Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 03:25 pm GMT

PDB ID	:	6SPB
EMDB ID	:	EMD-10280
Title	:	Pseudomonas aeruginosa 50s ribosome from a clinical isolate with a mutation in uL6
Authors	:	Halfon, Y.; Jimenez-Fernande, A.; La Ros, R.; Espinos, R.; Krogh Johansen, H.; Matzov, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Belousoff, M.; Molin, S.; Yonath, A.
Deposited on	:	2019-09-01
Resolution	:	2.82 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

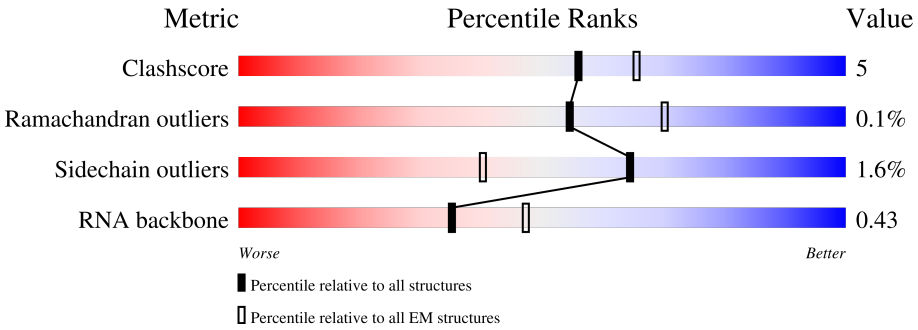
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.82 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	2888	50% 35% 12%
2	B	117	62% 23% 9% 5%
3	C	271	81% 18%
4	D	207	82% 17%
5	E	199	81% 19%
6	F	174	21% 70% 29%
7	G	169	12% 82% 17%

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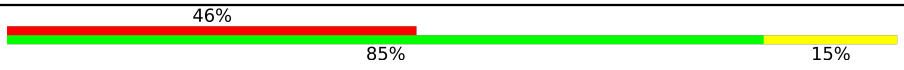
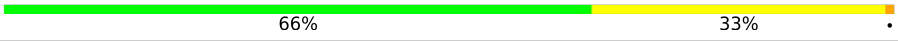
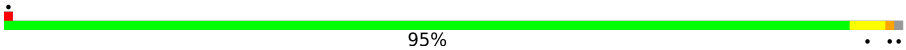
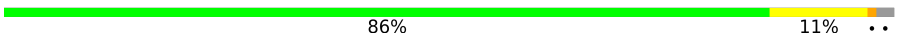
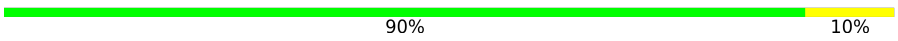
Mol	Chain	Length	Quality of chain
8	H	78	
9	I	140	
10	J	141	
11	K	120	
12	L	144	
13	M	136	
14	N	120	
15	O	115	
16	P	115	
17	Q	117	
18	R	102	
19	S	110	
20	T	94	
21	U	103	
22	V	188	
23	W	76	
24	X	77	
25	Y	60	
26	Z	57	
27	1	31	
28	2	53	
29	3	50	
30	4	44	
31	5	63	
32	6	38	

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 90362 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2885	61899	27618	11351	20046	2884	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	A	G	conflict	REF 470469287
A	2872	G	U	conflict	REF 470469287

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	117	2495	1114	448	816	117	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2048	1258	422	362	6	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	207	1549	960	297	287	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	199	1509	948	281	278	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	174	Total	C	N	O	S	0	0
			1278	806	225	244	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	7	LEU	ILE	conflict	UNP A0A072ZMU2
F	80	ALA	ARG	conflict	UNP A0A072ZMU2
F	81	ALA	GLU	conflict	UNP A0A072ZMU2

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	169	Total	C	N	O	S	0	0
			1264	795	233	234	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	GLY	deletion	UNP A0A2V3F3S9
G	?	-	TYR	deletion	UNP A0A2V3F3S9
G	?	-	LYS	deletion	UNP A0A2V3F3S9
G	?	-	ALA	deletion	UNP A0A2V3F3S9

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	78	Total	C	N	O	0	0
			577	363	104	110		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	140	Total	C	N	O	S	0	0
			1026	642	183	198	3		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1122	713	205	201	3		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	120	Total	C	N	O	S	0	0
			922	576	178	162	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1055	648	213	192	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	135	Total	C	N	O	S	0	0
			1069	679	209	178	3		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	118	Total	C	N	O	S	0	0
			945	590	190	160	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	113	Total	C	N	O	S	0	0
			891	563	168	159	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	117	Total 936	C 592	N 196	O 148	0	0

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total 801	C 509	N 154	O 136	S 2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	109	Total 825	C 510	N 160	O 152	S 3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	92	Total 701	C 449	N 124	O 128	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	2	ALA	ASN	conflict	UNP E2RXT1
T	3	ALA	GLN	conflict	UNP E2RXT1

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	103	Total 801	C 503	N 152	O 144	S 2	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	188	Total 1397	C 888	N 254	O 253	S 2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	6	VAL	LEU	conflict	UNP A0A072ZBM5
V	71	VAL	ALA	conflict	UNP A0A072ZBM5

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	76	Total	C	N	O	0	0
			574	365	110	99		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	40	LEU	GLN	conflict	UNP A0A071LFT4

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	77	Total	C	N	O	S	0	0
			626	389	134	101	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total	C	N	O	S	0	0
			468	286	96	85	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	8	GLU	-	insertion	UNP W6V2V8
Y	11	GLY	ALA	conflict	UNP W6V2V8
Y	12	PRO	GLN	conflict	UNP W6V2V8
Y	13	VAL	GLN	conflict	UNP W6V2V8
Y	14	THR	LEU	conflict	UNP W6V2V8
Y	15	GLY	ASN	conflict	UNP W6V2V8
Y	16	ASN	GLU	conflict	UNP W6V2V8
Y	17	ASN	GLN	conflict	UNP W6V2V8
Y	18	ILE	LEU	conflict	UNP W6V2V8
Y	19	SER	LEU	conflict	UNP W6V2V8
Y	20	HIS	GLY	conflict	UNP W6V2V8

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	57	Total	C	N	O	S	0	0
			445	277	87	79	2		

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	31	Total	C	N	O	S	0	0
			232	144	40	45	3		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	53	Total	C	N	O	S	0	0
			423	254	90	78	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	3	50	Total	C	N	O	0	0
			418	267	77	74		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	44	Total	C	N	O	S	1	0
			376	228	91	55	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

- Molecule 32 is a protein called 50S ribosomal protein L36.

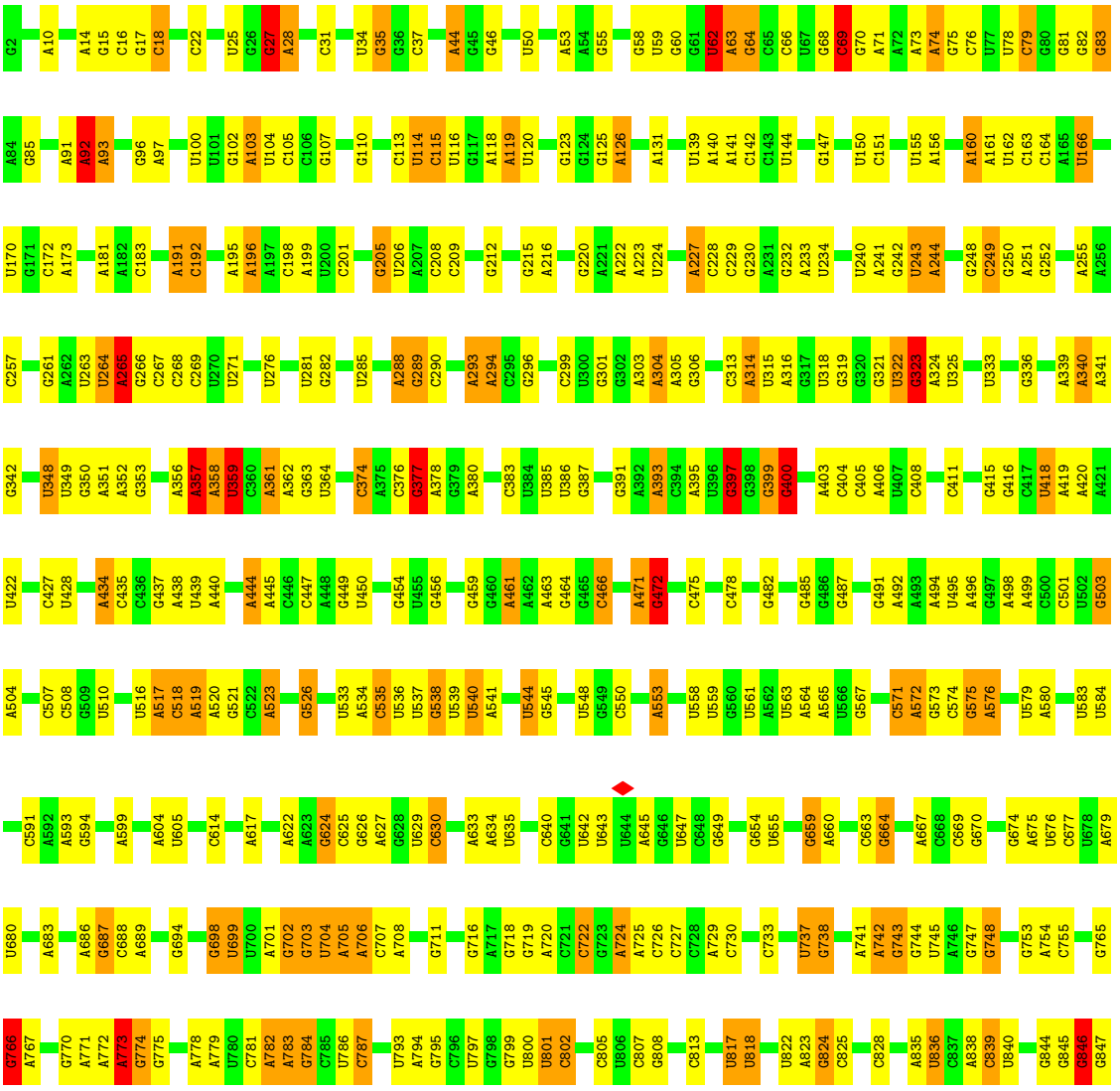
Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	38	Total	C	N	O	S	0	0
			303	184	69	46	4		

