L	62	PRO
14	L	64	VAL
14	L	67	HIS
14	L	82	ARG
14	L	83	VAL
14	L	134	PRO
15	M	7	VAL
16	N	30	TYR
16	N	89	VAL
17	O	5	GLN
17	O	111	PRO
19	Q	177	ALA
20	R	36	ASN
21	S	146	HIS
21	S	165	PRO
24	V	14	PHE
24	V	99	GLU
26	X	131	ASP
29	a	76	ASP
29	a	92	LYS
29	a	96	GLY
30	b	7	HIS
30	b	12	GLN
34	f	4	ARG
35	g	7	TYR
36	h	119	PHE
37	i	64	SER
39	k	23	VAL
39	k	59	SER
40	l	22	PRO
43	o	90	HIS
43	o	94	GLY
45	r	34	ALA
45	r	45	HIS
45	r	107	ARG
46	1	62	PHE
46	1	174	GLY
46	1	285	TYR
46	1	435	ALA
46	1	436	ASP
46	1	445	THR
4	A	110	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	47	LEU
5	B	147	ALA
5	B	274	TYR
5	B	314	ILE
5	B	394	LYS
6	C	58	ALA
6	C	66	SER
6	C	320	LYS
7	D	21	ARG
7	D	57	ASN
7	D	96	ALA
7	D	220	LYS
7	D	260	GLU
7	D	279	ARG
7	D	281	ALA
7	D	293	ARG
8	E	43	ASN
8	E	61	ARG
8	E	91	PRO
8	E	181	PRO
8	E	220	LYS
9	F	31	LYS
9	F	168	ARG
9	F	229	PHE
10	G	28	VAL
11	H	64	ARG
12	I	101	LYS
12	I	210	ARG
13	J	26	VAL
13	J	88	LYS
13	J	169	LYS
14	L	143	GLU
15	M	87	ALA
16	N	79	ALA
18	P	41	ILE
19	Q	178	ARG
20	R	39	GLN
22	T	18	PRO
22	T	44	GLY
22	T	55	LYS
26	X	86	ALA
27	Y	6	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	Z	91	LEU
29	a	60	HIS
29	a	62	HIS
29	a	97	ALA
31	c	32	LYS
31	c	80	GLU
31	c	81	LEU
32	d	93	ASN
33	e	34	ASN
36	h	122	LYS
39	k	61	PRO
43	o	33	LEU
43	o	98	LYS
45	r	123	PRO
46	1	61	PRO
46	1	239	LEU
46	1	288	ASN
46	1	385	SER
47	2	8	VAL
47	2	66	VAL
4	A	180	LEU
4	A	196	TRP
5	B	295	ASP
6	C	73	VAL
6	C	97	ARG
6	C	266	THR
6	C	273	LEU
7	D	129	GLU
7	D	152	ARG
7	D	187	SER
7	D	188	LYS
8	E	92	VAL
8	E	95	ASP
8	E	104	LYS
8	E	153	HIS
8	E	206	LYS
8	E	218	LEU
8	E	255	ARG
9	F	105	PRO
12	I	94	PHE
12	I	106	ALA
13	J	124	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	L	172	GLU
18	P	54	GLN
19	Q	52	PHE
19	Q	146	ARG
20	R	130	ASN
21	S	153	PRO
23	U	38	ASN
27	Y	11	ARG
27	Y	18	HIS
28	Z	8	GLY
28	Z	33	THR
29	a	93	ASN
32	d	38	PHE
34	f	80	ASN
34	f	107	PRO
40	l	47	THR
43	o	49	GLY
4	A	35	ALA
4	A	109	GLU
4	A	193	ARG
5	B	117	ARG
5	B	189	THR
5	B	310	SER
5	B	329	ASP
6	C	23	THR
6	C	49	ARG
7	D	20	PHE
7	D	32	ALA
8	E	85	LEU
8	E	118	PRO
8	E	122	LEU
8	E	183	ARG
8	E	203	LYS
8	E	254	LEU
10	G	43	GLN
10	G	165	GLU
11	H	51	LYS
12	I	77	VAL
12	I	109	ASP
16	N	182	HIS
19	Q	55	ARG
20	R	131	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	U	98	ASP
24	V	110	GLY
25	W	43	LYS
29	a	98	ALA
30	b	10	HIS
32	d	58	GLY
32	d	102	LEU
34	f	5	LEU
39	k	29	LYS
43	o	8	ARG
46	1	270	ALA
4	A	130	SER
5	B	137	TRP
5	B	139	ASP
5	B	194	LEU
5	B	387	ALA
7	D	125	VAL
7	D	263	LYS
8	E	229	PHE
8	E	245	ASP
9	F	99	GLY
10	G	123	ALA
10	G	125	LYS
11	H	110	SER
13	J	11	PRO
13	J	32	ARG
16	N	40	PRO
16	N	55	ALA
27	Y	85	VAL
28	Z	124	THR
30	b	21	ILE
31	c	77	ASN
34	f	106	TYR
35	g	84	ALA
38	j	5	THR
38	j	38	GLY
46	1	59	ALA
46	1	73	ARG
46	1	287	SER
47	2	27	LYS
5	B	17	LEU
5	B	112	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	144	ALA
6	C	198	ASN
8	E	40	CYS
8	E	100	THR
12	I	110	ARG
13	J	27	GLY
14	L	169	ILE
17	O	110	PRO
27	Y	63	LYS
27	Y	79	VAL
28	Z	4	PHE
38	j	9	GLY
38	j	75	ARG
44	p	4	ARG
45	r	103	ARG
5	B	110	ILE
5	B	259	PRO
7	D	114	GLY
39	k	63	GLY
46	1	211	GLY
14	L	100	PRO
46	1	201	VAL
7	D	261	VAL
12	I	47	PRO
46	1	339	GLY
5	B	321	VAL
8	E	90	LYS
9	F	100	ILE
10	G	58	PRO
14	L	28	GLN
36	h	38	GLY
37	i	63	VAL
45	r	44	ILE
9	F	199	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	187/199 (94%)	139 (74%)	48 (26%)	0	1
5	B	335/335 (100%)	265 (79%)	70 (21%)	1	2
6	C	305/305 (100%)	239 (78%)	66 (22%)	1	2
7	D	246/250 (98%)	178 (72%)	68 (28%)	0	1
8	E	209/209 (100%)	157 (75%)	52 (25%)	0	1
9	F	194/194 (100%)	145 (75%)	49 (25%)	0	1
10	G	206/226 (91%)	158 (77%)	48 (23%)	0	2
11	H	169/171 (99%)	125 (74%)	44 (26%)	0	1
12	I	180/180 (100%)	136 (76%)	44 (24%)	0	1
13	J	143/149 (96%)	115 (80%)	28 (20%)	1	3
14	L	176/177 (99%)	135 (77%)	41 (23%)	0	2
15	M	116/160 (72%)	95 (82%)	21 (18%)	1	5
16	N	171/172 (99%)	129 (75%)	42 (25%)	0	1
17	O	172/172 (100%)	146 (85%)	26 (15%)	2	9
18	P	134/134 (100%)	112 (84%)	22 (16%)	2	7
19	Q	163/164 (99%)	132 (81%)	31 (19%)	1	4
20	R	159/175 (91%)	120 (76%)	39 (24%)	0	1
21	S	156/192 (81%)	121 (78%)	35 (22%)	1	2
22	T	139/140 (99%)	112 (81%)	27 (19%)	1	3
23	U	89/114 (78%)	67 (75%)	22 (25%)	0	1
24	V	101/107 (94%)	77 (76%)	24 (24%)	0	1
25	W	55/126 (44%)	42 (76%)	13 (24%)	0	1
26	X	107/133 (80%)	89 (83%)	18 (17%)	1	7
27	Y	124/135 (92%)	96 (77%)	28 (23%)	1	2
28	Z	117/118 (99%)	94 (80%)	23 (20%)	1	3
29	a	119/120 (99%)	102 (86%)	17 (14%)	2	10
30	b	63/123 (51%)	45 (71%)	18 (29%)	0	1
31	c	79/97 (81%)	60 (76%)	19 (24%)	0	1
32	d	98/110 (89%)	66 (67%)	32 (33%)	0	0
33	e	114/121 (94%)	89 (78%)	25 (22%)	1	2
34	f	88/89 (99%)	73 (83%)	15 (17%)	1	6
35	g	98/100 (98%)	79 (81%)	19 (19%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	h	109/110 (99%)	92 (84%)	17 (16%)	2 8
37	i	86/89 (97%)	71 (83%)	15 (17%)	1 6
38	j	73/73 (100%)	60 (82%)	13 (18%)	1 5
39	k	64/65 (98%)	52 (81%)	12 (19%)	1 4
40	l	47/48 (98%)	39 (83%)	8 (17%)	1 6
41	m	48/116 (41%)	36 (75%)	12 (25%)	0 1
42	n	22/24 (92%)	17 (77%)	5 (23%)	0 2
43	o	92/94 (98%)	70 (76%)	22 (24%)	0 1
44	p	74/74 (100%)	61 (82%)	13 (18%)	1 6
45	r	109/109 (100%)	85 (78%)	24 (22%)	1 2
46	1	330/398 (83%)	309 (94%)	21 (6%)	14 39
47	2	53/59 (90%)	50 (94%)	3 (6%)	17 43
All	All	5919/6456 (92%)	4680 (79%)	1239 (21%)	2 2