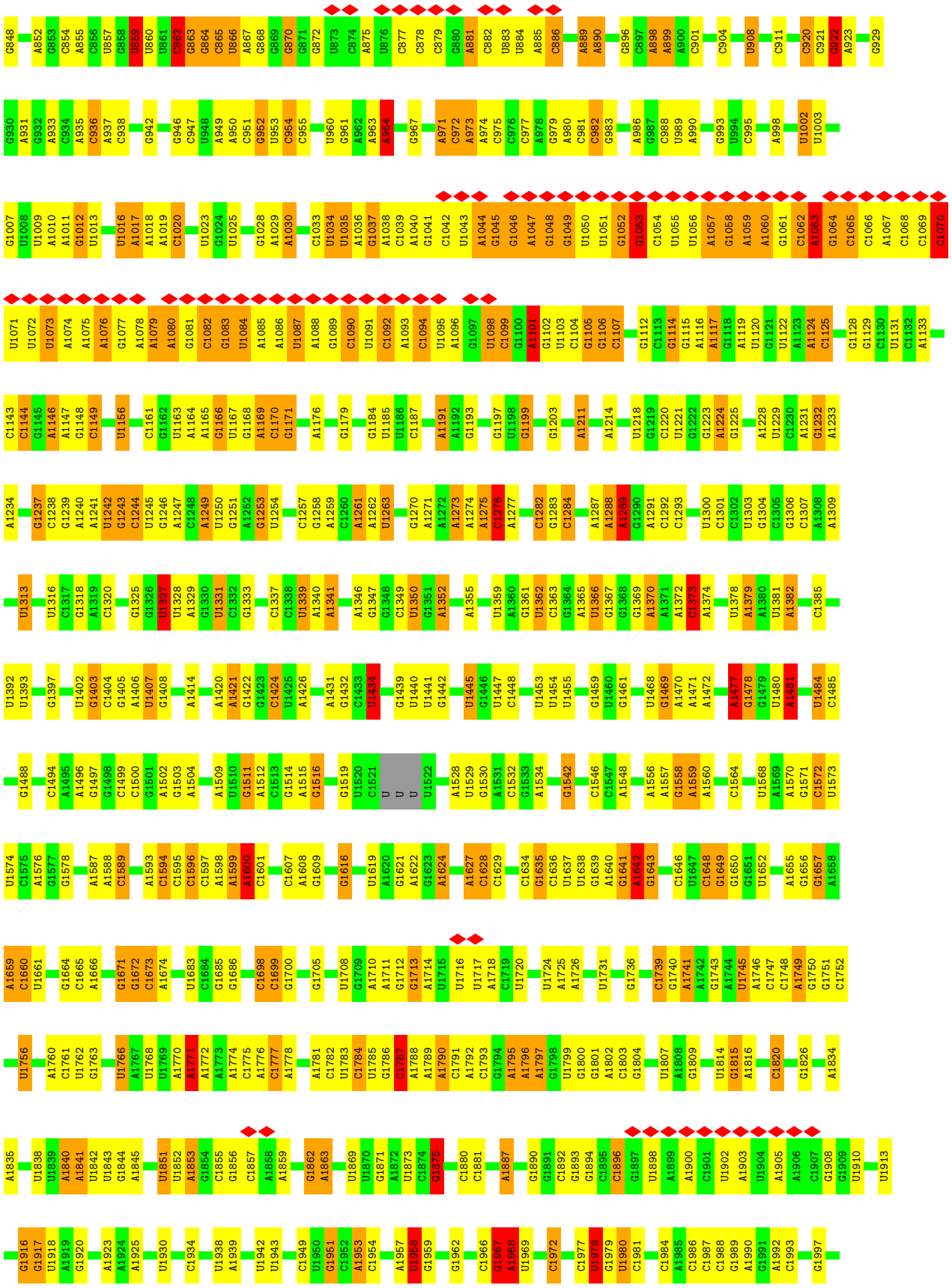
3 Residue-property plots (i)

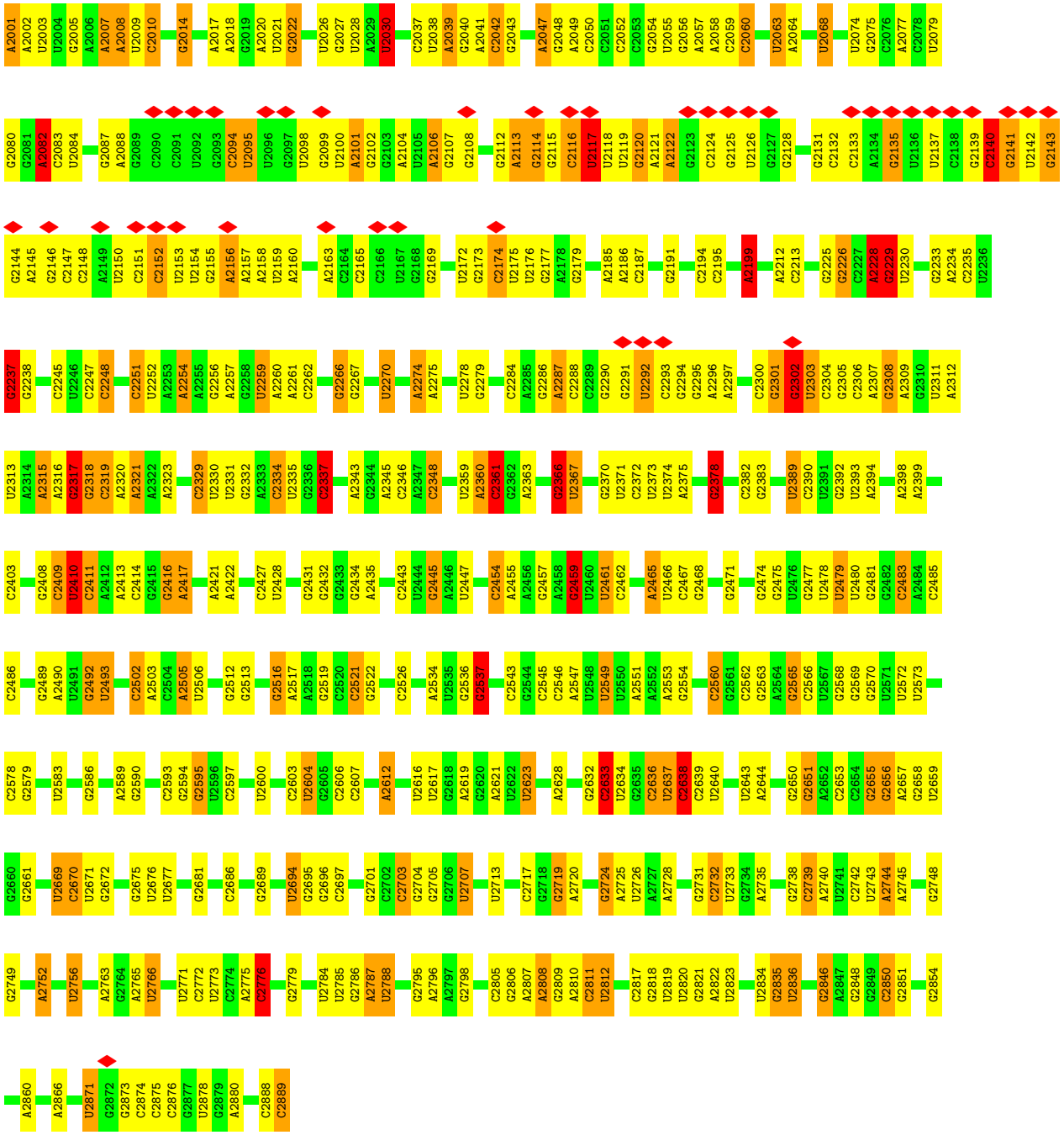
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S ribosomal RNA

Chain A:

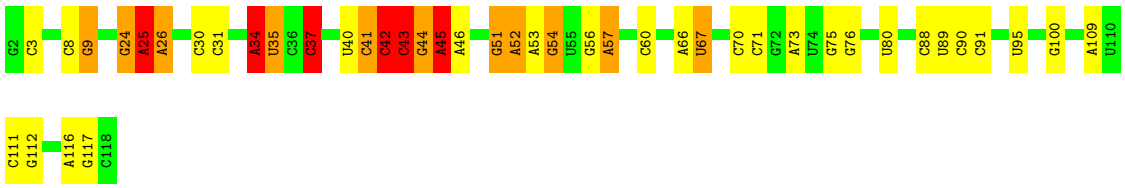






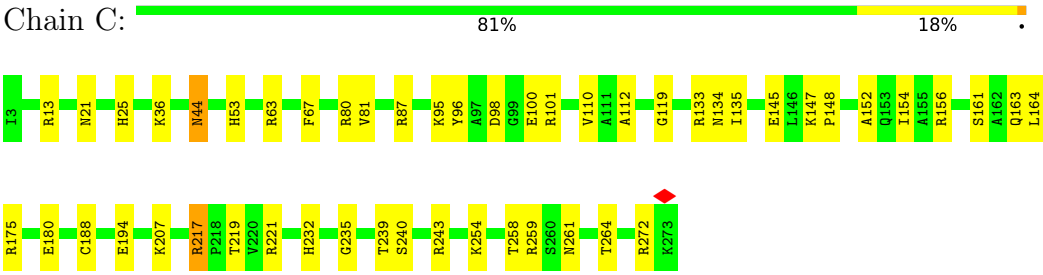
• Molecule 2: 5S rRNA

Chain B:



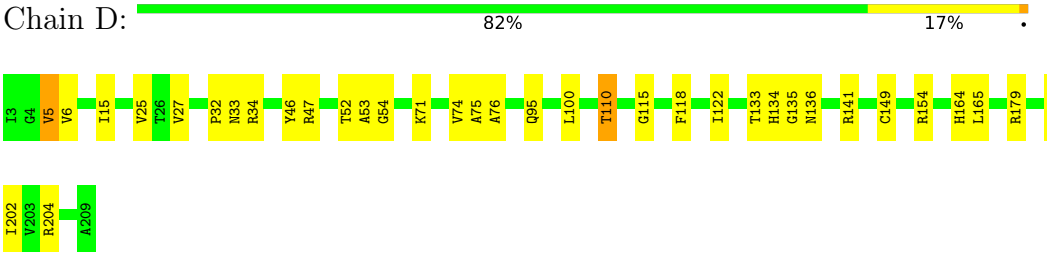
• Molecule 3: 50S ribosomal protein L2

Chain C:



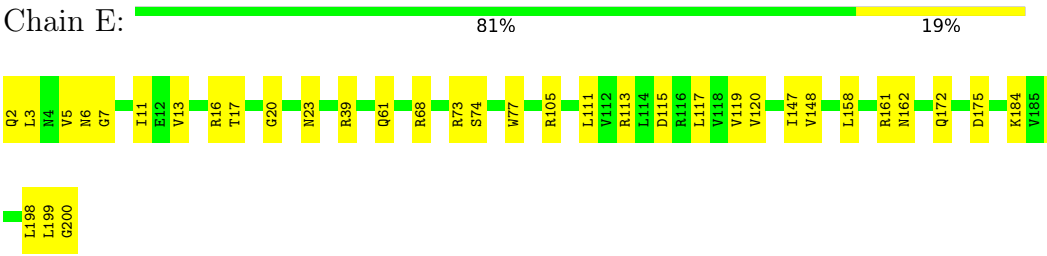
• Molecule 4: 50S ribosomal protein L3

Chain D:



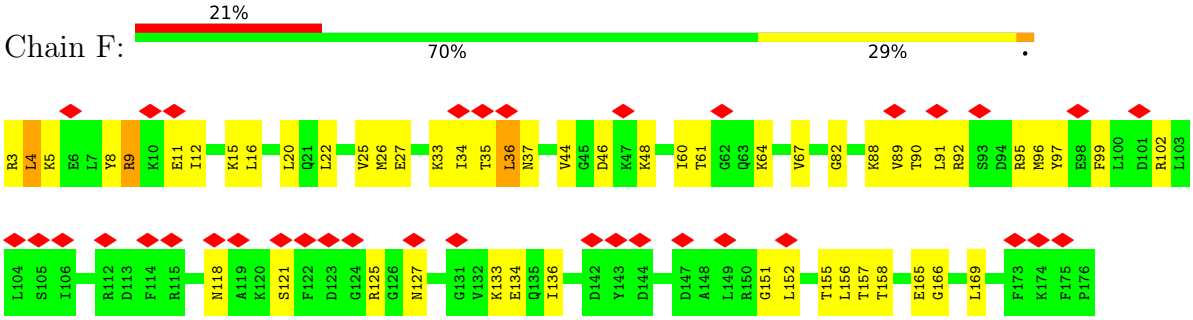
• Molecule 5: 50S ribosomal protein L4

Chain E:



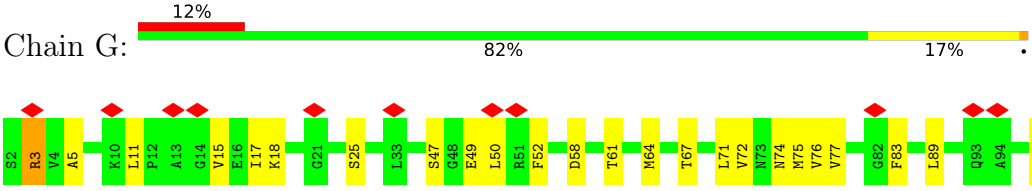
• Molecule 6: 50S ribosomal protein L5

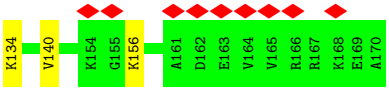
Chain F:



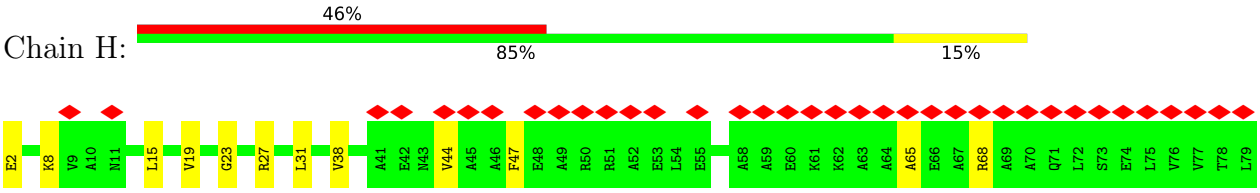
• Molecule 7: 50S ribosomal protein L6

Chain G:

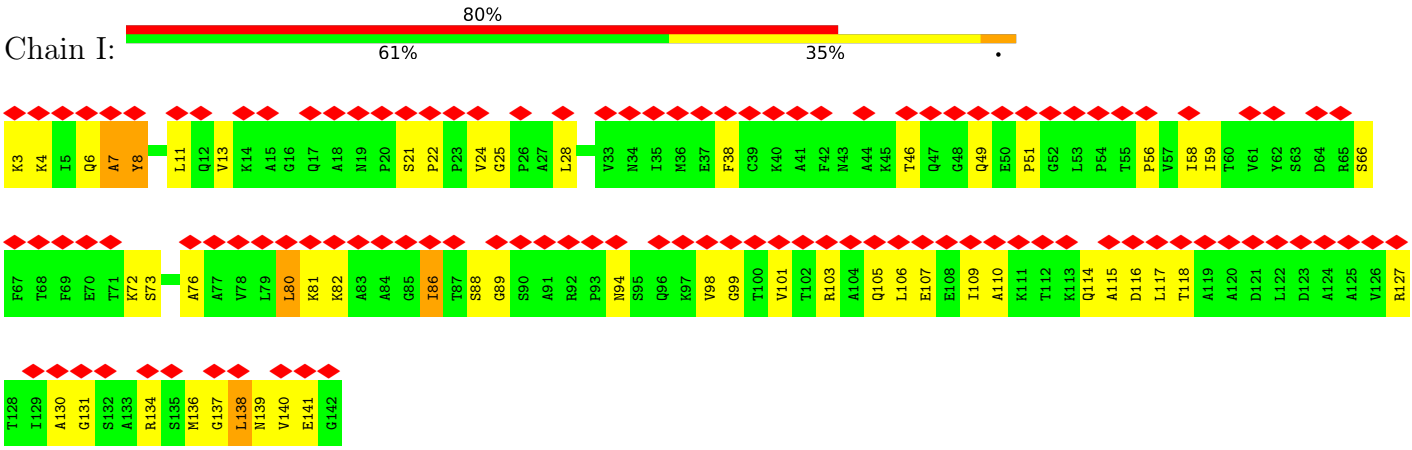




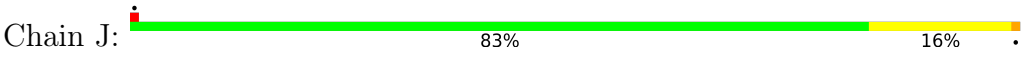
• Molecule 8: 50S ribosomal protein L9

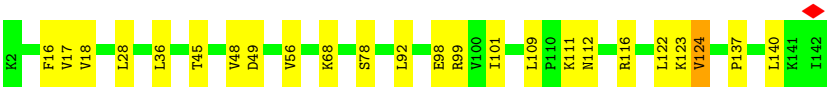


• Molecule 9: 50S ribosomal protein L11

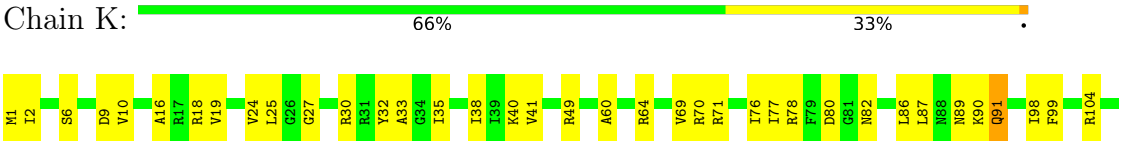


• Molecule 10: 50S ribosomal protein L13

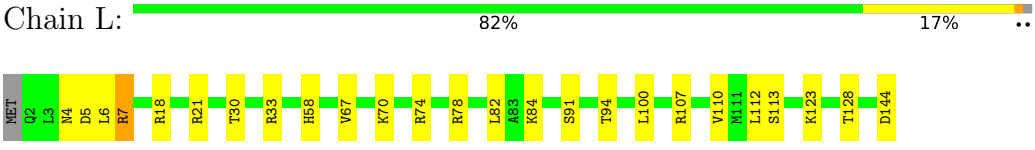




• Molecule 11: 50S ribosomal protein L14

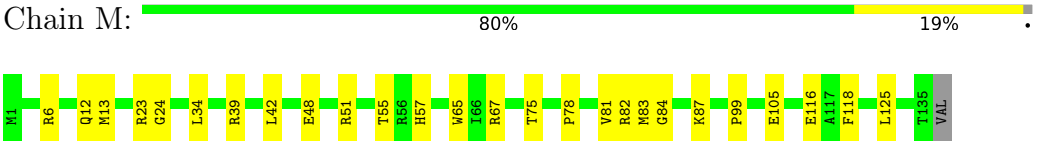


• Molecule 12: 50S ribosomal protein L15



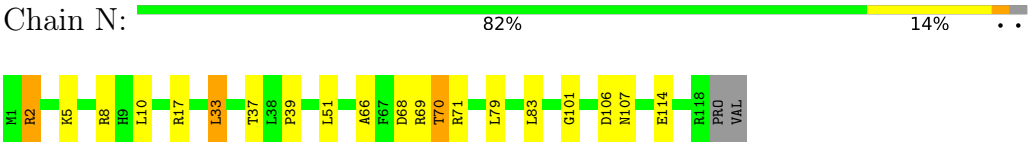
• Molecule 13: 50S ribosomal protein L16

Chain M:



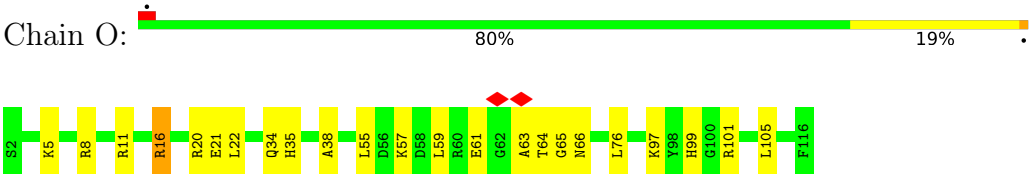
• Molecule 14: 50S ribosomal protein L17

Chain N:



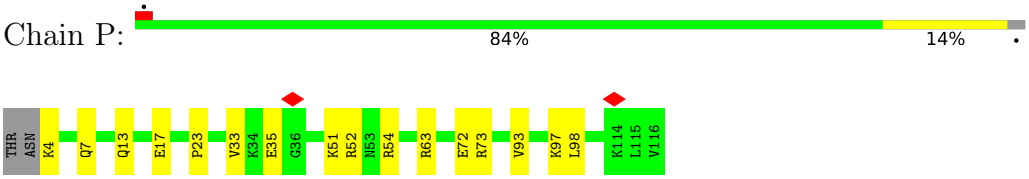
• Molecule 15: 50S ribosomal protein L18

Chain O:



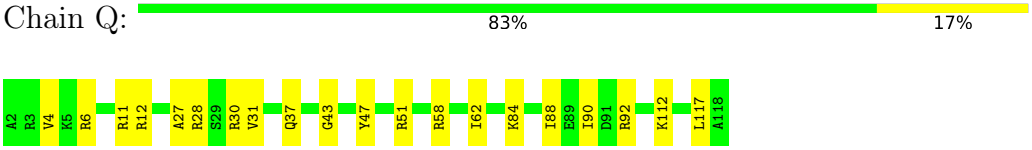
• Molecule 16: 50S ribosomal protein L19

Chain P:



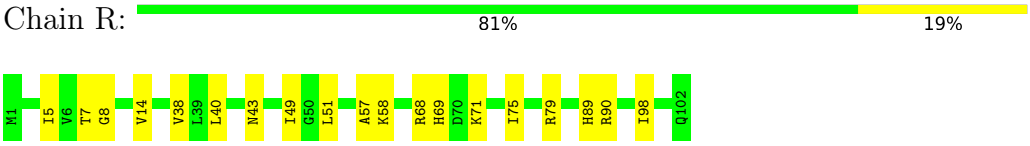
• Molecule 17: 50S ribosomal protein L20

Chain Q:



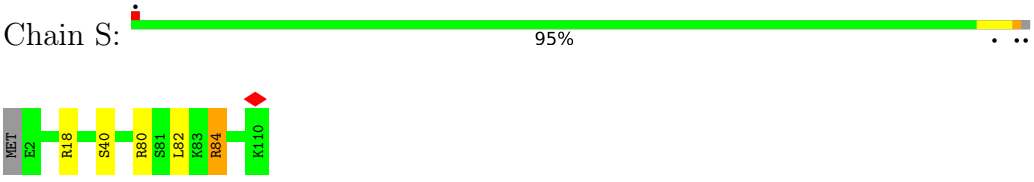
• Molecule 18: 50S ribosomal protein L21

Chain R:



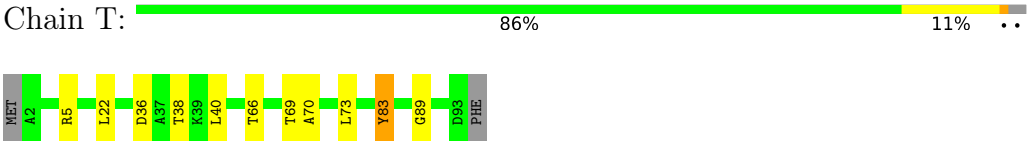
• Molecule 19: 50S ribosomal protein L22

Chain S:



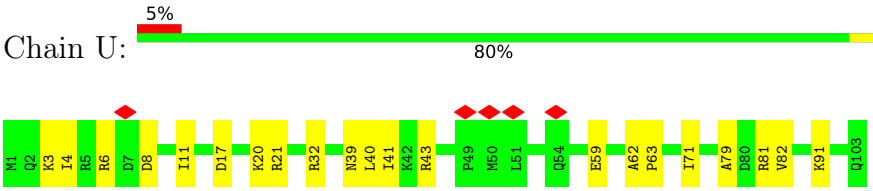
• Molecule 20: 50S ribosomal protein L23

Chain T:



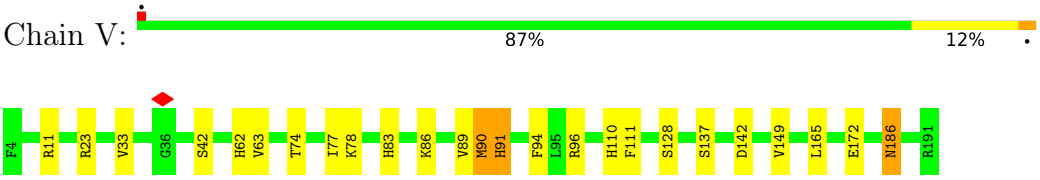
• Molecule 21: 50S ribosomal protein L24

Chain U:



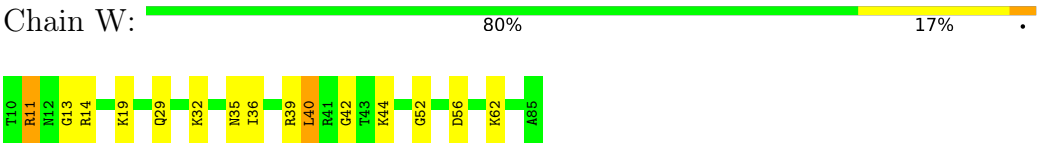
• Molecule 22: 50S ribosomal protein L25

Chain V:



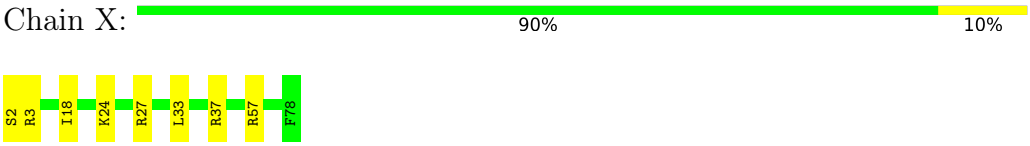
• Molecule 23: 50S ribosomal protein L27

Chain W:



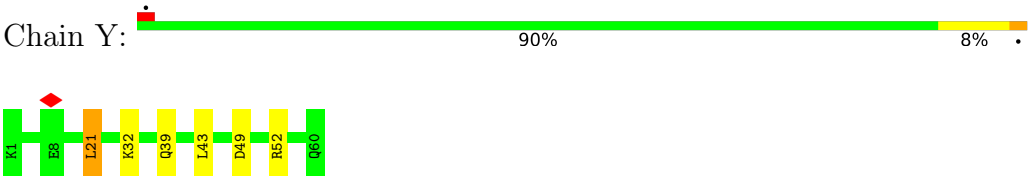
• Molecule 24: 50S ribosomal protein L28

Chain X:



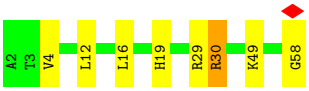
• Molecule 25: 50S ribosomal protein L29

Chain Y:



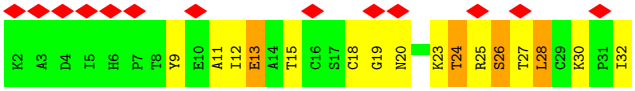
• Molecule 26: 50S ribosomal protein L30

Chain Z:



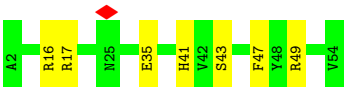
• Molecule 27: 50S ribosomal protein L31

Chain 1:



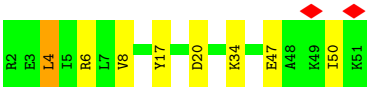
• Molecule 28: 50S ribosomal protein L32

Chain 2:



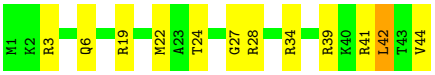
• Molecule 29: 50S ribosomal protein L33

Chain 3:



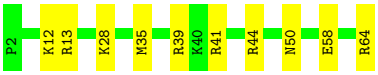
• Molecule 30: 50S ribosomal protein L34

Chain 4:



• Molecule 31: 50S ribosomal protein L35

Chain 5:



• Molecule 32: 50S ribosomal protein L36

Chain 6:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	319022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.381	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0166	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.75	60/69320 (0.1%)	1.43	1113/108135 (1.0%)
2	B	0.86	1/2789 (0.0%)	1.33	37/4345 (0.9%)
3	C	0.64	0/2084	0.72	0/2800
4	D	0.70	0/1572	0.80	2/2118 (0.1%)
5	E	0.58	0/1529	0.69	0/2060
6	F	0.36	0/1294	0.82	2/1754 (0.1%)
7	G	0.35	0/1280	0.62	0/1726
8	H	0.31	0/580	0.51	0/781
9	I	2.03	1/1041 (0.1%)	1.01	7/1408 (0.5%)
10	J	0.66	1/1148 (0.1%)	0.70	0/1549
11	K	0.64	0/931	0.74	1/1247 (0.1%)
12	L	0.55	0/1067	0.76	2/1422 (0.1%)
13	M	0.45	0/1089	0.61	0/1456
14	N	0.71	0/960	0.79	1/1282 (0.1%)
15	O	0.44	0/888	0.74	2/1183 (0.2%)
16	P	0.62	0/900	0.65	0/1203
17	Q	0.73	0/946	0.75	1/1257 (0.1%)
18	R	0.58	0/814	0.78	1/1091 (0.1%)
19	S	0.61	0/829	0.73	2/1104 (0.2%)
20	T	0.59	0/710	0.75	2/953 (0.2%)
21	U	0.48	0/809	0.71	0/1079
22	V	0.42	0/1420	0.67	0/1927
23	W	0.61	0/582	0.80	2/773 (0.3%)
24	X	0.61	0/637	0.73	1/849 (0.1%)
25	Y	0.47	0/471	0.82	1/630 (0.2%)
26	Z	0.56	0/449	0.75	1/602 (0.2%)
27	1	0.46	0/235	0.95	0/318
28	2	0.70	0/429	0.79	0/572
29	3	0.43	0/425	0.73	1/566 (0.2%)
30	4	0.72	0/379	0.92	1/496 (0.2%)
31	5	0.50	0/511	0.77	0/668
32	6	0.40	0/304	0.59	0/399
All	All	1.52	63/98422 (0.1%)	1.30	1180/147753 (0.8%)

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
3	C	0	1
4	D	0	2
6	F	0	3
9	I	0	5
11	K	0	1
14	N	0	2
16	P	0	1
18	R	0	2
20	T	0	1
22	V	0	5
23	W	0	2
27	1	0	7
32	6	0	1
All	All	0	33

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1092	C	N1-C6	163.76	2.35	1.37
1	A	1092	C	N3-C4	140.51	2.32	1.33
1	A	1092	C	C2-N3	124.00	2.35	1.35
1	A	1092	C	C4-C5	115.28	2.35	1.43
1	A	1092	C	C5-C6	112.80	2.24	1.34
1	A	1092	C	N1-C2	105.45	2.45	1.40
9	I	8	TYR	CA-CB	64.34	2.95	1.53
1	A	1908	G	O3'-P	21.34	1.86	1.61
1	A	1896	C	O3'-P	-14.31	1.44	1.61
1	A	519	A	N9-C4	-9.76	1.31	1.37
1	A	2254	A	N9-C4	-9.22	1.32	1.37
1	A	1133	A	N9-C4	-8.69	1.32	1.37
1	A	1011	A	N9-C4	-8.49	1.32	1.37
1	A	1790	A	N9-C4	-7.91	1.33	1.37
1	A	766	G	C2-N3	-7.59	1.26	1.32
1	A	572	A	N9-C4	-7.02	1.33	1.37
1	A	1771	A	N7-C5	-6.84	1.35	1.39
1	A	518	C	N3-C4	-6.55	1.29	1.33
1	A	687	G	N9-C8	-6.46	1.33	1.37
1	A	773	A	N9-C4	-6.40	1.34	1.37
1	A	191	A	N9-C4	-6.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	576	A	N9-C4	-6.36	1.34	1.37
1	A	1790	A	N3-C4	-6.34	1.31	1.34
1	A	1191	A	N9-C4	-6.31	1.34	1.37
1	A	1076	A	N9-C4	6.20	1.41	1.37
1	A	1627	A	N7-C5	-6.14	1.35	1.39
1	A	575	G	C8-N7	-5.94	1.27	1.30
1	A	517	A	N9-C4	-5.93	1.34	1.37
1	A	519	A	N3-C4	-5.77	1.31	1.34
1	A	1801	G	C6-N1	-5.72	1.35	1.39
1	A	1559	A	N9-C4	-5.70	1.34	1.37
1	A	198	C	C4-C5	-5.62	1.38	1.43
1	A	2005	G	C5-C4	-5.62	1.34	1.38
1	A	972	C	N3-C4	-5.60	1.30	1.33
1	A	1790	A	C2-N3	-5.59	1.28	1.33
1	A	64	G	N9-C8	-5.54	1.33	1.37
10	J	124	VAL	CB-CG2	-5.51	1.41	1.52
1	A	1341	A	N7-C5	-5.51	1.35	1.39
1	A	1616	G	N7-C5	-5.48	1.35	1.39
1	A	1010	A	N9-C4	-5.47	1.34	1.37
1	A	2007	A	N9-C4	-5.45	1.34	1.37
1	A	2809	G	C8-N7	-5.43	1.27	1.30
1	A	1247	A	C8-N7	-5.42	1.27	1.31
1	A	808	G	C8-N7	-5.33	1.27	1.30
1	A	784	G	N9-C8	-5.31	1.34	1.37
1	A	1801	G	N1-C2	-5.25	1.33	1.37
1	A	293	A	N7-C5	-5.21	1.36	1.39
1	A	964	A	N7-C5	-5.19	1.36	1.39
1	A	2670	C	N3-C4	-5.16	1.30	1.33
1	A	1313	U	C2-N3	-5.16	1.34	1.37
1	A	2315	A	C6-N1	-5.14	1.31	1.35
1	A	677	C	N3-C4	-5.14	1.30	1.33
1	A	1627	A	C8-N7	-5.12	1.27	1.31
1	A	1840	A	N9-C4	-5.12	1.34	1.37
1	A	2007	A	C6-N1	-5.10	1.31	1.35
1	A	961	G	N7-C5	-5.10	1.36	1.39
1	A	504	A	N7-C5	-5.09	1.36	1.39
1	A	1774	A	C8-N7	-5.09	1.27	1.31
1	A	1146	A	N9-C4	-5.08	1.34	1.37
1	A	53	A	N9-C4	-5.08	1.34	1.37
1	A	1655	A	N9-C4	-5.03	1.34	1.37
2	B	45	A	N9-C4	-5.03	1.34	1.37
1	A	2001	A	N9-C4	-5.01	1.34	1.37