All (1239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	5	ILE
4	A	16	PHE
4	A	30	ARG
4	A	37	ARG
4	A	40	TYR
4	A	41	ILE
4	A	63	PHE
4	A	64	ARG
4	A	70	LYS
4	A	73	THR
4	A	74	GLU
4	A	95	GLN
4	A	97	ASN
4	A	100	ASN
4	A	109	GLU
4	A	116	LEU
4	A	122	ASP
4	A	123	ARG
4	A	125	LYS
4	A	126	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	128	ARG
4	A	139	HIS
4	A	144	LYS
4	A	147	ARG
4	A	162	ASN
4	A	163	ARG
4	A	176	ASP
4	A	181	LYS
4	A	186	TYR
4	A	187	HIS
4	A	189	TYR
4	A	190	LYS
4	A	193	ARG
4	A	194	ASN
4	A	195	CYS
4	A	196	TRP
4	A	205	ASN
4	A	208	GLU
4	A	215	ASN
4	A	216	HIS
4	A	218	HIS
4	A	221	LYS
4	A	226	ARG
4	A	227	ARG
4	A	233	ARG
4	A	242	ARG
4	A	245	ARG
5	B	10	ARG
5	B	16	PHE
5	B	17	LEU
5	B	25	HIS
5	B	26	ARG
5	B	36	ASP
5	B	39	LYS
5	B	41	VAL
5	B	46	PHE
5	B	55	HIS
5	B	56	ILE
5	B	58	ARG
5	B	61	ASP
5	B	62	ARG
5	B	74	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	78	ILE
5	B	94	GLU
5	B	95	THR
5	B	99	LEU
5	B	100	ARG
5	B	101	THR
5	B	103	LYS
5	B	104	THR
5	B	106	PHE
5	B	116	ARG
5	B	117	ARG
5	B	119	TYR
5	B	122	TRP
5	B	123	HIS
5	B	146	LEU
5	B	149	ASP
5	B	154	LYS
5	B	156	TYR
5	B	165	HIS
5	B	167	GLN
5	B	169	ARG
5	B	174	ARG
5	B	189	THR
5	B	198	ARG
5	B	203	GLN
5	B	207	VAL
5	B	214	ASP
5	B	218	ASP
5	B	228	TYR
5	B	233	SER
5	B	235	TRP
5	B	236	HIS
5	B	245	HIS
5	B	249	ARG
5	B	257	TRP
5	B	258	HIS
5	B	261	ARG
5	B	264	PHE
5	B	289	GLN
5	B	291	TYR
5	B	309	LEU
5	B	314	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	323	TYR
5	B	326	VAL
5	B	328	ASN
5	B	329	ASP
5	B	347	LEU
5	B	348	ARG
5	B	355	THR
5	B	356	LYS
5	B	357	ARG
5	B	366	LYS
5	B	369	ASP
5	B	378	ARG
5	B	388	PHE
6	C	14	LYS
6	C	36	ILE
6	C	47	ASN
6	C	49	ARG
6	C	60	HIS
6	C	65	GLU
6	C	71	ARG
6	C	75	ARG
6	C	76	ILE
6	C	78	ARG
6	C	80	ARG
6	C	85	HIS
6	C	86	ARG
6	C	87	SER
6	C	92	PHE
6	C	94	ASN
6	C	95	MET
6	C	97	ARG
6	C	100	ARG
6	C	102	PHE
6	C	107	THR
6	C	112	HIS
6	C	113	ARG
6	C	122	TYR
6	C	126	SER
6	C	131	SER
6	C	142	HIS
6	C	150	LEU
6	C	156	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	C	160	SER
6	C	173	LYS
6	C	175	LYS
6	C	177	TRP
6	C	178	ASN
6	C	182	LYS
6	C	184	TYR
6	C	188	ARG
6	C	193	LYS
6	C	196	MET
6	C	198	ASN
6	C	201	ARG
6	C	212	ASN
6	C	215	ASN
6	C	219	LYS
6	C	222	ARG
6	C	262	GLU
6	C	264	TYR
6	C	267	TRP
6	C	281	MET
6	C	288	ASP
6	C	291	ARG
6	C	300	ARG
6	C	303	ARG
6	C	307	LYS
6	C	309	ILE
6	C	310	HIS
6	C	311	ARG
6	C	312	ARG
6	C	321	ASN
6	C	322	LEU
6	C	333	LYS
6	C	342	ARG
6	C	343	GLN
6	C	345	ARG
6	C	350	ARG
6	C	352	ASP
7	D	15	ARG
7	D	22	ARG
7	D	23	ARG
7	D	30	TYR
7	D	31	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D	33	ARG
7	D	35	ARG
7	D	39	GLN
7	D	42	ASN
7	D	44	TYR
7	D	45	ASN
7	D	50	ARG
7	D	59	ASP
7	D	63	GLN
7	D	66	TYR
7	D	79	TYR
7	D	81	HIS
7	D	90	VAL
7	D	92	LEU
7	D	94	ASN
7	D	95	TYR
7	D	99	TYR
7	D	104	LEU
7	D	107	ARG
7	D	111	ASN
7	D	113	PHE
7	D	116	ASP
7	D	118	ILE
7	D	119	TYR
7	D	124	GLU
7	D	129	GLU
7	D	131	ASN
7	D	136	ASP
7	D	157	ASN
7	D	168	ASP
7	D	177	THR
7	D	179	ARG
7	D	189	GLU
7	D	191	ASN
7	D	193	GLU
7	D	196	ARG
7	D	202	GLN
7	D	203	ASN
7	D	206	ASP
7	D	213	GLU
7	D	221	LYS
7	D	223	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D	229	ASN
7	D	232	THR
7	D	234	ASP
7	D	244	HIS
7	D	248	ARG
7	D	249	GLU
7	D	254	GLU
7	D	255	LYS
7	D	256	LYS
7	D	259	LYS
7	D	260	GLU
7	D	262	LYS
7	D	264	LYS
7	D	265	ARG
7	D	266	TRP
7	D	268	ARG
7	D	279	ARG
7	D	287	PHE
7	D	291	GLN
7	D	292	GLU
7	D	293	ARG
8	E	39	HIS
8	E	40	CYS
8	E	43	ASN
8	E	46	LEU
8	E	52	ARG
8	E	61	ARG
8	E	64	MET
8	E	67	ARG
8	E	68	LYS
8	E	95	ASP
8	E	101	ARG
8	E	104	LYS
8	E	111	TYR
8	E	112	TYR
8	E	114	THR
8	E	115	GLU
8	E	119	ARG
8	E	124	HIS
8	E	126	LYS
8	E	129	PHE
8	E	134	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	E	153	HIS
8	E	157	ARG
8	E	166	SER
8	E	171	VAL
8	E	175	LEU
8	E	178	ASN
8	E	179	ARG
8	E	186	HIS
8	E	187	GLN
8	E	203	LYS
8	E	206	LYS
8	E	212	TYR
8	E	217	LYS
8	E	219	ARG
8	E	230	ASP
8	E	233	LYS
8	E	237	GLU
8	E	241	GLN
8	E	242	ARG
8	E	245	ASP
8	E	246	GLN
8	E	250	ASP
8	E	252	GLN
8	E	256	ARG
8	E	262	GLN
8	E	266	TYR
8	E	268	ARG
8	E	277	ILE
8	E	280	HIS
8	E	282	LEU
8	E	284	PHE
9	F	27	PHE
9	F	33	LYS
9	F	34	ARG
9	F	41	GLN
9	F	43	MET
9	F	44	LEU
9	F	49	ARG
9	F	64	ARG
9	F	65	GLN
9	F	68	ARG
9	F	72	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	F	82	ASN
9	F	83	PHE
9	F	84	TYR
9	F	85	VAL
9	F	90	LYS
9	F	93	PHE
9	F	96	ARG
9	F	100	ILE
9	F	101	ASN
9	F	118	GLN
9	F	119	ILE
9	F	120	PHE
9	F	121	ASN
9	F	137	ILE
9	F	146	TYR
9	F	148	ASN
9	F	149	LEU
9	F	151	SER
9	F	154	GLU
9	F	176	LEU
9	F	192	LEU
9	F	194	HIS
9	F	197	TYR
9	F	201	LYS
9	F	202	ARG
9	F	204	LYS
9	F	209	PHE
9	F	213	PHE
9	F	214	LYS
9	F	224	LYS
9	F	226	THR
9	F	227	THR
9	F	228	HIS
9	F	234	ASP
9	F	239	GLU
9	F	245	LEU
9	F	247	ARG
9	F	248	ARG
10	G	28	VAL
10	G	29	ASN
10	G	31	LEU
10	G	32	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	G	38	ASN
10	G	39	PHE
10	G	44	ASP
10	G	46	GLN
10	G	49	ARG
10	G	50	ASP
10	G	56	LYS
10	G	60	TYR
10	G	62	ARG
10	G	67	ARG
10	G	71	TYR
10	G	73	ARG
10	G	85	GLN
10	G	88	ASP
10	G	89	ARG
10	G	90	GLN
10	G	100	HIS
10	G	101	LYS
10	G	102	TYR
10	G	103	ARG
10	G	108	GLN
10	G	112	GLN
10	G	125	LYS
10	G	131	LYS
10	G	141	ASN
10	G	150	LYS
10	G	162	ASP
10	G	169	PHE
10	G	170	LEU
10	G	175	ARG
10	G	177	MET
10	G	189	ARG
10	G	202	VAL
10	G	210	GLU
10	G	217	LYS
10	G	220	GLU
10	G	223	ARG
10	G	227	ASN
10	G	230	TYR
10	G	231	ASN
10	G	235	ARG
10	G	240	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	G	254	GLU
10	G	259	LYS
11	H	11	ASP
11	H	12	ILE
11	H	18	ILE
11	H	26	ILE
11	H	31	ARG
11	H	40	HIS
11	H	42	ASN
11	H	51	LYS
11	H	52	LYS
11	H	54	ARG
11	H	57	VAL
11	H	58	ASP
11	H	59	LYS
11	H	60	TRP
11	H	63	ASN
11	H	66	GLU
11	H	71	ARG
11	H	79	ASN
11	H	84	VAL
11	H	88	PHE
11	H	92	MET
11	H	96	TYR
11	H	105	ILE
11	H	106	GLN
11	H	107	GLU
11	H	108	ASN
11	H	113	GLU
11	H	115	ARG
11	H	117	PHE
11	H	118	LEU
11	H	122	TYR
11	H	123	ILE
11	H	124	ARG
11	H	125	ARG
11	H	128	MET
11	H	140	GLN
11	H	141	LYS
11	H	161	ILE
11	H	162	GLN
11	H	168	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	H	171	ASP
11	H	173	ARG
11	H	177	ASP
11	H	180	TYR
12	I	3	ARG
12	I	4	ARG
12	I	8	CYS
12	I	9	TYR
12	I	13	LYS
12	I	17	TYR
12	I	21	ARG
12	I	24	ARG
12	I	28	ASP
12	I	32	ARG
12	I	35	ASP
12	I	39	LYS
12	I	43	VAL
12	I	45	GLU
12	I	46	PHE
12	I	58	GLU
12	I	71	CYS
12	I	74	LYS
12	I	78	LYS
12	I	83	ASP
12	I	86	HIS
12	I	88	ARG
12	I	92	HIS
12	I	94	PHE
12	I	95	HIS
12	I	100	ASN
12	I	101	LYS
12	I	102	MET
12	I	110	ARG
12	I	111	LEU
12	I	119	PHE
12	I	126	VAL
12	I	128	ARG
12	I	143	GLN
12	I	146	GLU
12	I	159	PHE
12	I	171	TRP
12	I	177	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	I	179	ASP
12	I	181	PHE
12	I	182	GLU
12	I	203	HIS
12	I	207	ASP
12	I	208	LYS
13	J	15	LEU
13	J	23	ASN
13	J	32	ARG
13	J	33	LEU
13	J	35	ARG
13	J	54	ARG
13	J	55	TYR
13	J	58	ARG
13	J	81	GLU
13	J	83	LEU
13	J	85	LYS
13	J	87	LEU
13	J	90	ARG
13	J	96	LYS
13	J	97	ASN
13	J	98	ASN
13	J	101	ASP
13	J	113	ILE
13	J	128	LEU
13	J	129	ASP
13	J	139	PHE
13	J	146	ARG
13	J	150	CYS
13	J	154	LYS
13	J	155	HIS
13	J	164	ARG
13	J	171	ASP
13	J	178	ASN
14	L	5	ARG
14	L	10	LEU
14	L	13	HIS
14	L	19	GLN
14	L	28	GLN
14	L	31	ARG
14	L	34	ARG
14	L	36	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	L	39	ARG
14	L	45	ARG
14	L	49	ARG
14	L	56	ARG
14	L	65	ARG
14	L	66	TYR
14	L	67	HIS
14	L	74	ARG
14	L	79	GLU
14	L	82	ARG
14	L	92	ARG
14	L	99	ASP
14	L	101	ARG
14	L	103	ARG
14	L	111	GLN
14	L	113	ASN
14	L	115	GLN
14	L	119	GLU
14	L	123	LYS
14	L	127	PHE
14	L	129	ARG
14	L	130	LYS
14	L	146	LEU
14	L	158	ARG
14	L	162	LYS
14	L	163	ARG
14	L	165	LYS
14	L	172	GLU
14	L	176	PHE
14	L	186	ARG
14	L	195	ARG
14	L	201	GLU
14	L	205	GLN
15	M	8	GLU
15	M	11	ARG
15	M	17	PHE
15	M	29	ASP
15	M	32	ASP
15	M	33	GLN
15	M	34	ASN
15	M	38	VAL
15	M	47	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	M	56	GLN
15	M	57	LEU
15	M	59	ASP
15	M	61	ILE
15	M	66	HIS
15	M	70	GLN
15	M	79	LYS
15	M	89	THR
15	M	90	ARG
15	M	91	TRP
15	M	98	ARG
15	M	119	ARG
16	N	4	TYR
16	N	9	GLU
16	N	11	TRP
16	N	26	ARG
16	N	29	GLN
16	N	49	ARG
16	N	50	ARG
16	N	53	TYR
16	N	54	LYS
16	N	59	TYR
16	N	63	ARG
16	N	67	ARG
16	N	71	ARG
16	N	72	LYS
16	N	80	THR
16	N	86	HIS
16	N	87	HIS
16	N	91	GLN
16	N	92	LEU
16	N	104	GLU
16	N	108	ARG
16	N	119	TYR
16	N	123	GLU
16	N	126	THR
16	N	127	TYR
16	N	131	GLU
16	N	136	ASP
16	N	138	PHE
16	N	139	HIS
16	N	147	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	N	150	TRP
16	N	162	ARG
16	N	169	ARG
16	N	174	LEU
16	N	178	HIS
16	N	182	HIS
16	N	189	ARG
16	N	192	TRP
16	N	195	ARG
16	N	196	ASN
16	N	199	GLN
16	N	203	TYR
17	O	5	GLN
17	O	42	ASN
17	O	46	ASN
17	O	49	ARG
17	O	57	PHE
17	O	59	ARG
17	O	60	LYS
17	O	61	ARG
17	O	62	MET
17	O	74	ARG
17	O	78	ARG
17	O	82	ARG
17	O	85	ARG
17	O	110	PRO
17	O	113	ASP
17	O	140	ARG
17	O	160	ARG
17	O	167	HIS
17	O	173	GLN
17	O	178	ARG
17	O	184	ASN
17	O	187	LYS
17	O	188	LYS
17	O	191	ARG
17	O	192	PHE
17	O	194	GLU
18	P	3	ARG
18	P	9	GLU
18	P	10	ASN
18	P	13	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	P	18	ARG
18	P	23	ARG
18	P	24	VAL
18	P	28	ASN
18	P	30	ARG
18	P	40	HIS
18	P	42	ARG
18	P	61	ARG
18	P	69	ARG
18	P	70	CYS
18	P	78	TRP
18	P	90	PHE
18	P	91	LEU
18	P	110	ASP
18	P	128	ARG
18	P	133	HIS
18	P	135	ARG
18	P	154	GLU
19	Q	5	ILE
19	Q	9	LYS
19	Q	14	ARG
19	Q	15	ARG
19	Q	16	LYS
19	Q	32	TYR
19	Q	37	ARG
19	Q	44	ASN
19	Q	54	SER
19	Q	58	ARG
19	Q	61	LEU
19	Q	65	ARG
19	Q	68	ARG
19	Q	72	LEU
19	Q	75	ARG
19	Q	79	THR
19	Q	85	THR
19	Q	89	ASP
19	Q	91	ARG
19	Q	93	GLN
19	Q	97	LYS
19	Q	108	ARG
19	Q	110	ARG
19	Q	112	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Q	119	LYS
19	Q	146	ARG
19	Q	150	ARG
19	Q	166	TYR
19	Q	173	LYS
19	Q	180	ARG
19	Q	181	ARG
20	R	5	ARG
20	R	6	LEU
20	R	9	ARG
20	R	23	TRP
20	R	30	ASN
20	R	39	GLN
20	R	40	GLN
20	R	47	ASP
20	R	50	ILE
20	R	58	HIS
20	R	60	ARG
20	R	74	ARG
20	R	81	ARG
20	R	86	ASN
20	R	89	MET
20	R	99	MET
20	R	104	ARG
20	R	105	LEU
20	R	107	ARG
20	R	108	ARG
20	R	109	TYR
20	R	113	LYS
20	R	114	LYS
20	R	117	ARG
20	R	118	HIS
20	R	120	TYR
20	R	124	TYR
20	R	131	VAL
20	R	133	LYS
20	R	136	ARG
20	R	138	LEU
20	R	141	HIS
20	R	163	ARG
20	R	168	GLU
20	R	172	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R	175	GLU
20	R	177	LEU
20	R	178	GLN
20	R	180	LYS
21	S	2	LYS
21	S	15	ARG
21	S	28	TYR
21	S	29	ARG
21	S	37	HIS
21	S	44	PHE
21	S	47	PHE
21	S	48	VAL
21	S	53	LYS
21	S	57	SER
21	S	64	CYS
21	S	68	PHE
21	S	70	LYS
21	S	82	LEU
21	S	83	ARG
21	S	84	TYR
21	S	86	SER
21	S	90	THR
21	S	95	ARG
21	S	99	ASP
21	S	100	LEU
21	S	101	THR
21	S	127	MET
21	S	128	LYS
21	S	138	ARG
21	S	146	HIS
21	S	147	ASP
21	S	150	ILE
21	S	151	LYS
21	S	156	HIS
21	S	157	ARG
21	S	159	LEU
21	S	162	GLN
21	S	168	THR
21	S	171	ARG
22	T	5	LYS
22	T	7	LYS
22	T	9	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	T	13	TYR
22	T	19	PHE
22	T	30	TYR
22	T	32	ARG
22	T	33	ILE
22	T	35	LYS
22	T	36	LYS
22	T	38	ASP
22	T	41	ASP
22	T	54	HIS
22	T	60	LYS
22	T	70	HIS
22	T	76	VAL
22	T	88	ARG
22	T	102	ARG
22	T	103	ASP
22	T	107	LYS
22	T	113	ASP
22	T	118	GLU
22	T	121	GLU
22	T	139	HIS
22	T	142	ARG
22	T	144	ASN
22	T	152	GLU
23	U	21	PHE
23	U	23	LEU
23	U	27	HIS
23	U	33	ILE
23	U	38	ASN
23	U	39	PHE
23	U	40	GLU
23	U	42	PHE
23	U	46	ARG
23	U	50	ASN
23	U	52	LYS
23	U	62	THR
23	U	64	GLU
23	U	65	ARG
23	U	67	LYS
23	U	69	LYS
23	U	82	TYR
23	U	89	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	U	90	TYR
23	U	98	ASP
23	U	101	ARG
23	U	113	ARG
24	V	13	LYS
24	V	14	PHE
24	V	15	ARG
24	V	18	LEU
24	V	27	ASN
24	V	30	ASP
24	V	36	ASN
24	V	46	LYS
24	V	48	ARG
24	V	50	ASN
24	V	51	ARG
24	V	59	ASP
24	V	60	MET
24	V	73	ARG
24	V	77	HIS
24	V	84	GLN
24	V	91	LYS
24	V	98	PHE
24	V	100	ASP
24	V	107	ASN
24	V	109	LYS
24	V	111	GLU
24	V	123	LYS
24	V	128	LEU
25	W	3	VAL
25	W	4	GLU
25	W	8	PHE
25	W	12	LYS
25	W	17	HIS
25	W	25	ASP
25	W	33	ASN
25	W	44	ARG
25	W	50	ASN
25	W	55	TYR
25	W	56	ARG
25	W	57	ARG
25	W	59	HIS
26	X	39	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	X	45	THR
26	X	48	ARG
26	X	60	TYR
26	X	62	ARG
26	X	72	ASP
26	X	79	PHE
26	X	84	GLU
26	X	94	ASN
26	X	117	TYR
26	X	120	ASP
26	X	129	ARG
26	X	133	GLU
26	X	137	TYR
26	X	139	ARG
26	X	144	TYR
26	X	148	ASP
26	X	151	ASN
27	Y	2	LYS
27	Y	4	ASN
27	Y	11	ARG
27	Y	15	ARG
27	Y	17	ARG
27	Y	18	HIS
27	Y	19	PHE
27	Y	27	ARG
27	Y	36	LYS
27	Y	45	ARG
27	Y	49	ILE
27	Y	50	ARG
27	Y	53	ASP
27	Y	56	GLN
27	Y	59	ARG
27	Y	62	TYR
27	Y	65	GLN
27	Y	72	GLN
27	Y	82	ILE
27	Y	83	GLU
27	Y	84	ARG
27	Y	87	ARG
27	Y	91	ASN
27	Y	112	ASP
27	Y	114	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	Y	115	ARG
27	Y	126	ARG
27	Y	127	GLN
28	Z	4	PHE
28	Z	17	ARG
28	Z	21	ARG
28	Z	27	LYS
28	Z	30	ASP
28	Z	36	ARG
28	Z	38	TYR
28	Z	54	THR
28	Z	57	MET
28	Z	60	LYS
28	Z	64	LYS
28	Z	78	ASN
28	Z	88	ASP
28	Z	92	ASP
28	Z	93	LYS
28	Z	98	LYS
28	Z	102	ARG
28	Z	108	ARG
28	Z	109	LYS
28	Z	112	ARG
28	Z	121	ARG
28	Z	122	TYR
28	Z	136	PHE
29	a	7	LYS
29	a	10	LYS
29	a	14	HIS
29	a	19	HIS
29	a	21	ARG
29	a	40	HIS
29	a	41	HIS
29	a	46	ASP
29	a	49	HIS
29	a	52	TYR
29	a	59	ARG
29	a	61	TYR
29	a	63	LEU
29	a	77	LYS
29	a	84	GLU
29	a	105	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	132	ARG
30	b	6	ASN
30	b	7	HIS
30	b	12	GLN
30	b	16	TRP
30	b	18	ARG
30	b	19	ASN
30	b	22	LYS
30	b	23	LYS
30	b	25	ARG
30	b	27	GLN
30	b	28	ARG
30	b	30	GLU
30	b	39	PHE
30	b	43	MET
30	b	44	ARG
30	b	51	LYS
30	b	55	LYS
30	b	65	MET
31	c	18	LEU
31	c	27	TYR
31	c	31	TYR
31	c	37	MET
31	c	39	ARG
31	c	42	LYS
31	c	44	LYS
31	c	52	CYS
31	c	55	LEU
31	c	56	ARG
31	c	59	GLU
31	c	66	LEU
31	c	72	HIS
31	c	73	HIS
31	c	74	TYR
31	c	77	ASN
31	c	78	ASN
31	c	81	LEU
31	c	88	TYR
32	d	18	ASN
32	d	19	GLU
32	d	23	ARG
32	d	26	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	d	28	ASN
32	d	31	LYS
32	d	32	ARG
32	d	38	PHE
32	d	39	LYS
32	d	44	ARG
32	d	67	ARG
32	d	73	TRP
32	d	78	ARG
32	d	79	ASN
32	d	83	ARG
32	d	85	ARG
32	d	86	VAL
32	d	87	ARG
32	d	91	LYS
32	d	93	ASN
32	d	94	GLU
32	d	95	ASP
32	d	101	LYS
32	d	103	TYR
32	d	108	TYR
32	d	109	VAL
32	d	116	ASN
32	d	117	LEU
32	d	118	GLN
32	d	119	THR
32	d	121	ASN
32	d	123	ASP
33	e	11	LYS
33	e	16	ARG
33	e	21	ILE
33	e	26	ASP
33	e	36	ARG
33	e	42	ASP
33	e	43	ASN
33	e	46	ARG
33	e	49	PHE
33	e	52	GLN
33	e	57	ASN
33	e	64	LYS
33	e	68	HIS
33	e	77	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	e	78	LEU
33	e	85	LEU
33	e	92	ASN
33	e	95	TYR
33	e	106	LYS
33	e	107	ASN
33	e	108	ARG
33	e	113	GLU
33	e	124	ASN
33	e	126	ASN
33	e	128	ARG
34	f	4	ARG
34	f	5	LEU
34	f	7	SER
34	f	14	TYR
34	f	16	ARG
34	f	19	ARG
34	f	22	ARG
34	f	24	HIS
34	f	36	ARG
34	f	49	TYR
34	f	51	TYR
34	f	52	LYS
34	f	71	TRP
34	f	101	ILE
34	f	109	ARG
35	g	3	GLN
35	g	4	ARG
35	g	5	LEU
35	g	12	SER
35	g	14	ASN
35	g	29	ARG
35	g	32	TYR
35	g	52	ARG
35	g	54	ARG
35	g	57	ARG
35	g	60	ARG
35	g	66	ARG
35	g	75	SER
35	g	81	SER
35	g	88	ARG
35	g	93	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	g	95	PHE
35	g	114	GLN
35	g	115	LYS
36	h	8	ASP
36	h	10	ARG
36	h	15	GLU
36	h	23	ASP
36	h	28	LEU
36	h	48	ARG
36	h	51	ARG
36	h	67	GLU
36	h	68	ASN
36	h	72	PHE
36	h	73	TYR
36	h	89	ARG
36	h	93	ARG
36	h	97	LYS
36	h	100	GLU
36	h	119	PHE
36	h	122	LYS
37	i	3	LEU
37	i	4	ARG
37	i	12	ASN
37	i	20	ASN
37	i	27	SER
37	i	30	ARG
37	i	33	LEU
37	i	42	ASP
37	i	46	GLU
37	i	50	PHE
37	i	54	GLU
37	i	68	ARG
37	i	85	ARG
37	i	88	GLU
37	i	103	LYS
38	j	10	LYS
38	j	25	LYS
38	j	27	TYR
38	j	39	TYR
38	j	45	ARG
38	j	47	TYR
38	j	48	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	j	55	ARG
38	j	56	ARG
38	j	57	ASN
38	j	71	TYR
38	j	79	ARG
38	j	80	GLU
39	k	14	THR
39	k	19	ASP
39	k	21	LYS
39	k	27	LYS
39	k	30	ASP
39	k	35	LYS
39	k	37	ARG
39	k	51	GLU
39	k	54	GLU
39	k	56	LEU
39	k	60	LEU
39	k	70	LYS
40	l	11	ARG
40	l	12	PHE
40	l	16	LYS
40	l	17	GLN
40	l	21	ARG
40	l	36	ARG
40	l	46	ARG
40	l	49	LEU
41	m	79	GLU
41	m	84	GLN
41	m	87	GLN
41	m	89	TYR
41	m	90	ASN
41	m	96	CYS
41	m	97	ARG
41	m	104	HIS
41	m	106	ARG
41	m	109	ASN
41	m	111	ARG
41	m	119	ASN
42	n	8	LYS
42	n	9	ARG
42	n	18	ARG
42	n	20	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	n	21	ARG
43	o	6	LYS
43	o	11	PHE
43	o	24	THR
43	o	26	TYR
43	o	33	LEU
43	o	36	GLN
43	o	42	ASP
43	o	45	GLN
43	o	48	TYR
43	o	57	ARG
43	o	58	LYS
43	o	59	LYS
43	o	61	LYS
43	o	64	LYS
43	o	69	ARG
43	o	76	ASN
43	o	78	ARG
43	o	79	SER
43	o	81	ARG
43	o	82	MET
43	o	99	ARG
43	o	102	GLN
44	p	3	LYS
44	p	4	ARG
44	p	16	THR
44	p	30	GLU
44	p	34	HIS
44	p	48	LYS
44	p	49	ARG
44	p	69	TRP
44	p	71	TYR
44	p	84	ARG
44	p	85	ARG
44	p	87	LYS
44	p	92	GLN
45	r	7	TRP
45	r	11	ARG
45	r	13	CYS
45	r	15	SER
45	r	16	PHE
45	r	18	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	r	26	SER
45	r	28	GLU
45	r	30	ASN
45	r	33	LYS
45	r	35	ARG
45	r	39	ARG
45	r	46	HIS
45	r	64	ILE
45	r	66	ARG
45	r	67	ARG
45	r	71	ARG
45	r	73	PRO
45	r	83	ASN
45	r	102	TYR
45	r	106	LEU
45	r	107	ARG
45	r	112	ARG
45	r	115	SER
46	1	60	ASP
46	1	66	ARG
46	1	82	SER
46	1	130	VAL
46	1	149	LEU
46	1	205	ARG
46	1	207	MET
46	1	226	LYS
46	1	235	TYR
46	1	239	LEU
46	1	243	MET
46	1	271	ARG
46	1	273	ARG
46	1	275	GLN
46	1	346	SER
46	1	351	PHE
46	1	355	LEU
46	1	393	GLN
46	1	412	GLU
46	1	457	TYR
46	1	461	PHE
47	2	8	VAL
47	2	21	LEU
47	2	32	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	19	HIS
4	A	100	ASN
4	A	132	ASN
4	A	194	ASN
4	A	209	HIS
4	A	215	ASN
5	B	123	HIS
5	B	167	GLN
5	B	179	HIS
5	B	203	GLN
5	B	258	HIS
5	B	275	HIS
5	B	276	HIS
5	B	301	ASN
5	B	302	ASN
5	B	322	HIS
5	B	380	GLN
6	C	50	GLN
6	C	85	HIS
6	C	94	ASN
6	C	112	HIS
6	C	142	HIS
6	C	178	ASN
6	C	198	ASN
6	C	203	GLN
6	C	223	ASN
6	C	286	ASN
6	C	338	ASN
6	C	343	GLN
7	D	45	ASN
7	D	94	ASN
7	D	111	ASN
7	D	122	GLN
7	D	131	ASN
7	D	157	ASN
7	D	191	ASN
7	D	195	HIS
7	D	198	HIS
7	D	202	GLN
7	D	244	HIS
7	D	250	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D	282	GLN
8	E	43	ASN
8	E	124	HIS
8	E	153	HIS
8	E	178	ASN
8	E	186	HIS
8	E	224	GLN
8	E	246	GLN
9	F	58	HIS
9	F	82	ASN
9	F	153	ASN
9	F	165	ASN
9	F	174	ASN
9	F	194	HIS
9	F	237	ASN
9	F	250	ASN
10	G	29	ASN
10	G	64	GLN
10	G	81	ASN
10	G	108	GLN
10	G	112	GLN
10	G	153	GLN
10	G	227	ASN
10	G	231	ASN
11	H	40	HIS
11	H	63	ASN
11	H	106	GLN
12	I	59	GLN
12	I	100	ASN
12	I	144	ASN
12	I	163	GLN
12	I	213	HIS
13	J	155	HIS
14	L	6	ASN
14	L	28	GLN
14	L	104	ASN
14	L	113	ASN
14	L	159	ASN
15	M	33	GLN
15	M	34	ASN
15	M	48	GLN
15	M	66	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	N	8	GLN
16	N	90	ASN
16	N	178	HIS
16	N	181	HIS
16	N	182	HIS
16	N	196	ASN
16	N	201	HIS
17	O	65	ASN
17	O	96	GLN
17	O	173	GLN
18	P	25	HIS
18	P	28	ASN
18	P	54	GLN
18	P	64	ASN
18	P	72	GLN
18	P	80	GLN
18	P	97	ASN
18	P	133	HIS
18	P	145	HIS
19	Q	7	HIS
19	Q	40	ASN
19	Q	57	ASN
20	R	66	ASN
20	R	75	HIS
20	R	118	HIS
20	R	143	HIS
21	S	37	HIS
21	S	91	HIS
21	S	92	ASN
21	S	122	HIS
21	S	125	GLN
21	S	163	HIS
22	T	58	HIS
22	T	70	HIS
22	T	139	HIS
23	U	55	ASN
24	V	36	ASN
25	W	17	HIS
25	W	59	HIS
26	X	93	ASN
26	X	111	GLN
27	Y	24	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	Y	56	GLN
27	Y	72	GLN
27	Y	86	GLN
27	Y	100	HIS
27	Y	127	GLN
28	Z	79	HIS
29	a	41	HIS
29	a	62	HIS
29	a	66	ASN
29	a	67	GLN
30	b	6	ASN
30	b	7	HIS
30	b	12	GLN
30	b	19	ASN
30	b	27	GLN
30	b	42	ASN
31	c	19	GLN
31	c	40	GLN
31	c	73	HIS
31	c	77	ASN
32	d	30	HIS
32	d	93	ASN
32	d	100	ASN
33	e	24	GLN
33	e	43	ASN
33	e	126	ASN
34	f	21	GLN
34	f	24	HIS
34	f	55	ASN
34	f	80	ASN
35	g	18	ASN
35	g	110	GLN
35	g	112	GLN
36	h	68	ASN
36	h	98	HIS
38	j	16	HIS
38	j	48	ASN
40	l	19	GLN
40	l	25	GLN
41	m	84	GLN
41	m	87	GLN
41	m	109	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	o	21	HIS
43	o	25	GLN
43	o	45	GLN
43	o	76	ASN
43	o	90	HIS
44	p	92	GLN
45	r	6	GLN
45	r	12	ASN
45	r	21	ASN
45	r	31	ASN
45	r	36	ASN
45	r	41	ASN
45	r	70	GLN
45	r	83	ASN
46	1	127	GLN
46	1	154	GLN
46	1	244	ASN
46	1	275	GLN
46	1	277	ASN
46	1	398	GLN
46	1	414	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3647/3722 (97%)	1611 (44%)	629 (17%)
2	7	119/120 (99%)	31 (26%)	9 (7%)
3	8	155/156 (99%)	61 (39%)	22 (14%)
All	All	3921/3998 (98%)	1703 (43%)	660 (16%)