All (1180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1908	G	OP1-P-O3'	-37.38	22.97	105.20
1	A	1908	G	P-O3'-C3'	-28.87	85.05	119.70
1	A	1092	C	N1-C2-O2	20.76	131.35	118.90
1	A	1896	C	O3'-P-O5'	18.26	138.69	104.00
1	A	1896	C	P-O3'-C3'	17.24	140.38	119.70
1	A	1908	G	OP2-P-O3'	16.96	142.52	105.20
1	A	1070	C	N1-C2-O2	15.11	127.97	118.90
9	I	8	TYR	CA-CB-CG	14.81	141.53	113.40
2	B	43	C	O4'-C1'-N1	13.85	119.28	108.20
1	A	1062	C	C2-N1-C1'	13.63	133.79	118.80
1	A	1070	C	C2-N1-C1'	13.24	133.36	118.80
1	A	863	G	O5'-P-OP1	-13.01	93.99	105.70
9	I	8	TYR	CB-CA-C	12.89	136.18	110.40
1	A	1622	A	N7-C8-N9	12.14	119.87	113.80
1	A	1062	C	N1-C2-O2	12.13	126.18	118.90
1	A	1896	C	OP2-P-O3'	-12.12	78.54	105.20
1	A	2003	U	N3-C2-O2	-11.54	114.12	122.20
1	A	2604	U	N3-C2-O2	-11.51	114.14	122.20
1	A	265	A	O4'-C1'-N9	11.49	117.39	108.20
1	A	2021	U	N3-C2-O2	-11.43	114.20	122.20
1	A	293	A	N7-C8-N9	11.29	119.45	113.80
1	A	2410	U	N3-C2-O2	-11.14	114.40	122.20
1	A	1761	C	N1-C2-O2	11.11	125.56	118.90
1	A	1092	C	C5-C4-N4	11.00	127.90	120.20
1	A	2410	U	N1-C2-O2	10.96	130.47	122.80
1	A	964	A	N7-C8-N9	10.88	119.24	113.80
1	A	818	U	C2-N1-C1'	10.88	130.75	117.70
1	A	1622	A	C8-N9-C4	-10.85	101.46	105.80
1	A	964	A	C8-N9-C4	-10.84	101.46	105.80
1	A	540	U	N3-C2-O2	-10.83	114.62	122.20
1	A	2410	U	C2-N1-C1'	10.70	130.54	117.70
1	A	1070	C	N3-C2-O2	-10.59	114.49	121.90
1	A	1125	C	N3-C2-O2	-10.51	114.55	121.90
2	B	42	C	C6-N1-C2	-10.48	116.11	120.30
1	A	2259	U	N3-C2-O2	-10.46	114.88	122.20
2	B	42	C	N1-C2-O2	10.40	125.14	118.90
1	A	1125	C	N1-C2-O2	10.36	125.11	118.90
1	A	2670	C	N3-C2-O2	-10.32	114.67	121.90
1	A	818	U	N1-C2-O2	10.32	130.02	122.80
1	A	1092	C	N1-C2-N3	-10.27	112.01	119.20
1	A	519	A	C2-N3-C4	-10.26	105.47	110.60
1	A	2367	U	N3-C2-O2	-10.19	115.07	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	519	A	N3-C4-N9	-10.17	119.27	127.40
1	A	2742	C	N1-C2-O2	10.17	125.00	118.90
1	A	1020	C	N3-C2-O2	-10.15	114.80	121.90
2	B	42	C	N3-C2-O2	-10.09	114.84	121.90
1	A	2254	A	N3-C4-N9	-10.04	119.37	127.40
1	A	503	G	O4'-C1'-N9	10.04	116.23	108.20
1	A	540	U	N1-C2-O2	9.92	129.75	122.80
1	A	818	U	N3-C2-O2	-9.87	115.29	122.20
1	A	1131	U	N3-C2-O2	-9.86	115.30	122.20
1	A	1020	C	C2-N1-C1'	9.82	129.60	118.80
1	A	1596	C	N1-C2-O2	9.82	124.79	118.90
1	A	2583	U	N3-C2-O2	-9.76	115.37	122.20
1	A	1301	C	C6-N1-C2	-9.76	116.40	120.30
1	A	2811	C	C6-N1-C2	-9.75	116.40	120.30
1	A	1671	G	C6-C5-N7	-9.74	124.56	130.40
1	A	1622	A	C5-N7-C8	-9.74	99.03	103.90
1	A	1020	C	N1-C2-O2	9.70	124.72	118.90
1	A	64	G	N7-C8-N9	9.65	117.92	113.10
1	A	1596	C	C2-N1-C1'	9.63	129.40	118.80
1	A	1107	C	N3-C2-O2	-9.59	115.19	121.90
1	A	113	C	N3-C2-O2	-9.55	115.22	121.90
1	A	2653	C	N3-C2-O2	-9.49	115.26	121.90
1	A	1062	C	C6-N1-C1'	-9.47	109.43	120.80
1	A	2303	U	C5-C4-O4	-9.47	120.22	125.90
1	A	1671	G	C4-C5-N7	9.46	114.58	110.80
1	A	1092	C	N3-C4-N4	-9.45	111.39	118.00
1	A	2653	C	N1-C2-O2	9.43	124.56	118.90
1	A	1300	U	C2-N1-C1'	9.42	129.00	117.70
1	A	1761	C	N3-C2-O2	-9.41	115.31	121.90
1	A	1011	A	C2-N3-C4	-9.40	105.90	110.60
1	A	955	C	C6-N1-C2	-9.37	116.55	120.30
1	A	1062	C	N3-C2-O2	-9.32	115.37	121.90
1	A	501	C	N1-C2-O2	9.31	124.49	118.90
1	A	2653	C	C2-N1-C1'	9.30	129.03	118.80
1	A	1070	C	C6-N1-C1'	-9.29	109.65	120.80
1	A	1107	C	N1-C2-O2	9.27	124.46	118.90
25	Y	21	LEU	CA-CB-CG	9.26	136.60	115.30
1	A	1092	C	C6-N1-C2	9.26	124.00	120.30
30	4	42	LEU	CA-CB-CG	9.25	136.58	115.30
1	A	1671	G	N7-C8-N9	9.22	117.71	113.10
1	A	2742	C	C2-N1-C1'	9.21	128.93	118.80
1	A	1745	U	N1-C2-O2	9.18	129.23	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1070	C	C5-C6-N1	9.16	125.58	121.00
1	A	293	A	C5-N7-C8	-9.15	99.33	103.90
6	F	36	LEU	CA-CB-CG	9.12	136.29	115.30
1	A	1745	U	N3-C2-O2	-9.12	115.82	122.20
1	A	1791	C	C6-N1-C2	-9.11	116.66	120.30
2	B	42	C	C2-N1-C1'	9.09	128.80	118.80
1	A	63	A	O5'-P-OP2	-9.08	97.53	105.70
1	A	340	A	N7-C8-N9	9.06	118.33	113.80
1	A	126	A	N7-C8-N9	9.05	118.33	113.80
1	A	113	C	N1-C2-O2	9.04	124.33	118.90
1	A	113	C	C2-N1-C1'	9.00	128.70	118.80
1	A	1980	U	N3-C2-O2	-8.93	115.95	122.20
2	B	37	C	N1-C2-O2	8.93	124.25	118.90
1	A	2374	U	N3-C2-O2	-8.92	115.95	122.20
1	A	1107	C	C2-N1-C1'	8.92	128.61	118.80
1	A	1627	A	C8-N9-C4	-8.91	102.23	105.80
1	A	1062	C	C6-N1-C2	-8.84	116.77	120.30
1	A	1761	C	C6-N1-C2	-8.83	116.77	120.30
1	A	1987	C	C6-N1-C2	-8.82	116.77	120.30
1	A	1784	C	C6-N1-C2	-8.81	116.78	120.30
1	A	2742	C	N3-C2-O2	-8.80	115.74	121.90
1	A	293	A	C8-N9-C4	-8.79	102.28	105.80
1	A	1918	U	C5-C6-N1	8.75	127.07	122.70
1	A	1634	C	N1-C2-O2	8.68	124.11	118.90
1	A	1131	U	N1-C2-O2	8.67	128.87	122.80
1	A	964	A	C5-N7-C8	-8.62	99.59	103.90
1	A	2021	U	N1-C2-O2	8.62	128.83	122.80
1	A	2254	A	N3-C4-C5	8.60	132.82	126.80
1	A	2633	C	C6-N1-C2	-8.56	116.88	120.30
1	A	1671	G	C5-N7-C8	-8.55	100.02	104.30
1	A	519	A	N3-C4-C5	8.54	132.78	126.80
1	A	1289	A	O4'-C1'-N9	8.53	115.03	108.20
1	A	2293	C	C2-N1-C1'	8.53	128.18	118.80
1	A	2812	U	C2-N1-C1'	8.52	127.92	117.70
1	A	2254	A	C2-N3-C4	-8.49	106.35	110.60
1	A	519	A	C8-N9-C4	-8.48	102.41	105.80
1	A	1943	U	N3-C2-O2	-8.45	116.29	122.20
1	A	2739	C	N1-C2-O2	8.42	123.95	118.90
1	A	836	U	C2-N1-C1'	8.41	127.79	117.70
1	A	1980	U	N1-C2-O2	8.40	128.68	122.80
1	A	2303	U	N3-C4-O4	8.38	125.27	119.40
2	B	37	C	C6-N1-C2	-8.37	116.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1070	C	C6-N1-C2	-8.36	116.96	120.30
1	A	2003	U	C2-N1-C1'	8.34	127.71	117.70
1	A	2653	C	C6-N1-C2	-8.34	116.96	120.30
1	A	2382	C	C2-N1-C1'	8.32	127.96	118.80
1	A	1300	U	N3-C2-O2	-8.28	116.40	122.20
1	A	1881	C	C2-N1-C1'	8.25	127.88	118.80
1	A	208	C	C6-N1-C2	-8.25	117.00	120.30
1	A	1011	A	N3-C4-N9	-8.23	120.81	127.40
1	A	113	C	C6-N1-C2	-8.18	117.03	120.30
1	A	519	A	C5-N7-C8	-8.17	99.81	103.90
1	A	1761	C	C2-N1-C1'	8.15	127.76	118.80
1	A	1953	A	N7-C8-N9	8.15	117.87	113.80
1	A	2670	C	N1-C2-O2	8.15	123.79	118.90
1	A	501	C	N3-C2-O2	-8.14	116.20	121.90
1	A	1125	C	C6-N1-C2	-8.14	117.05	120.30
1	A	862	C	N1-C2-O2	8.14	123.78	118.90
1	A	69	C	N1-C2-O2	8.11	123.76	118.90
1	A	2288	C	N1-C2-O2	8.10	123.76	118.90
1	A	540	U	C2-N1-C1'	8.08	127.40	117.70
1	A	126	A	C5-N7-C8	-8.07	99.86	103.90
1	A	1634	C	N3-C2-O2	-8.07	116.25	121.90
1	A	544	U	N3-C2-O2	-8.06	116.56	122.20
1	A	2284	C	C6-N1-C2	-8.06	117.08	120.30
1	A	1943	U	N1-C2-O2	8.05	128.43	122.80
1	A	340	A	C8-N9-C4	-8.04	102.58	105.80
1	A	2257	A	O4'-C1'-N9	8.04	114.63	108.20
1	A	518	C	N3-C2-O2	-8.02	116.29	121.90
1	A	818	U	C6-N1-C1'	-8.01	109.99	121.20
1	A	1627	A	N7-C8-N9	8.01	117.80	113.80
1	A	1596	C	N3-C2-O2	-8.00	116.30	121.90
1	A	614	C	C6-N1-C2	-8.00	117.10	120.30
1	A	2431	G	O5'-P-OP2	-8.00	98.50	105.70
1	A	2199	A	N7-C8-N9	7.99	117.80	113.80
1	A	519	A	N7-C8-N9	7.99	117.79	113.80
1	A	982	C	C6-N1-C2	-7.98	117.11	120.30
1	A	1282	C	N1-C2-O2	7.98	123.69	118.90
1	A	1300	U	N1-C2-O2	7.97	128.38	122.80
1	A	2639	C	N1-C2-O2	7.97	123.68	118.90
1	A	79	C	C6-N1-C2	-7.97	117.11	120.30
1	A	1131	U	C2-N1-C1'	7.97	127.27	117.70
1	A	1763	G	C2-N3-C4	7.97	115.89	111.90
1	A	115	C	C6-N1-C2	-7.96	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2021	U	C2-N1-C1'	7.94	127.23	117.70
1	A	973	A	C5-N7-C8	-7.93	99.93	103.90
1	A	2638	C	N1-C2-O2	7.92	123.65	118.90
1	A	862	C	N3-C2-O2	-7.92	116.36	121.90
1	A	1092	C	C2-N3-C4	7.90	123.85	119.90
1	A	2811	C	C5-C6-N1	7.90	124.95	121.00
1	A	1062	C	C5-C6-N1	7.89	124.95	121.00
1	A	79	C	C5-C6-N1	7.87	124.93	121.00
1	A	971	A	N7-C8-N9	7.86	117.73	113.80
1	A	1801	G	N1-C2-N2	-7.86	109.13	116.20
1	A	2703	C	C6-N1-C2	-7.85	117.16	120.30
1	A	1011	A	N3-C4-C5	7.84	132.29	126.80
1	A	2583	U	N1-C2-O2	7.83	128.28	122.80
1	A	1619	U	N3-C2-O2	-7.83	116.72	122.20
1	A	2003	U	N1-C2-O2	7.79	128.25	122.80
2	B	37	C	N3-C2-O2	-7.79	116.45	121.90
2	B	25	A	P-O3'-C3'	7.77	129.02	119.70
1	A	2319	C	C6-N1-C2	-7.76	117.19	120.30
1	A	166	U	C5-C6-N1	7.76	126.58	122.70
1	A	1313	U	N3-C2-O2	-7.76	116.77	122.20
2	B	43	C	C6-N1-C2	-7.75	117.20	120.30
1	A	1747	C	C6-N1-C2	-7.71	117.22	120.30
1	A	2583	U	C2-N1-C1'	7.71	126.95	117.70
1	A	2633	C	C5-C6-N1	7.70	124.85	121.00
1	A	995	C	C6-N1-C2	-7.70	117.22	120.30
1	A	1053	G	N3-C4-C5	-7.68	124.76	128.60
9	I	8	TYR	N-CA-C	-7.66	90.31	111.00
1	A	659	G	C4-N9-C1'	7.65	136.44	126.50
1	A	922	G	C4-N9-C1'	7.64	136.44	126.50
1	A	659	G	C8-N9-C1'	-7.64	117.07	127.00
1	A	1092	C	N3-C2-O2	-7.62	116.56	121.90
1	A	2259	U	C2-N1-C1'	7.62	126.84	117.70
9	I	8	TYR	N-CA-CB	7.61	124.30	110.60
1	A	2199	A	C5-N7-C8	-7.61	100.10	103.90
1	A	2367	U	C2-N1-C1'	7.57	126.79	117.70
1	A	1968	A	N7-C8-N9	7.56	117.58	113.80
2	B	31	C	C2-N1-C1'	7.56	127.11	118.80
1	A	2726	U	N1-C2-O2	7.55	128.09	122.80
1	A	518	C	N1-C2-O2	7.55	123.43	118.90
1	A	126	A	C8-N9-C4	-7.54	102.78	105.80
1	A	66	C	C6-N1-C2	-7.54	117.28	120.30
1	A	1596	C	C6-N1-C1'	-7.54	111.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2836	U	N1-C2-O2	7.53	128.07	122.80
1	A	2100	U	N3-C2-O2	-7.53	116.93	122.20
1	A	1125	C	C2-N1-C1'	7.53	127.08	118.80
1	A	2042	C	C2-N1-C1'	7.52	127.07	118.80
1	A	2739	C	C2-N1-C1'	7.50	127.05	118.80
1	A	973	A	O4'-C1'-N9	7.50	114.20	108.20
1	A	2050	C	C6-N1-C2	-7.50	117.30	120.30
1	A	908	U	N3-C2-O2	-7.47	116.97	122.20
1	A	2367	U	N1-C2-O2	7.47	128.03	122.80
1	A	2670	C	C6-N1-C2	-7.47	117.31	120.30
1	A	1616	G	N1-C2-N2	-7.47	109.48	116.20
1	A	955	C	C5-C6-N1	7.46	124.73	121.00
1	A	393	A	N7-C8-N9	7.46	117.53	113.80
1	A	1986	C	C6-N1-C2	-7.46	117.32	120.30
1	A	1009	U	C2-N1-C1'	7.43	126.61	117.70
1	A	974	A	N7-C8-N9	7.42	117.51	113.80
1	A	299	C	C5-C6-N1	7.42	124.71	121.00
1	A	2604	U	N1-C2-O2	7.42	127.99	122.80
1	A	1073	U	N3-C2-O2	-7.41	117.02	122.20
1	A	79	C	C2-N1-C1'	7.39	126.93	118.80