All (1703) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	2	G
1	5	5	A
1	5	6	C
1	5	8	U
1	5	12	A
1	5	13	U
1	5	20	U
1	5	21	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	25	A
1	5	33	A
1	5	34	A
1	5	39	A
1	5	40	G
1	5	42	A
1	5	43	U
1	5	47	A
1	5	48	G
1	5	49	U
1	5	50	C
1	5	51	A
1	5	54	G
1	5	56	A
1	5	58	G
1	5	59	A
1	5	64	A
1	5	65	A
1	5	66	A
1	5	69	A
1	5	70	A
1	5	71	C
1	5	72	C
1	5	74	G
1	5	80	C
1	5	81	C
1	5	84	A
1	5	85	G
1	5	88	A
1	5	89	C
1	5	91	G
1	5	92	C
1	5	93	G
1	5	94	A
1	5	95	G
1	5	96	U
1	5	98	A
1	5	99	A
1	5	101	A
1	5	107	G
1	5	108	A
1	5	109	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	110	C
1	5	111	C
1	5	112	C
1	5	115	C
1	5	118	C
1	5	119	G
1	5	120	A
1	5	121	A
1	5	126	C
1	5	128	C
1	5	129	C
1	5	130	C
1	5	131	C
1	5	132	G
1	5	134	G
1	5	135	G
1	5	136	C
1	5	137	G
1	5	138	G
1	5	139	G
1	5	143	C
1	5	144	G
1	5	145	G
1	5	150	U
1	5	152	U
1	5	157	U
1	5	158	A
1	5	159	C
1	5	164	G
1	5	170	C
1	5	171	U
1	5	172	C
1	5	173	C
1	5	178	C
1	5	182	G
1	5	183	C
1	5	184	U
1	5	185	C
1	5	186	G
1	5	187	U
1	5	188	G
1	5	189	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	195	C
1	5	196	C
1	5	197	A
1	5	198	A
1	5	200	U
1	5	201	C
1	5	202	C
1	5	203	U
1	5	205	C
1	5	206	U
1	5	210	C
1	5	211	G
1	5	216	C
1	5	217	C
1	5	218	A
1	5	219	G
1	5	220	C
1	5	221	C
1	5	224	U
1	5	225	G
1	5	226	G
1	5	227	A
1	5	232	G
1	5	233	U
1	5	234	G
1	5	235	A
1	5	236	G
1	5	238	C
1	5	239	C
1	5	245	C
1	5	246	G
1	5	255	C
1	5	257	C
1	5	262	G
1	5	264	C
1	5	265	C
1	5	266	C
1	5	267	G
1	5	270	U
1	5	274	C
1	5	275	C
1	5	276	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	277	G
1	5	278	G
1	5	280	G
1	5	281	U
1	5	288	G
1	5	292	G
1	5	293	G
1	5	294	G
1	5	296	A
1	5	297	U
1	5	300	A
1	5	305	A
1	5	306	A
1	5	309	C
1	5	310	G
1	5	315	G
1	5	316	U
1	5	317	A
1	5	319	A
1	5	322	C
1	5	323	C
1	5	324	A
1	5	325	U
1	5	330	G
1	5	334	A
1	5	337	U
1	5	338	A
1	5	339	C
1	5	340	C
1	5	342	G
1	5	343	C
1	5	345	C
1	5	347	A
1	5	349	A
1	5	350	C
1	5	352	G
1	5	353	A
1	5	354	U
1	5	355	A
1	5	357	U
1	5	358	C
1	5	360	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	361	C
1	5	362	A
1	5	363	A
1	5	370	U
1	5	381	U
1	5	383	A
1	5	384	A
1	5	385	A
1	5	386	A
1	5	387	G
1	5	388	A
1	5	390	C
1	5	395	A
1	5	399	G
1	5	406	C
1	5	407	A
1	5	408	A
1	5	409	G
1	5	410	A
1	5	412	G
1	5	413	G
1	5	414	C
1	5	415	G
1	5	417	G
1	5	418	A
1	5	431	G
1	5	432	U
1	5	433	A
1	5	434	A
1	5	440	U
1	5	444	G
1	5	445	U
1	5	449	C
1	5	450	G
1	5	451	C
1	5	452	A
1	5	453	G
1	5	454	U
1	5	455	C
1	5	456	C
1	5	458	C
1	5	466	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	467	U
1	5	468	U
1	5	469	C
1	5	470	A
1	5	471	A
1	5	473	C
1	5	484	U
1	5	485	C
1	5	486	C
1	5	487	G
1	5	491	G
1	5	496	G
1	5	498	C
1	5	500	G
1	5	502	C
1	5	503	C
1	5	504	G
1	5	506	C
1	5	509	A
1	5	510	U
1	5	511	C
1	5	513	U
1	5	514	U
1	5	515	C
1	5	516	C
1	5	519	C
1	5	647	G
1	5	648	G
1	5	649	A
1	5	650	C
1	5	653	U
1	5	654	C
1	5	656	C
1	5	658	C
1	5	664	G
1	5	665	C
1	5	666	G
1	5	667	A
1	5	668	C
1	5	669	C
1	5	671	G
1	5	672	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	681	G
1	5	682	G
1	5	683	C
1	5	684	G
1	5	685	C
1	5	686	A
1	5	687	U
1	5	689	U
1	5	690	C
1	5	692	A
1	5	694	C
1	5	695	G
1	5	696	C
1	5	697	G
1	5	702	U
1	5	703	G
1	5	704	C
1	5	705	G
1	5	707	C
1	5	716	C
1	5	717	U
1	5	718	C
1	5	721	G
1	5	724	C
1	5	727	C
1	5	728	U
1	5	729	G
1	5	730	G
1	5	731	G
1	5	732	A
1	5	737	C
1	5	739	G
1	5	742	G
1	5	743	G
1	5	745	G
1	5	746	A
1	5	747	A
1	5	748	G
1	5	749	G
1	5	912	G
1	5	915	A
1	5	917	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	918	G
1	5	926	G
1	5	927	G
1	5	928	C
1	5	929	A
1	5	930	G
1	5	931	C
1	5	932	A
1	5	933	G
1	5	934	C
1	5	935	A
1	5	936	C
1	5	937	U
1	5	938	C
1	5	939	G
1	5	940	C
1	5	944	A
1	5	945	U
1	5	946	C
1	5	950	G
1	5	952	G
1	5	955	G
1	5	956	A
1	5	957	G
1	5	958	G
1	5	959	G
1	5	960	A
1	5	961	G
1	5	962	C
1	5	963	G
1	5	964	A
1	5	965	G
1	5	966	A
1	5	967	C
1	5	968	C
1	5	969	C
1	5	971	U
1	5	972	C
1	5	973	G
1	5	974	C
1	5	975	C
1	5	976	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	977	C
1	5	978	G
1	5	979	C
1	5	980	U
1	5	982	U
1	5	983	C
1	5	985	C
1	5	990	C
1	5	1051	G
1	5	1072	C
1	5	1075	G
1	5	1076	C
1	5	1077	C
1	5	1078	A
1	5	1082	C
1	5	1083	U
1	5	1084	C
1	5	1086	C
1	5	1168	G
1	5	1177	U
1	5	1181	C
1	5	1193	C
1	5	1210	C
1	5	1211	G
1	5	1212	G
1	5	1214	C
1	5	1215	C
1	5	1218	G
1	5	1219	G
1	5	1221	G
1	5	1222	A
1	5	1233	G
1	5	1235	G
1	5	1236	C
1	5	1237	C
1	5	1238	A
1	5	1239	C
1	5	1240	G
1	5	1242	G
1	5	1243	C
1	5	1244	G
1	5	1245	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1255	A
1	5	1264	C
1	5	1265	G
1	5	1266	G
1	5	1267	C
1	5	1268	G
1	5	1269	G
1	5	1270	A
1	5	1271	G
1	5	1272	C
1	5	1273	G
1	5	1274	A
1	5	1275	G
1	5	1277	G
1	5	1279	A
1	5	1280	C
1	5	1282	G
1	5	1283	G
1	5	1284	G
1	5	1285	U
1	5	1288	G
1	5	1289	C
1	5	1290	G
1	5	1291	G
1	5	1292	C
1	5	1293	G
1	5	1294	A
1	5	1295	C
1	5	1296	G
1	5	1297	U
1	5	1298	C
1	5	1300	G
1	5	1301	C
1	5	1304	C
1	5	1313	C
1	5	1314	C
1	5	1319	U
1	5	1325	C
1	5	1326	A
1	5	1330	A
1	5	1333	A
1	5	1337	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1338	G
1	5	1344	C
1	5	1354	A
1	5	1357	C
1	5	1358	G
1	5	1359	G
1	5	1360	G
1	5	1362	G
1	5	1364	U
1	5	1365	C
1	5	1366	G
1	5	1367	C
1	5	1368	A
1	5	1369	C
1	5	1370	G
1	5	1371	A
1	5	1372	A
1	5	1377	G
1	5	1378	C
1	5	1379	C
1	5	1380	G
1	5	1381	U
1	5	1382	G
1	5	1387	A
1	5	1390	G
1	5	1394	G
1	5	1397	A
1	5	1398	A
1	5	1399	G
1	5	1402	C
1	5	1407	C
1	5	1408	G
1	5	1410	U
1	5	1411	C
1	5	1420	A
1	5	1421	G
1	5	1426	G
1	5	1427	A
1	5	1428	U
1	5	1429	C
1	5	1435	G
1	5	1436	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1439	C
1	5	1440	U
1	5	1441	C
1	5	1444	G
1	5	1445	U
1	5	1446	C
1	5	1448	G
1	5	1455	G
1	5	1456	C
1	5	1457	G
1	5	1458	C
1	5	1465	G
1	5	1466	G
1	5	1474	C
1	5	1475	G
1	5	1478	C
1	5	1479	G
1	5	1480	C
1	5	1481	C
1	5	1482	G
1	5	1483	C
1	5	1484	G
1	5	1485	C
1	5	1487	G
1	5	1488	G
1	5	1489	G
1	5	1490	G
1	5	1493	G
1	5	1497	A
1	5	1498	G
1	5	1499	C
1	5	1500	A
1	5	1501	C
1	5	1503	A
1	5	1504	G
1	5	1514	U
1	5	1516	G
1	5	1518	A
1	5	1519	C
1	5	1520	C
1	5	1522	G
1	5	1523	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1525	A
1	5	1530	G
1	5	1534	A
1	5	1535	C
1	5	1542	U
1	5	1543	G
1	5	1547	A
1	5	1563	A
1	5	1564	A
1	5	1566	C
1	5	1568	C
1	5	1571	G
1	5	1572	U
1	5	1578	U
1	5	1583	A
1	5	1590	C
1	5	1591	U
1	5	1596	U
1	5	1597	G
1	5	1604	G
1	5	1611	C
1	5	1612	G
1	5	1613	A
1	5	1614	C
1	5	1624	G
1	5	1625	G
1	5	1631	A
1	5	1633	G
1	5	1634	A
1	5	1636	U
1	5	1637	A
1	5	1638	A
1	5	1639	U
1	5	1640	C
1	5	1641	G
1	5	1642	A
1	5	1643	A
1	5	1650	A
1	5	1654	G
1	5	1656	U
1	5	1661	C
1	5	1662	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1670	G
1	5	1671	U
1	5	1673	U
1	5	1674	C
1	5	1676	C
1	5	1678	C
1	5	1679	A
1	5	1680	G
1	5	1681	G
1	5	1684	A
1	5	1685	G
1	5	1687	U
1	5	1691	G
1	5	1692	C
1	5	1694	C
1	5	1696	C
1	5	1697	G
1	5	1698	C
1	5	1699	A
1	5	1719	A
1	5	1720	C
1	5	1721	G
1	5	1722	C
1	5	1723	A
1	5	1724	G
1	5	1725	U
1	5	1727	U
1	5	1730	U
1	5	1733	G
1	5	1734	G
1	5	1735	U
1	5	1736	A
1	5	1741	G
1	5	1742	A
1	5	1746	A
1	5	1750	G
1	5	1751	A
1	5	1753	G
1	5	1754	U
1	5	1755	C
1	5	1756	U
1	5	1757	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1758	G
1	5	1759	G
1	5	1760	G
1	5	1761	G
1	5	1764	G
1	5	1765	A
1	5	1766	A
1	5	1767	A
1	5	1768	C
1	5	1769	G
1	5	1770	A
1	5	1772	C
1	5	1776	A
1	5	1777	C
1	5	1779	U
1	5	1781	U
1	5	1787	A
1	5	1788	A
1	5	1790	U
1	5	1791	U
1	5	1799	G
1	5	1800	U
1	5	1803	G
1	5	1804	A
1	5	1805	A
1	5	1817	U
1	5	1818	G
1	5	1819	G
1	5	1820	C
1	5	1822	U
1	5	1825	A
1	5	1827	C
1	5	1830	G
1	5	1832	C
1	5	1833	G
1	5	1834	U
1	5	1835	G
1	5	1836	G
1	5	1840	G
1	5	1843	A
1	5	1847	C
1	5	1848	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1849	U
1	5	1850	A
1	5	1851	G
1	5	1855	G
1	5	1864	G
1	5	1866	U
1	5	1867	A
1	5	1869	G
1	5	1878	G
1	5	1881	C
1	5	1882	U
1	5	1886	G
1	5	1890	G
1	5	1891	A
1	5	1897	A
1	5	1899	G
1	5	1900	C
1	5	1903	G
1	5	1907	A
1	5	1910	G
1	5	1912	G
1	5	1913	C
1	5	1916	G
1	5	1917	A
1	5	1918	U
1	5	1919	G
1	5	1920	C
1	5	1921	C
1	5	1922	G
1	5	1923	A
1	5	1925	G
1	5	1929	A
1	5	1930	U
1	5	1931	C
1	5	1932	A
1	5	1935	C
1	5	1936	C
1	5	1938	C
1	5	1940	G
1	5	1941	A
1	5	1947	U
1	5	1948	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1951	G
1	5	1952	G
1	5	1956	A
1	5	1959	U
1	5	1961	G
1	5	1962	A
1	5	1964	A
1	5	1965	G
1	5	1966	C
1	5	1971	C
1	5	1974	U
1	5	1975	G
1	5	1976	G
1	5	1977	C
1	5	1979	A
1	5	1980	U
1	5	1981	G
1	5	1983	A
1	5	1984	A
1	5	1985	G
1	5	1986	U
1	5	1987	C
1	5	1988	G
1	5	1992	U
1	5	1993	C
1	5	1997	U
1	5	1998	A
1	5	1999	A
1	5	2001	G
1	5	2002	A
1	5	2003	G
1	5	2004	U
1	5	2005	G
1	5	2007	G
1	5	2008	U
1	5	2009	A
1	5	2010	A
1	5	2015	U
1	5	2018	C
1	5	2019	C
1	5	2020	U
1	5	2023	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2024	G
1	5	2025	A
1	5	2026	A
1	5	2033	A
1	5	2034	G
1	5	2040	A
1	5	2044	U
1	5	2045	G
1	5	2046	G
1	5	2047	A
1	5	2048	U
1	5	2052	G
1	5	2055	G
1	5	2056	G
1	5	2057	A
1	5	2059	C
1	5	2060	G
1	5	2062	C
1	5	2063	G
1	5	2064	G
1	5	2069	A
1	5	2070	U
1	5	2077	C
1	5	2083	C
1	5	2084	C
1	5	2085	G
1	5	2088	A
1	5	2089	G
1	5	2090	U
1	5	2091	C
1	5	2092	G
1	5	2093	A
1	5	2094	G
1	5	2095	A
1	5	2096	G
1	5	2097	U
1	5	2100	A
1	5	2105	A
1	5	2107	C
1	5	2108	G
1	5	2109	G
1	5	2110	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2111	G
1	5	2112	G
1	5	2113	G
1	5	2114	G
1	5	2115	G
1	5	2116	C
1	5	2117	G
1	5	2118	G
1	5	2119	C
1	5	2120	G
1	5	2121	C
1	5	2122	G
1	5	2123	C
1	5	2124	G
1	5	2125	C
1	5	2126	G
1	5	2127	C
1	5	2247	C
1	5	2248	C
1	5	2250	C
1	5	2251	G
1	5	2252	G
1	5	2253	A
1	5	2254	G
1	5	2255	C
1	5	2256	C
1	5	2257	C
1	5	2258	C
1	5	2259	G
1	5	2260	C
1	5	2261	G
1	5	2262	G
1	5	2263	A
1	5	2264	C
1	5	2265	G
1	5	2266	C
1	5	2267	U
1	5	2268	A
1	5	2269	C
1	5	2270	G
1	5	2273	G
1	5	2275	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2277	C
1	5	2279	A
1	5	2282	A
1	5	2283	G
1	5	2288	G
1	5	2289	C
1	5	2299	G
1	5	2300	A
1	5	2301	G
1	5	2305	U
1	5	2309	G
1	5	2312	U
1	5	2313	A
1	5	2314	G
1	5	2316	G
1	5	2319	C
1	5	2321	G
1	5	2322	G
1	5	2324	C
1	5	2325	C
1	5	2328	G
1	5	2329	U
1	5	2330	G
1	5	2331	G
1	5	2332	A
1	5	2333	G
1	5	2334	C
1	5	2337	C
1	5	2339	G
1	5	2342	G
1	5	2343	G
1	5	2347	A
1	5	2348	G
1	5	2349	A
1	5	2350	U
1	5	2351	C
1	5	2357	G
1	5	2360	A
1	5	2361	G
1	5	2362	U
1	5	2366	A
1	5	2367	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2368	A
1	5	2369	U
1	5	2370	A
1	5	2372	U
1	5	2378	G
1	5	2382	A
1	5	2384	U
1	5	2389	A
1	5	2390	G
1	5	2391	G
1	5	2395	A
1	5	2396	A
1	5	2397	G
1	5	2398	U
1	5	2399	G
1	5	2407	G
1	5	2409	U
1	5	2417	A
1	5	2422	C
1	5	2425	U
1	5	2426	U
1	5	2428	A
1	5	2429	A
1	5	2432	U
1	5	2433	G
1	5	2434	G
1	5	2437	C
1	5	2438	A
1	5	2439	G
1	5	2440	U
1	5	2441	C
1	5	2443	G
1	5	2447	U
1	5	2448	G
1	5	2450	G
1	5	2454	U
1	5	2456	G
1	5	2464	C
1	5	2465	C
1	5	2468	U
1	5	2469	C
1	5	2470	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2471	G
1	5	2472	A
1	5	2474	G
1	5	2475	G
1	5	2476	G
1	5	2487	G
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2502	G
1	5	2503	G
1	5	2504	C
1	5	2505	C
1	5	2506	G
1	5	2507	A
1	5	2508	U
1	5	2509	C
1	5	2510	G
1	5	2511	A
1	5	2512	A
1	5	2513	A
1	5	2514	G
1	5	2526	C
1	5	2527	A
1	5	2529	A
1	5	2530	U
1	5	2532	C
1	5	2537	A
1	5	2544	G
1	5	2545	U
1	5	2546	G
1	5	2547	G
1	5	2549	G
1	5	2551	A
1	5	2552	G
1	5	2553	A
1	5	2554	U
1	5	2555	G
1	5	2560	C
1	5	2566	G
1	5	2571	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2572	C
1	5	2577	C
1	5	2581	A
1	5	2583	C
1	5	2586	G
1	5	2587	A
1	5	2588	C
1	5	2589	C
1	5	2600	A
1	5	2601	A
1	5	2602	G
1	5	2615	C
1	5	2616	C
1	5	2620	G
1	5	2623	A
1	5	2627	C
1	5	2630	U
1	5	2631	U
1	5	2638	G
1	5	2639	U
1	5	2640	G
1	5	2643	G
1	5	2645	G
1	5	2648	G
1	5	2649	G
1	5	2653	C
1	5	2658	G
1	5	2659	A
1	5	2660	A
1	5	2661	U
1	5	2662	G
1	5	2664	G
1	5	2666	U
1	5	2667	C
1	5	2670	C
1	5	2673	G
1	5	2674	A
1	5	2675	G
1	5	2678	A
1	5	2684	C
1	5	2687	U
1	5	2688	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2689	C
1	5	2692	U
1	5	2694	G
1	5	2696	A
1	5	2704	C
1	5	2710	C
1	5	2711	G
1	5	2712	G
1	5	2713	C
1	5	2714	G
1	5	2716	C
1	5	2722	G
1	5	2725	A
1	5	2726	G
1	5	2735	G
1	5	2737	C
1	5	2740	U
1	5	2743	A
1	5	2744	A
1	5	2745	A
1	5	2747	U
1	5	2751	G
1	5	2752	G
1	5	2754	G
1	5	2756	G
1	5	2760	G
1	5	2762	G
1	5	2764	A
1	5	2765	A
1	5	2766	A
1	5	2767	U
1	5	2768	C
1	5	2769	U
1	5	2770	C
1	5	2783	A
1	5	2786	C
1	5	2787	A
1	5	2788	U
1	5	2790	U
1	5	2794	C
1	5	2796	G
1	5	2797	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2798	A
1	5	2799	G
1	5	2806	A
1	5	2807	A
1	5	2808	G
1	5	2812	A
1	5	2813	A
1	5	2814	C
1	5	2815	A
1	5	2818	C
1	5	2820	C
1	5	2821	U
1	5	2824	C
1	5	2826	U
1	5	2827	G
1	5	2828	U
1	5	2829	U
1	5	2832	A
1	5	2833	A
1	5	2834	C
1	5	2835	A
1	5	2838	G
1	5	2841	G
1	5	2842	G
1	5	2848	G
1	5	2849	A
1	5	2850	A
1	5	2852	U
1	5	2854	G
1	5	2855	G
1	5	2858	A
1	5	2859	G
1	5	2860	C
1	5	2866	C
1	5	2867	C
1	5	2873	U
1	5	2874	U
1	5	2875	C
1	5	2876	G
1	5	2879	A
1	5	2880	U
1	5	2888	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2892	C
1	5	2897	G
1	5	2898	G
1	5	2900	U
1	5	2904	U
1	5	2905	C
1	5	2910	G
1	5	3591	C
1	5	3592	G
1	5	3594	C
1	5	3595	U
1	5	3596	A
1	5	3597	G
1	5	3605	C
1	5	3606	U
1	5	3615	G
1	5	3616	U
1	5	3617	G
1	5	3620	G
1	5	3621	A
1	5	3623	C
1	5	3625	G
1	5	3626	G
1	5	3627	G
1	5	3635	A
1	5	3636	C
1	5	3643	A
1	5	3644	U
1	5	3649	A
1	5	3650	C
1	5	3658	C
1	5	3660	C
1	5	3662	A
1	5	3663	A
1	5	3664	G
1	5	3667	C
1	5	3668	C
1	5	3670	C
1	5	3671	G
1	5	3672	G
1	5	3673	C
1	5	3674	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	3675	G
1	5	3677	U
1	5	3678	G
1	5	3679	U
1	5	3680	U
1	5	3681	G
1	5	3682	A
1	5	3688	U
1	5	3692	A
1	5	3698	G
1	5	3699	C
1	5	3709	U
1	5	3710	G
1	5	3711	A
1	5	3712	A
1	5	3713	U
1	5	3715	U
1	5	3716	C
1	5	3717	A
1	5	3718	A
1	5	3727	A
1	5	3728	A
1	5	3729	U
1	5	3733	A
1	5	3735	G
1	5	3736	A
1	5	3737	A
1	5	3738	G
1	5	3739	C
1	5	3743	G
1	5	3744	G
1	5	3745	U
1	5	3748	A
1	5	3756	A
1	5	3759	A
1	5	3760	A
1	5	3770	U
1	5	3772	U
1	5	3773	U
1	5	3774	A
1	5	3775	A
1	5	3776	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	3777	G
1	5	3784	A
1	5	3785	A
1	5	3786	U
1	5	3791	C
1	5	3799	A
1	5	3800	A
1	5	3802	U
1	5	3803	A
1	5	3807	A
1	5	3809	G
1	5	3810	C
1	5	3811	G
1	5	3813	A
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3822	U
1	5	3831	U
1	5	3838	U
1	5	3839	G
1	5	3840	U
1	5	3843	C
1	5	3849	A
1	5	3851	U
1	5	3859	G
1	5	3861	A
1	5	3865	A
1	5	3867	A
1	5	3876	A
1	5	3877	A
1	5	3878	C
1	5	3879	G
1	5	3880	G
1	5	3881	G
1	5	3882	C
1	5	3887	C
1	5	3889	G
1	5	3895	G
1	5	3897	G
1	5	3898	G
1	5	3899	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	3900	G
1	5	3901	A
1	5	3902	A
1	5	3905	A
1	5	3906	A
1	5	3907	G
1	5	3908	A
1	5	3912	U
1	5	3913	G
1	5	3914	U
1	5	3915	U
1	5	3916	G
1	5	3917	A
1	5	3923	A
1	5	3925	U
1	5	3926	C
1	5	3938	G
1	5	3939	G
1	5	3943	A
1	5	4069	U
1	5	4070	U
1	5	4073	A
1	5	4075	U
1	5	4076	G
1	5	4083	U
1	5	4084	G
1	5	4085	A
1	5	4086	G
1	5	4087	G
1	5	4088	C
1	5	4089	G
1	5	4091	G
1	5	4092	G
1	5	4093	G
1	5	4094	G
1	5	4095	G
1	5	4097	G
1	5	4104	G
1	5	4105	A
1	5	4107	G
1	5	4114	C
1	5	4115	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4116	C
1	5	4117	U
1	5	4118	U
1	5	4119	C
1	5	4120	U
1	5	4121	G
1	5	4122	G
1	5	4125	C
1	5	4126	C
1	5	4127	A
1	5	4129	G
1	5	4132	C
1	5	4140	C
1	5	4143	G
1	5	4145	C
1	5	4158	C
1	5	4162	C
1	5	4164	C
1	5	4166	G
1	5	4168	G
1	5	4169	G
1	5	4171	C
1	5	4172	A
1	5	4173	G
1	5	4180	G
1	5	4183	G
1	5	4184	G
1	5	4191	G
1	5	4195	G
1	5	4196	G
1	5	4197	G
1	5	4199	C
1	5	4203	A
1	5	4205	A
1	5	4206	C
1	5	4208	U
1	5	4212	A
1	5	4213	A
1	5	4214	A
1	5	4215	C
1	5	4216	G
1	5	4217	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4218	U
1	5	4219	A
1	5	4220	A
1	5	4221	C
1	5	4222	G
1	5	4225	G
1	5	4226	G
1	5	4228	G
1	5	4229	U
1	5	4232	U
1	5	4233	A
1	5	4234	A
1	5	4235	G
1	5	4236	G
1	5	4239	A
1	5	4241	C
1	5	4249	G
1	5	4251	A
1	5	4252	C
1	5	4254	G
1	5	4255	A
1	5	4257	A
1	5	4258	C
1	5	4265	U
1	5	4267	G
1	5	4268	A
1	5	4271	A
1	5	4274	A
1	5	4276	G
1	5	4279	A
1	5	4280	A
1	5	4281	A
1	5	4282	A
1	5	4283	G
1	5	4286	C
1	5	4287	G
1	5	4288	C
1	5	4290	U
1	5	4291	G
1	5	4296	U
1	5	4297	G
1	5	4305	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4306	U
1	5	4311	A
1	5	4314	C
1	5	4316	G
1	5	4318	C
1	5	4323	A
1	5	4329	G
1	5	4330	G
1	5	4332	C
1	5	4335	C
1	5	4336	A
1	5	4337	C
1	5	4339	A
1	5	4344	U
1	5	4348	A
1	5	4349	C
1	5	4350	C
1	5	4352	U
1	5	4353	U
1	5	4354	U
1	5	4356	G
1	5	4364	G
1	5	4368	G
1	5	4369	A
1	5	4373	G
1	5	4374	U
1	5	4375	C
1	5	4376	A
1	5	4377	G
1	5	4378	A
1	5	4379	A
1	5	4385	A
1	5	4386	C
1	5	4387	C
1	5	4388	A
1	5	4391	G
1	5	4393	G
1	5	4394	A
1	5	4395	U
1	5	4396	A
1	5	4401	G
1	5	4419	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4422	A
1	5	4425	G
1	5	4426	C
1	5	4434	C
1	5	4436	U
1	5	4437	U
1	5	4438	U
1	5	4439	U
1	5	4440	G
1	5	4441	A
1	5	4443	C
1	5	4444	C
1	5	4448	G
1	5	4449	A
1	5	4450	U
1	5	4451	G
1	5	4452	U
1	5	4454	G
1	5	4459	U
1	5	4463	U
1	5	4464	A
1	5	4465	U
1	5	4466	C
1	5	4467	A
1	5	4469	U
1	5	4471	U
1	5	4472	G
1	5	4473	A
1	5	4475	G
1	5	4476	C
1	5	4484	A
1	5	4488	A
1	5	4489	G
1	5	4491	G
1	5	4498	U
1	5	4500	U
1	5	4503	A
1	5	4510	A
1	5	4511	A
1	5	4512	U
1	5	4513	A
1	5	4518	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4519	C
1	5	4520	G
1	5	4522	G
1	5	4523	A
1	5	4524	G
1	5	4528	G
1	5	4529	G
1	5	4530	U
1	5	4531	U
1	5	4532	U
1	5	4534	G
1	5	4536	C
1	5	4537	C
1	5	4543	G
1	5	4544	A
1	5	4546	A
1	5	4548	A
1	5	4549	G
1	5	4550	G
1	5	4552	U
1	5	4557	U
1	5	4560	C
1	5	4569	U
1	5	4570	G
1	5	4572	U
1	5	4574	U
1	5	4575	G
1	5	4581	G
1	5	4583	C
1	5	4584	A
1	5	4585	U
1	5	4586	G
1	5	4589	A
1	5	4590	A
1	5	4592	C
1	5	4599	A
1	5	4600	G
1	5	4601	U
1	5	4603	C
1	5	4605	A
1	5	4606	G
1	5	4608	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4617	G
1	5	4623	G
1	5	4624	A
1	5	4636	U
1	5	4637	G
1	5	4641	U
1	5	4646	U
1	5	4647	G
1	5	4648	A
1	5	4652	G
1	5	4656	A
1	5	4657	U
1	5	4661	G
1	5	4664	A
1	5	4669	A
1	5	4670	C
1	5	4671	C
1	5	4672	A
1	5	4676	G
1	5	4677	U
1	5	4678	G
1	5	4679	G
1	5	4687	A
1	5	4693	C
1	5	4694	G
1	5	4695	C
1	5	4700	A
1	5	4701	A
1	5	4709	U
1	5	4714	C
1	5	4715	C
1	5	4717	A
1	5	4718	G
1	5	4719	G
1	5	4720	C
1	5	4721	G
1	5	4722	G
1	5	4729	A
1	5	4730	C
1	5	4731	G
1	5	4732	G
1	5	4733	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4734	A
1	5	4735	G
1	5	4737	G
1	5	4738	C
1	5	4741	C
1	5	4743	G
1	5	4745	G
1	5	4746	C
1	5	4748	U
1	5	4749	C
1	5	4750	G
1	5	4751	G
1	5	4753	U
1	5	4756	C
1	5	4757	C
1	5	4758	U
1	5	4760	G
1	5	4763	U
1	5	4764	A
1	5	4770	U
1	5	4771	C
1	5	4774	C
1	5	4860	G
1	5	4865	C
1	5	4869	U
1	5	4871	C
1	5	4872	G
1	5	4873	G
1	5	4874	A
1	5	4875	G
1	5	4876	U
1	5	4877	G
1	5	4878	C
1	5	4881	U
1	5	4882	U
1	5	4883	C
1	5	4884	G
1	5	4885	U
1	5	4886	C
1	5	4888	U
1	5	4889	G
1	5	4890	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4891	G
1	5	4893	A
1	5	4895	C
1	5	4896	G
1	5	4900	C
1	5	4901	G
1	5	4903	G
1	5	4906	C
1	5	4910	G
1	5	4911	A
1	5	4912	G
1	5	4913	G
1	5	4915	G
1	5	4919	G
1	5	4926	C
1	5	4927	G
1	5	4928	C
1	5	4929	C
1	5	4930	C
1	5	4932	U
1	5	4933	C
1	5	4934	A
1	5	4936	G
1	5	4937	C
1	5	4938	A
1	5	4939	C
1	5	4942	C
1	5	4945	G
1	5	4946	U
1	5	4947	U
1	5	4948	C
1	5	4949	G
1	5	4950	U
1	5	4951	G
1	5	4952	G
1	5	4953	G
1	5	4957	C
1	5	4959	U
1	5	4961	G
1	5	4962	C
1	5	4964	C
1	5	4965	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4966	A
1	5	4967	A
1	5	4977	A
1	5	4979	A
1	5	4980	C
1	5	4981	G
1	5	4982	A
1	5	4985	U
1	5	4988	U
1	5	4989	U
1	5	4990	C
1	5	4991	U
1	5	4992	G
1	5	4993	G
1	5	4999	G
1	5	5002	U
1	5	5006	U
1	5	5013	C
1	5	5014	A
1	5	5016	A
1	5	5017	G
1	5	5018	C
1	5	5019	A
1	5	5021	C
1	5	5023	C
1	5	5026	U
1	5	5027	C
1	5	5028	G
1	5	5034	A
1	5	5035	U
1	5	5040	U
1	5	5041	G
1	5	5042	A
1	5	5045	G
1	5	5047	C
1	5	5048	A
1	5	5049	G
1	5	5050	C
1	5	5052	C
1	5	5053	U
1	5	5054	C
1	5	5056	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	5057	C
1	5	5058	A
1	5	5060	A
1	5	5061	A
1	5	5062	G
1	5	5063	G
1	5	5069	U
2	7	7	G
2	7	11	A
2	7	17	C
2	7	21	G
2	7	22	A
2	7	23	A
2	7	24	C
2	7	27	G
2	7	30	C
2	7	31	G
2	7	42	A
2	7	53	U
2	7	54	A
2	7	57	C
2	7	60	G
2	7	63	C
2	7	64	G
2	7	65	G
2	7	70	G
2	7	73	U
2	7	74	A
2	7	79	U
2	7	80	U
2	7	90	A
2	7	100	A
2	7	105	C
2	7	106	G
2	7	110	G
2	7	112	U
2	7	115	A
2	7	120	U
3	8	2	G
3	8	3	A
3	8	9	A
3	8	11	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	8	13	G
3	8	16	G
3	8	23	C
3	8	32	C
3	8	33	G
3	8	34	U
3	8	35	C
3	8	37	A
3	8	38	U
3	8	39	G
3	8	40	A
3	8	46	G
3	8	48	A
3	8	50	C
3	8	51	U
3	8	59	A
3	8	61	A
3	8	62	A
3	8	63	U
3	8	64	U
3	8	65	A
3	8	70	G
3	8	71	A
3	8	74	U
3	8	75	G
3	8	80	A
3	8	81	C
3	8	82	A
3	8	83	C
3	8	84	A
3	8	85	U
3	8	86	U
3	8	87	G
3	8	90	C
3	8	94	G
3	8	95	A
3	8	97	A
3	8	98	C
3	8	99	U
3	8	103	A
3	8	104	A
3	8	105	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	8	109	C
3	8	110	U
3	8	111	U
3	8	112	G
3	8	114	G
3	8	118	C
3	8	121	G
3	8	122	G
3	8	125	C
3	8	126	C
3	8	127	U
3	8	137	A
3	8	147	G
3	8	151	G
3	8	153	C

All (660) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	1	C
1	5	20	U
1	5	33	A
1	5	39	A
1	5	42	A
1	5	47	A
1	5	48	G
1	5	51	A
1	5	53	C
1	5	54	G
1	5	55	G
1	5	62	A
1	5	64	A
1	5	65	A
1	5	66	A
1	5	84	A
1	5	85	G
1	5	88	A
1	5	94	A
1	5	97	G
1	5	98	A
1	5	99	A
1	5	100	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	107	G
1	5	111	C
1	5	112	C
1	5	119	G
1	5	120	A
1	5	125	C
1	5	134	G
1	5	136	C
1	5	143	C
1	5	149	A
1	5	151	G
1	5	158	A
1	5	159	C
1	5	163	A
1	5	170	C
1	5	172	C
1	5	183	C
1	5	186	G
1	5	187	U
1	5	197	A
1	5	207	G
1	5	209	U
1	5	216	C
1	5	218	A
1	5	219	G
1	5	226	G
1	5	235	A
1	5	237	G
1	5	245	C
1	5	253	G
1	5	265	C
1	5	266	C
1	5	268	G
1	5	275	C
1	5	276	C
1	5	280	G
1	5	292	G
1	5	293	G
1	5	296	A
1	5	298	G
1	5	315	G
1	5	333	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	337	U
1	5	340	C
1	5	349	A
1	5	353	A
1	5	354	U
1	5	360	A
1	5	361	C
1	5	362	A
1	5	371	A
1	5	385	A
1	5	387	G
1	5	388	A
1	5	393	U
1	5	394	G
1	5	405	U
1	5	406	C
1	5	407	A
1	5	410	A
1	5	414	C
1	5	417	G
1	5	421	C
1	5	432	U
1	5	435	A
1	5	451	C
1	5	454	U
1	5	485	C
1	5	486	C
1	5	493	G
1	5	495	C
1	5	496	G
1	5	497	G
1	5	502	C
1	5	505	G
1	5	514	U
1	5	647	G
1	5	648	G
1	5	655	C
1	5	658	C
1	5	659	G
1	5	664	G
1	5	666	G
1	5	668	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	684	G
1	5	686	A
1	5	693	C
1	5	704	C
1	5	727	C
1	5	728	U
1	5	732	A
1	5	733	A
1	5	738	C
1	5	746	A
1	5	747	A
1	5	909	A
1	5	911	U
1	5	917	A
1	5	920	C
1	5	927	G
1	5	930	G
1	5	931	C
1	5	932	A
1	5	936	C
1	5	943	A
1	5	946	C
1	5	956	A
1	5	957	G
1	5	958	G
1	5	961	G
1	5	962	C
1	5	965	G
1	5	968	C
1	5	974	C
1	5	977	C
1	5	978	G
1	5	979	C
1	5	986	C
1	5	987	C
1	5	989	U
1	5	1067	G
1	5	1068	G
1	5	1074	G
1	5	1076	C
1	5	1186	U
1	5	1210	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1211	G
1	5	1214	C
1	5	1217	G
1	5	1221	G
1	5	1232	G
1	5	1235	G
1	5	1236	C
1	5	1237	C
1	5	1238	A
1	5	1239	C
1	5	1241	C
1	5	1243	C
1	5	1244	G
1	5	1254	A
1	5	1264	C
1	5	1266	G
1	5	1268	G
1	5	1272	C
1	5	1274	A
1	5	1279	A
1	5	1280	C
1	5	1281	G
1	5	1293	G
1	5	1296	G
1	5	1319	U
1	5	1324	A
1	5	1325	C
1	5	1329	G
1	5	1334	A
1	5	1356	U
1	5	1357	C
1	5	1359	G
1	5	1364	U
1	5	1365	C
1	5	1368	A
1	5	1370	G
1	5	1371	A
1	5	1377	G
1	5	1378	C
1	5	1379	C
1	5	1380	G
1	5	1386	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1398	A
1	5	1405	C
1	5	1406	G
1	5	1407	C
1	5	1410	U
1	5	1419	G
1	5	1420	A
1	5	1426	G
1	5	1428	U
1	5	1438	U
1	5	1439	C
1	5	1440	U
1	5	1445	U
1	5	1464	C
1	5	1474	C
1	5	1479	G
1	5	1480	C
1	5	1481	C
1	5	1484	G
1	5	1488	G
1	5	1489	G
1	5	1500	A
1	5	1509	C
1	5	1521	C
1	5	1522	G
1	5	1539	G
1	5	1554	A
1	5	1562	G
1	5	1563	A
1	5	1564	A
1	5	1596	U
1	5	1613	A
1	5	1614	C
1	5	1615	C
1	5	1617	G
1	5	1627	G
1	5	1633	G
1	5	1636	U
1	5	1640	C
1	5	1650	A
1	5	1654	G
1	5	1671	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1676	C
1	5	1681	G
1	5	1682	A
1	5	1696	C
1	5	1697	G
1	5	1698	C
1	5	1724	G
1	5	1725	U
1	5	1742	A
1	5	1763	C
1	5	1764	G
1	5	1804	A
1	5	1808	C
1	5	1819	G
1	5	1835	G
1	5	1864	G
1	5	1865	G
1	5	1869	G
1	5	1876	U
1	5	1881	C
1	5	1884	C
1	5	1887	G
1	5	1890	G
1	5	1891	A
1	5	1912	G
1	5	1919	G
1	5	1920	C
1	5	1921	C
1	5	1925	G
1	5	1928	C
1	5	1930	U
1	5	1935	C
1	5	1938	C
1	5	1945	G
1	5	1946	G
1	5	1961	G
1	5	1963	C
1	5	1974	U
1	5	1975	G
1	5	1980	U
1	5	1983	A
1	5	1992	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1998	A
1	5	2007	G
1	5	2008	U
1	5	2009	A
1	5	2014	C
1	5	2025	A
1	5	2034	G
1	5	2035	C
1	5	2044	U
1	5	2046	G
1	5	2057	A
1	5	2068	C
1	5	2075	G
1	5	2077	C
1	5	2083	C
1	5	2088	A
1	5	2089	G
1	5	2090	U
1	5	2093	A
1	5	2094	G
1	5	2096	G
1	5	2107	C
1	5	2111	G
1	5	2114	G
1	5	2116	C
1	5	2118	G
1	5	2119	C
1	5	2122	G
1	5	2123	C
1	5	2124	G
1	5	2126	G
1	5	2246	C
1	5	2248	C
1	5	2250	C
1	5	2251	G
1	5	2256	C
1	5	2257	C
1	5	2258	C
1	5	2260	C
1	5	2261	G
1	5	2262	G
1	5	2264	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2265	G
1	5	2266	C
1	5	2267	U
1	5	2268	A
1	5	2269	C
1	5	2272	C
1	5	2276	A
1	5	2278	G
1	5	2289	C
1	5	2313	A
1	5	2321	G
1	5	2323	C
1	5	2324	C
1	5	2325	C
1	5	2328	G
1	5	2329	U
1	5	2331	G
1	5	2332	A
1	5	2347	A
1	5	2361	G
1	5	2362	U
1	5	2370	A
1	5	2389	A
1	5	2394	G
1	5	2396	A
1	5	2398	U
1	5	2417	A
1	5	2436	U
1	5	2438	A
1	5	2447	U
1	5	2448	G
1	5	2459	G
1	5	2464	C
1	5	2468	U
1	5	2470	C
1	5	2474	G
1	5	2479	G
1	5	2487	G
1	5	2490	U
1	5	2502	G
1	5	2507	A
1	5	2509	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2512	A
1	5	2513	A
1	5	2514	G
1	5	2515	G
1	5	2529	A
1	5	2533	C
1	5	2544	G
1	5	2545	U
1	5	2546	G
1	5	2553	A
1	5	2554	U
1	5	2576	G
1	5	2581	A
1	5	2583	C
1	5	2587	A
1	5	2588	C
1	5	2589	C
1	5	2591	A
1	5	2600	A
1	5	2614	C
1	5	2618	G
1	5	2622	G
1	5	2631	U
1	5	2652	G
1	5	2658	G
1	5	2661	U
1	5	2665	U
1	5	2666	U
1	5	2673	G
1	5	2674	A
1	5	2677	G
1	5	2683	C
1	5	2686	G
1	5	2688	G
1	5	2695	A
1	5	2703	G
1	5	2711	G
1	5	2732	G
1	5	2744	A
1	5	2761	U
1	5	2768	C
1	5	2769	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2782	U
1	5	2786	C
1	5	2796	G
1	5	2803	U
1	5	2806	A
1	5	2811	G
1	5	2812	A
1	5	2817	C
1	5	2825	A
1	5	2827	G
1	5	2828	U
1	5	2833	A
1	5	2834	C
1	5	2837	U
1	5	2843	U
1	5	2848	G
1	5	2851	G
1	5	2858	A
1	5	2859	G
1	5	2879	A
1	5	2895	A
1	5	2896	G
1	5	3590	G
1	5	3593	C
1	5	3615	G
1	5	3620	G
1	5	3622	C
1	5	3625	G
1	5	3626	G
1	5	3636	C
1	5	3648	A
1	5	3653	A
1	5	3654	G
1	5	3663	A
1	5	3666	C
1	5	3667	C
1	5	3671	G
1	5	3676	G
1	5	3679	U
1	5	3681	G
1	5	3683	C
1	5	3692	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	3697	U
1	5	3712	A
1	5	3717	A
1	5	3727	A
1	5	3730	U
1	5	3735	G
1	5	3736	A
1	5	3773	U
1	5	3774	A
1	5	3776	G
1	5	3784	A
1	5	3799	A
1	5	3802	U
1	5	3803	A
1	5	3809	G
1	5	3813	A
1	5	3817	A
1	5	3839	G
1	5	3845	A
1	5	3856	A
1	5	3860	A
1	5	3862	A
1	5	3875	G
1	5	3876	A
1	5	3877	A
1	5	3879	G
1	5	3888	G
1	5	3905	A
1	5	3922	G
1	5	3938	G
1	5	3944	G
1	5	4069	U
1	5	4075	U
1	5	4084	G
1	5	4085	A
1	5	4086	G
1	5	4095	G
1	5	4096	C
1	5	4097	G
1	5	4102	C
1	5	4103	C
1	5	4115	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4118	U
1	5	4119	C
1	5	4120	U
1	5	4121	G
1	5	4123	C
1	5	4124	G
1	5	4127	A
1	5	4144	C
1	5	4163	U
1	5	4165	C
1	5	4170	A
1	5	4173	G
1	5	4183	G
1	5	4195	G
1	5	4197	G
1	5	4219	A
1	5	4221	C
1	5	4227	U
1	5	4228	G
1	5	4229	U
1	5	4232	U
1	5	4233	A
1	5	4239	A
1	5	4240	G
1	5	4250	G
1	5	4251	A
1	5	4254	G
1	5	4257	A
1	5	4269	G
1	5	4270	C
1	5	4275	G
1	5	4276	G
1	5	4280	A
1	5	4282	A
1	5	4283	G
1	5	4287	G
1	5	4291	G
1	5	4295	U
1	5	4297	G
1	5	4322	G
1	5	4330	G
1	5	4334	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4338	G
1	5	4348	A
1	5	4349	C
1	5	4368	G
1	5	4374	U
1	5	4375	C
1	5	4378	A
1	5	4385	A
1	5	4395	U
1	5	4419	U
1	5	4425	G
1	5	4436	U
1	5	4440	G
1	5	4448	G
1	5	4449	A
1	5	4451	G
1	5	4454	G
1	5	4463	U
1	5	4464	A
1	5	4472	G
1	5	4474	A
1	5	4475	G
1	5	4481	U
1	5	4488	A
1	5	4489	G
1	5	4497	U
1	5	4498	U
1	5	4507	A
1	5	4518	A
1	5	4519	C
1	5	4522	G
1	5	4527	G
1	5	4528	G
1	5	4531	U
1	5	4533	A
1	5	4535	A
1	5	4536	C
1	5	4543	G
1	5	4547	C
1	5	4548	A
1	5	4560	C
1	5	4574	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4583	C
1	5	4600	G
1	5	4605	A
1	5	4610	A
1	5	4645	C
1	5	4647	G
1	5	4656	A
1	5	4670	C
1	5	4677	U
1	5	4678	G
1	5	4691	A
1	5	4693	C
1	5	4700	A
1	5	4718	G
1	5	4719	G
1	5	4720	C
1	5	4730	C
1	5	4731	G
1	5	4737	G
1	5	4739	C
1	5	4740	G
1	5	4745	G
1	5	4756	C
1	5	4762	A
1	5	4763	U
1	5	4871	C
1	5	4872	G
1	5	4873	G
1	5	4874	A
1	5	4884	G
1	5	4885	U
1	5	4887	C
1	5	4888	U
1	5	4889	G
1	5	4900	C
1	5	4911	A
1	5	4926	C
1	5	4929	C
1	5	4935	C
1	5	4936	G
1	5	4938	A
1	5	4948	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	4949	G
1	5	4950	U
1	5	4951	G
1	5	4981	G
1	5	4990	C
1	5	4991	U
1	5	5022	U
1	5	5026	U
1	5	5027	C
1	5	5041	G
1	5	5046	U
1	5	5049	G
1	5	5056	A
1	5	5059	C
1	5	5060	A
1	5	5061	A
1	5	5062	G
1	5	5068	G
2	7	7	G
2	7	21	G
2	7	42	A
2	7	56	G
2	7	58	A
2	7	60	G
2	7	63	C
2	7	72	U
2	7	75	G
3	8	2	G
3	8	9	A
3	8	10	G
3	8	14	U
3	8	33	G
3	8	34	U
3	8	37	A
3	8	64	U
3	8	70	G
3	8	73	U
3	8	81	C
3	8	83	C
3	8	85	U
3	8	94	G
3	8	95	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	8	98	C
3	8	110	U
3	8	111	U
3	8	124	U
3	8	125	C
3	8	126	C
3	8	131	G

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 133 ligands modelled in this entry, 133 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	12

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
8	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	72:ALA	C	84:VAL	N	23.51
1	5	4776:G	O3'	4859:C	P	17.87
1	5	757:G	O3'	906:C	P	16.89
1	5	519:C	O3'	642:G	P	16.61
1	5	2910:G	O3'	3583:U	P	16.04
1	5	2131:C	O3'	2243:C	P	14.89
1	5	997:C	O3'	1047:C	P	13.99
1	5	1051:G	O3'	1064:G	P	9.59
1	5	1222:A	O3'	1232:G	P	3.97
1	5	1699:A	O3'	1718:C	P	3.33
1	5	1100:U	O3'	1167:C	P	3.02
1	5	4939:C	O3'	4941:G	P	2.74
1	5	4942:C	O3'	4944:C	P	2.72

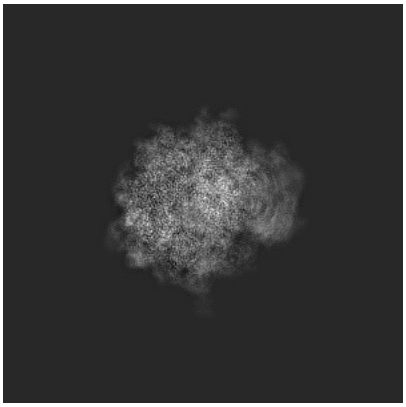
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2650. These allow visual inspection of the internal detail of the map and identification of artifacts.

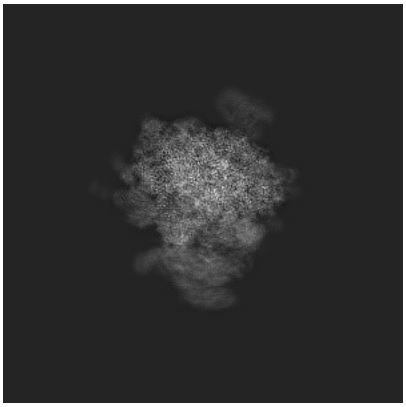
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

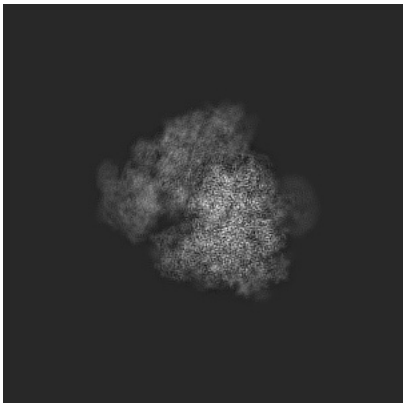
6.1.1 Primary map



X



Y

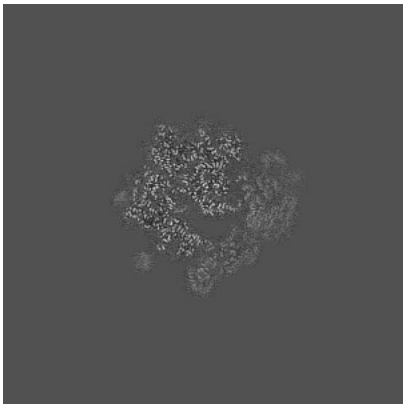


Z

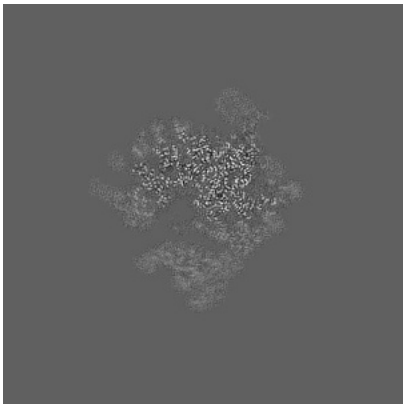
The images above show the map projected in three orthogonal directions.

6.2 Central slices

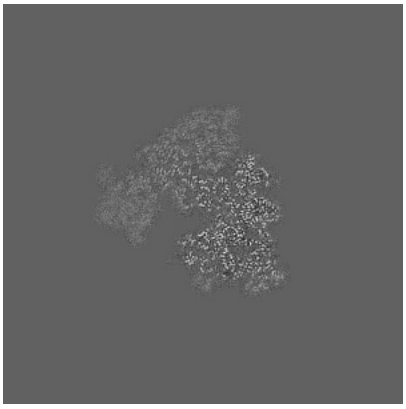
6.2.1 Primary map



X Index: 210



Y Index: 210

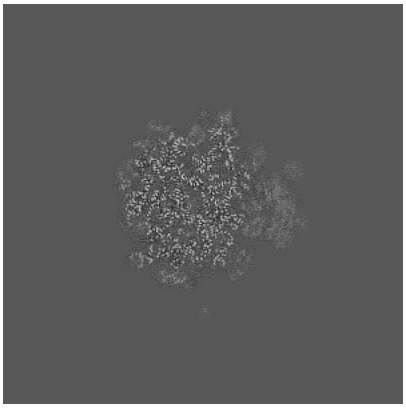


Z Index: 210

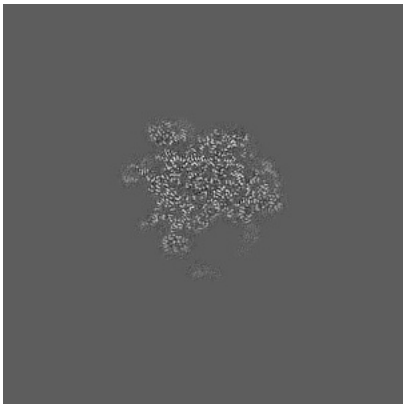
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

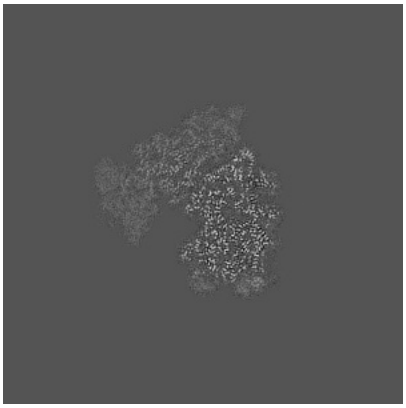
6.3.1 Primary map



X Index: 233



Y Index: 168

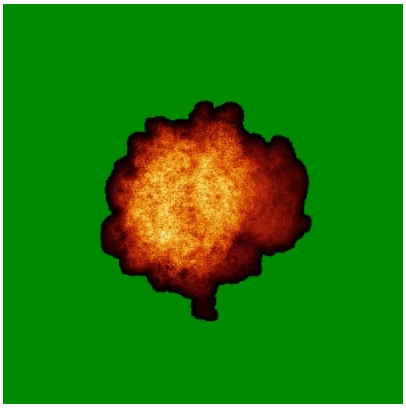


Z Index: 219

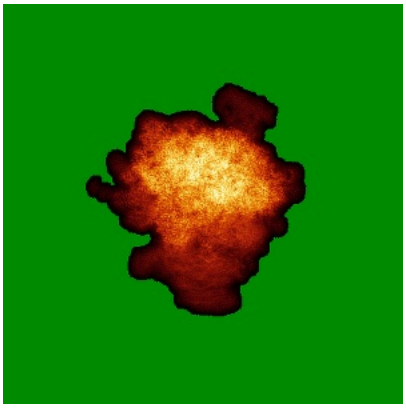
The images above show the largest variance slices of the map in three orthogonal directions.

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

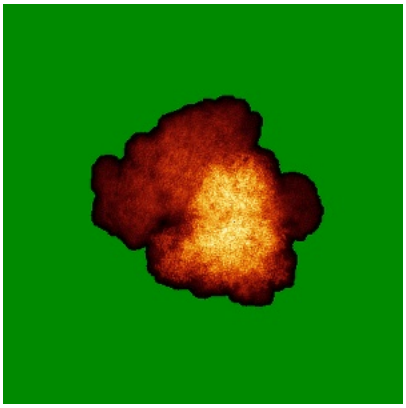
6.4.1 Primary map



X



Y

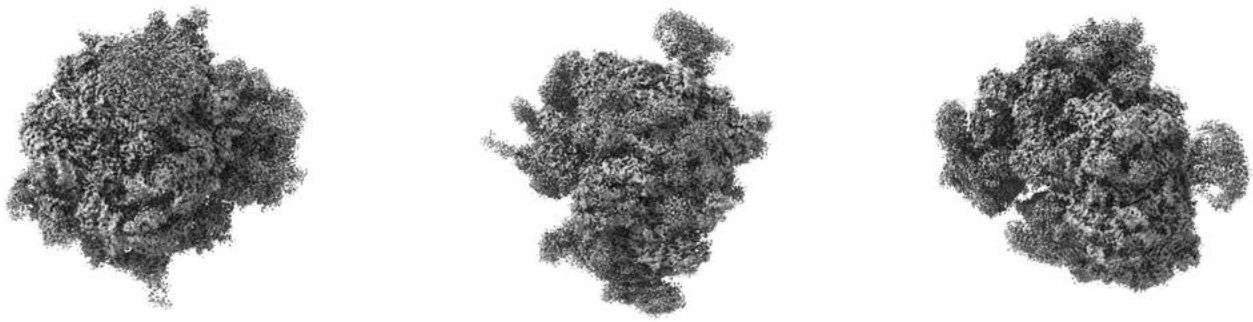


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

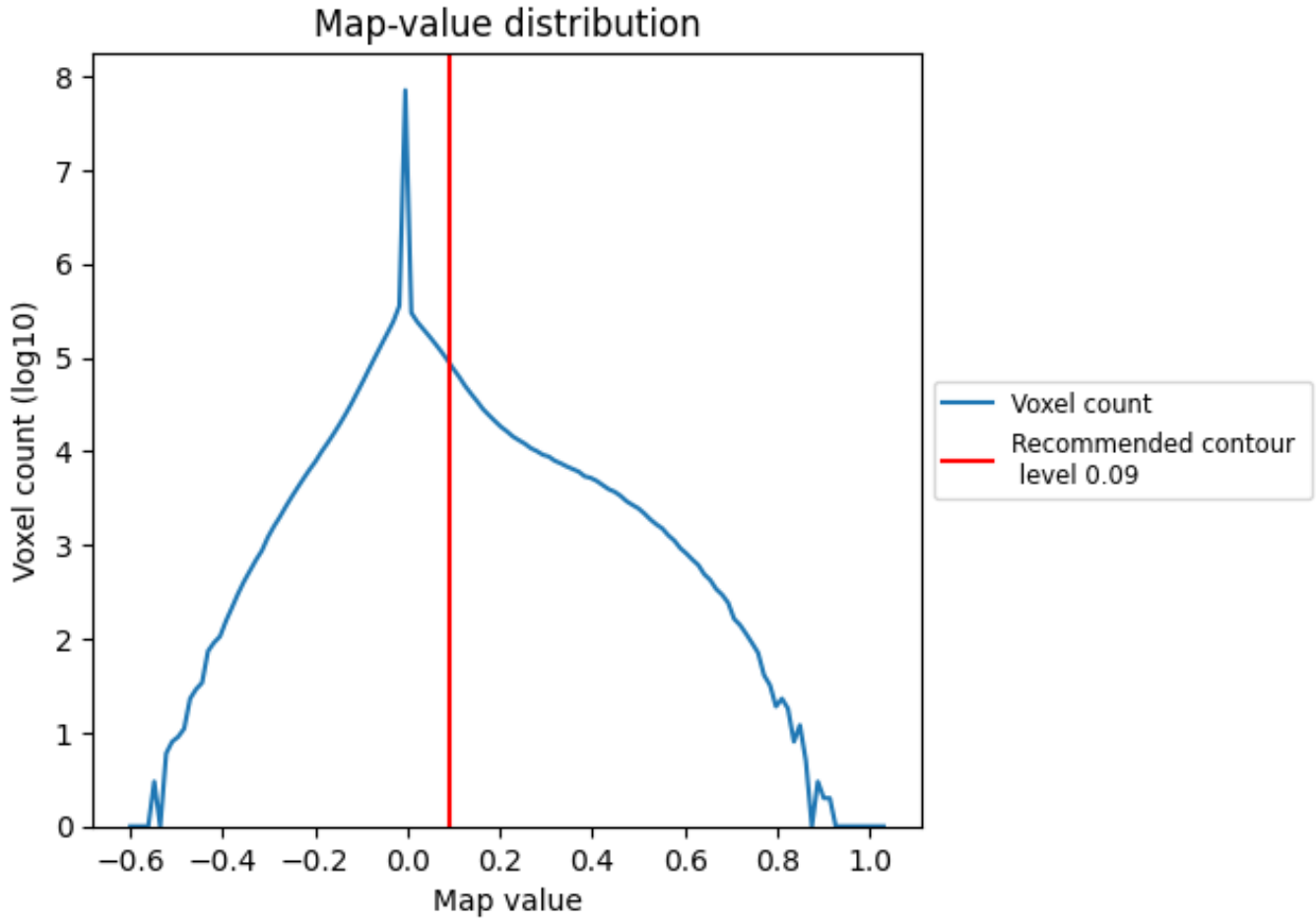
6.6 Mask visualisation (i)

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

7 Map analysis

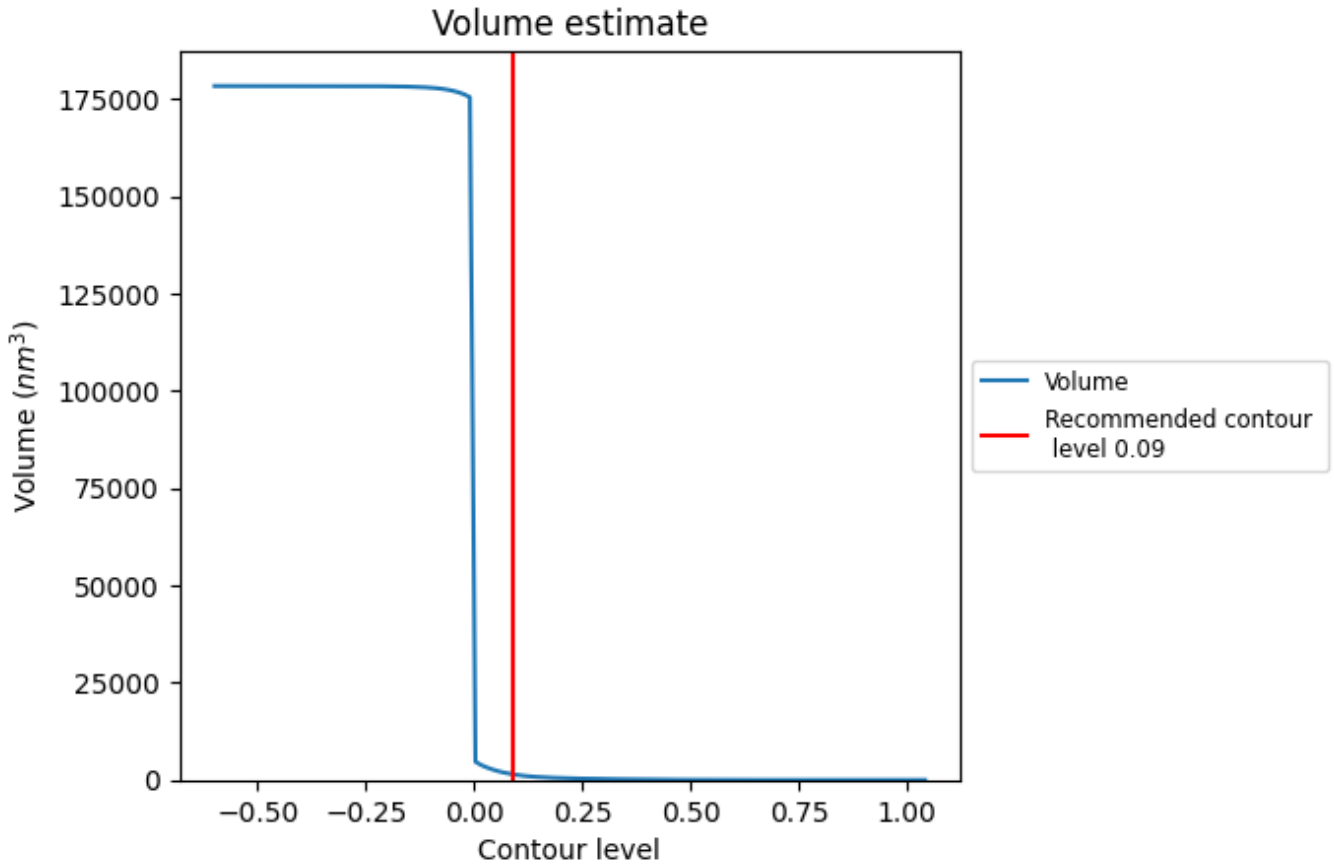
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

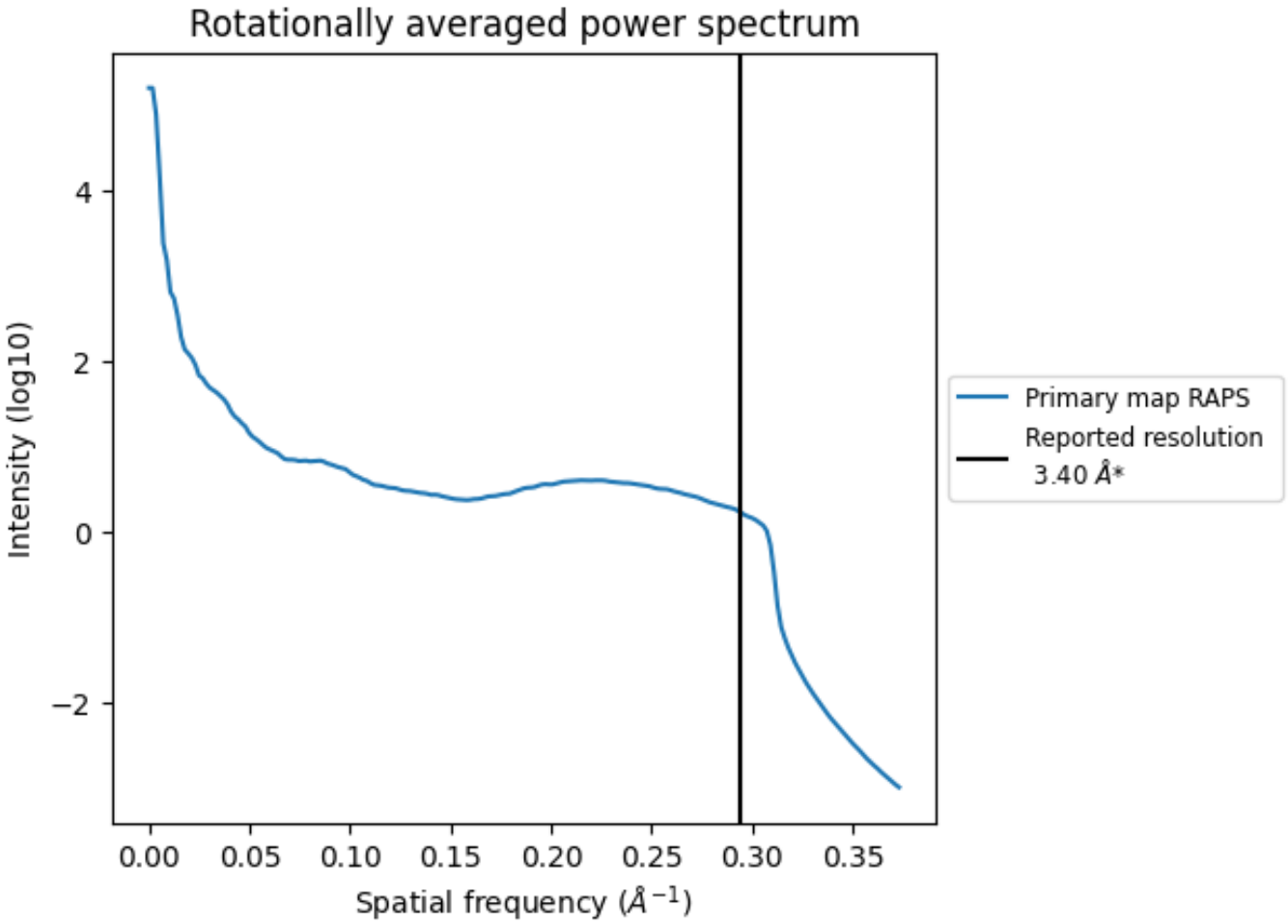
7.2 Volume estimate



The volume at the recommended contour level is 1453 nm^3; this corresponds to an approximate mass of 1312 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

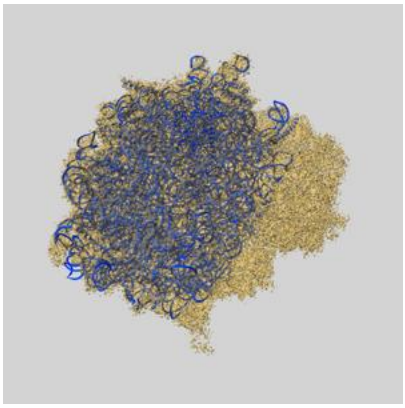
8 Fourier-Shell correlation

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

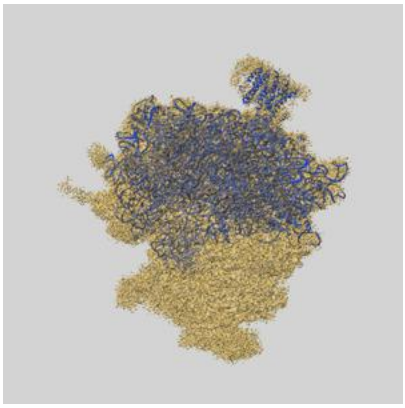
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2650 and PDB model 3J7Q. Per-residue inclusion information can be found in section 3 on page 15.

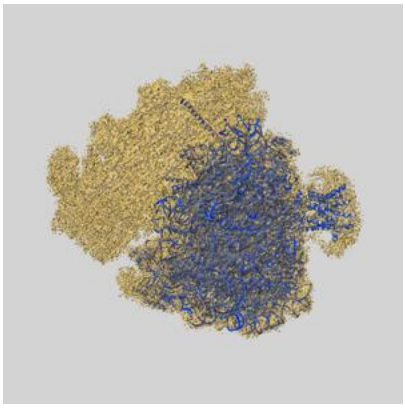
9.1 Map-model overlay



X



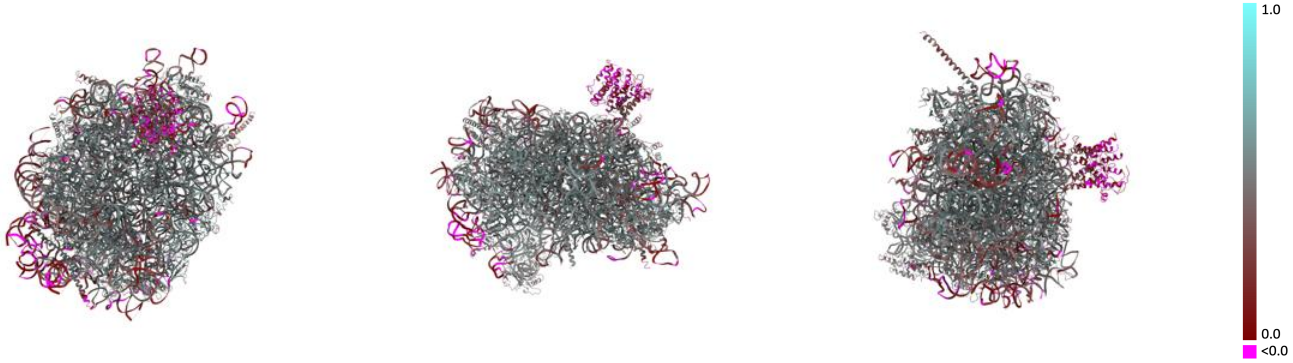
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

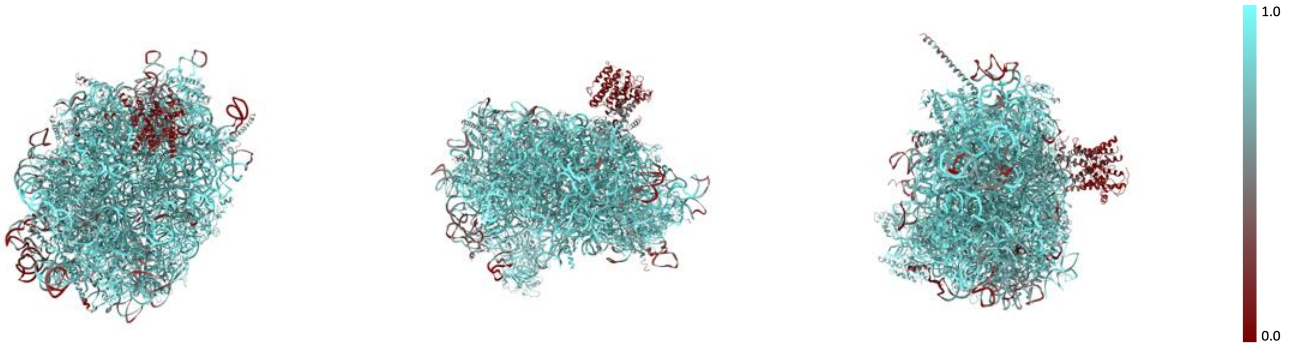
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

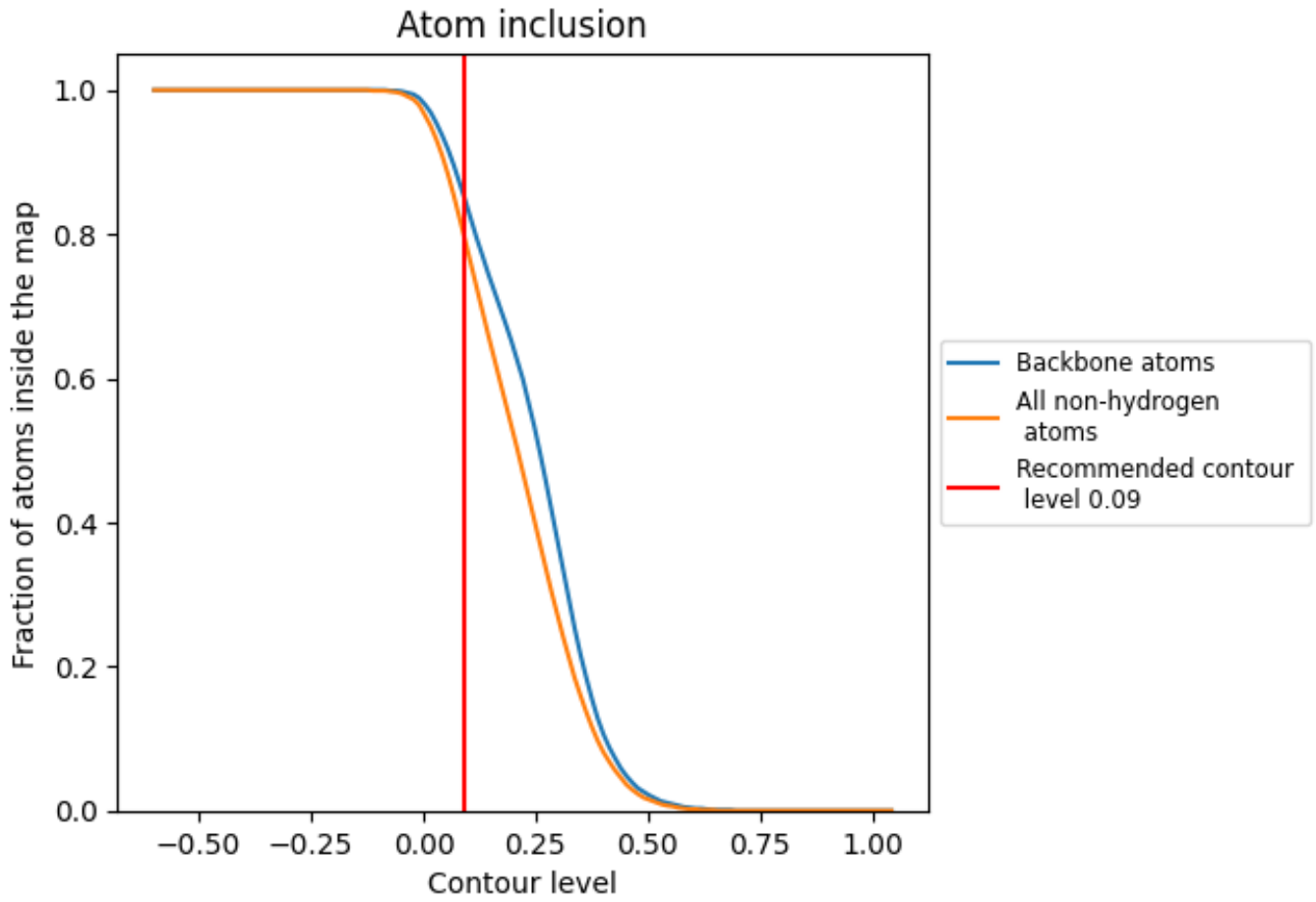
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.4410
1	0.2230	0.1560
2	0.2590	0.1820
3	0.0280	0.0620
5	0.8090	0.4170
7	0.9290	0.4920
8	0.8500	0.4530
A	0.8620	0.5200
B	0.8600	0.5130
C	0.8300	0.5000
D	0.8060	0.4580
E	0.7580	0.4480
F	0.8320	0.5010
G	0.7680	0.4560
H	0.8280	0.5050
I	0.8010	0.4800
J	0.7620	0.4510
L	0.7750	0.4650
M	0.8310	0.5010
N	0.8720	0.5200
O	0.8570	0.5230
P	0.8350	0.5160
Q	0.8610	0.5230
R	0.7790	0.4670
S	0.8610	0.5190
T	0.8250	0.5020
U	0.7200	0.4240
V	0.8430	0.5190
W	0.8210	0.5040
X	0.7870	0.4910
Y	0.8100	0.4990
Z	0.8310	0.4950
a	0.8630	0.5160
b	0.6780	0.4120
c	0.8080	0.4850

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.7990	0.4790
e	0.8470	0.5210
f	0.8780	0.5260
g	0.8150	0.5080
h	0.7890	0.4880
i	0.8040	0.4890
j	0.8470	0.5010
k	0.7540	0.4600
l	0.8350	0.5180
m	0.8490	0.5220
n	0.7710	0.4760
o	0.8010	0.5020
p	0.8200	0.5160
r	0.8390	0.5060