1	A	44	A	O4'-C1'-N9	7.39	114.11	108.20
1	A	2638	C	C2-N1-C1'	7.39	126.93	118.80
1	A	2293	C	N1-C2-O2	7.39	123.33	118.90
1	A	1133	A	N3-C4-C5	7.39	131.97	126.80
1	A	2052	C	C5-C6-N1	7.38	124.69	121.00
1	A	1648	C	C6-N1-C2	-7.37	117.35	120.30
1	A	1020	C	C6-N1-C1'	-7.36	111.97	120.80
2	B	67	U	N1-C2-O2	7.35	127.94	122.80
1	A	2836	U	N3-C2-O2	-7.35	117.06	122.20
18	R	40	LEU	CA-CB-CG	7.34	132.19	115.30
1	A	971	A	C8-N9-C4	-7.33	102.87	105.80
1	A	1407	U	N1-C2-O2	7.33	127.93	122.80
2	B	37	C	C2-N1-C1'	7.33	126.86	118.80
1	A	1301	C	C5-C6-N1	7.31	124.66	121.00
1	A	1756	U	N3-C2-O2	-7.31	117.08	122.20
1	A	2639	C	N3-C2-O2	-7.30	116.79	121.90
1	A	1009	U	N3-C2-O2	-7.29	117.10	122.20
1	A	2637	U	C5-C6-N1	7.29	126.34	122.70
1	A	1594	C	C6-N1-C2	-7.28	117.39	120.30
1	A	92	A	O4'-C1'-N9	7.26	114.01	108.20
1	A	2100	U	N1-C2-O2	7.25	127.88	122.80
1	A	1104	C	N3-C2-O2	-7.25	116.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	C	C6-N1-C2	-7.24	117.40	120.30
1	A	859	U	C2-N1-C1'	7.24	126.39	117.70
1	A	535	C	N3-C2-O2	-7.24	116.83	121.90
1	A	22	C	C6-N1-C2	-7.24	117.41	120.30
1	A	766	G	N7-C8-N9	7.22	116.71	113.10
1	A	1938	U	N3-C2-O2	-7.22	117.14	122.20
1	A	1073	U	N1-C2-O2	7.21	127.85	122.80
1	A	686	A	O4'-C1'-N9	7.21	113.97	108.20
1	A	1968	A	C8-N9-C4	-7.21	102.92	105.80
1	A	677	C	N1-C2-O2	7.20	123.22	118.90
1	A	150	U	C5-C6-N1	7.19	126.30	122.70
1	A	2308	G	C4-N9-C1'	7.19	135.84	126.50
1	A	2443	C	C6-N1-C2	-7.19	117.42	120.30
1	A	1166	G	P-O3'-C3'	7.17	128.30	119.70
1	A	836	U	N3-C2-O2	-7.16	117.19	122.20
1	A	1289	A	C5-N7-C8	-7.16	100.32	103.90
1	A	862	C	C6-N1-C2	-7.15	117.44	120.30
1	A	2675	G	N7-C8-N9	7.14	116.67	113.10
1	A	2675	G	C8-N9-C4	-7.14	103.54	106.40
1	A	1787	C	N3-C2-O2	-7.14	116.90	121.90
1	A	1857	C	N1-C2-O2	7.14	123.18	118.90
1	A	364	U	N1-C2-O2	7.12	127.79	122.80
1	A	2348	C	N1-C2-O2	7.12	123.17	118.90
1	A	2549	U	N3-C2-O2	-7.12	117.22	122.20
1	A	1875	G	N7-C8-N9	7.11	116.66	113.10
1	A	2100	U	C2-N1-C1'	7.11	126.23	117.70
1	A	340	A	C5-N7-C8	-7.10	100.35	103.90
1	A	1930	U	N3-C2-O2	-7.09	117.24	122.20
1	A	2194	C	C6-N1-C2	-7.09	117.47	120.30
1	A	1441	U	N1-C2-O2	7.08	127.75	122.80
1	A	738	G	O4'-C1'-N9	7.07	113.85	108.20
1	A	973	A	C4-C5-N7	7.05	114.23	110.70
1	A	2050	C	N3-C2-O2	-7.05	116.97	121.90
1	A	922	G	C8-N9-C1'	-7.04	117.85	127.00
1	A	1671	G	C4-N9-C1'	7.03	135.64	126.50
1	A	663	C	C6-N1-C2	-7.03	117.49	120.30
1	A	1938	U	C2-N1-C1'	7.03	126.13	117.70
1	A	364	U	N3-C2-O2	-7.01	117.29	122.20
1	A	1660	C	C6-N1-C2	-7.01	117.50	120.30
1	A	1301	C	C2-N1-C1'	7.01	126.51	118.80
1	A	2636	C	C6-N1-C2	-7.00	117.50	120.30
1	A	828	C	N1-C2-O2	6.98	123.09	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	933	A	C5-N7-C8	-6.98	100.41	103.90
1	A	126	A	O4'-C1'-N9	6.97	113.78	108.20
1	A	1370	A	N7-C8-N9	6.97	117.29	113.80
1	A	544	U	N1-C2-O2	6.97	127.68	122.80
1	A	1053	G	N3-C4-N9	6.97	130.18	126.00
1	A	359	U	N1-C2-O2	6.97	127.68	122.80
1	A	2063	U	N3-C2-O2	-6.96	117.32	122.20
1	A	1379	A	N7-C8-N9	6.95	117.28	113.80
1	A	766	G	C8-N9-C4	-6.95	103.62	106.40
1	A	1053	G	C4-N9-C1'	6.95	135.53	126.50
1	A	1363	C	N1-C2-O2	6.94	123.06	118.90
1	A	2254	A	C4-C5-C6	-6.93	113.53	117.00
1	A	1441	U	N3-C2-O2	-6.93	117.35	122.20
2	B	35	U	C2-N1-C1'	6.93	126.01	117.70
1	A	971	A	C5-N7-C8	-6.93	100.44	103.90
1	A	535	C	N1-C2-O2	6.92	123.06	118.90
1	A	1133	A	C2-N3-C4	-6.92	107.14	110.60
1	A	1385	C	C2-N1-C1'	6.92	126.42	118.80
1	A	1775	C	C6-N1-C2	-6.92	117.53	120.30
1	A	2726	U	N3-C2-O2	-6.90	117.37	122.20
1	A	1191	A	C6-N1-C2	6.90	122.74	118.60
1	A	1790	A	N3-C4-N9	-6.89	121.89	127.40
2	B	31	C	N1-C2-O2	6.89	123.03	118.90
1	A	357	A	C8-N9-C4	-6.89	103.05	105.80
1	A	722	C	C6-N1-C2	-6.88	117.55	120.30
1	A	2252	U	N3-C2-O2	-6.88	117.39	122.20
1	A	989	U	N1-C2-O2	6.87	127.61	122.80
1	A	1009	U	N1-C2-O2	6.87	127.61	122.80
1	A	1923	A	C2-N3-C4	-6.87	107.17	110.60
1	A	2007	A	C6-N1-C2	6.87	122.72	118.60
1	A	1790	A	C8-N9-C4	-6.86	103.06	105.80
1	A	1445	U	N3-C2-O2	-6.86	117.40	122.20
1	A	2578	C	C5-C6-N1	6.85	124.43	121.00
1	A	1249	A	C2-N3-C4	6.84	114.02	110.60
1	A	1318	G	N1-C6-O6	-6.84	115.80	119.90
1	A	2374	U	C2-N1-C1'	6.84	125.91	117.70
1	A	377	G	C4-C5-N7	6.84	113.54	110.80
1	A	1652	U	N3-C2-O2	-6.84	117.41	122.20
1	A	1953	A	C8-N9-C4	-6.84	103.06	105.80
1	A	2063	U	N1-C2-O2	6.84	127.58	122.80
1	A	1441	U	C2-N1-C1'	6.83	125.90	117.70
1	A	2334	C	C6-N1-C2	-6.83	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2756	U	N3-C2-O2	-6.83	117.42	122.20
1	A	1407	U	C5-C6-N1	6.83	126.12	122.70
1	A	1407	U	N3-C2-O2	-6.83	117.42	122.20
1	A	2315	A	C6-N1-C2	6.83	122.70	118.60
1	A	69	C	N3-C2-O2	-6.82	117.13	121.90
1	A	920	C	P-O3'-C3'	6.82	127.88	119.70
1	A	972	C	N3-C2-O2	-6.81	117.14	121.90
1	A	348	U	N3-C2-O2	-6.80	117.44	122.20
2	B	35	U	N1-C2-O2	6.78	127.55	122.80
1	A	974	A	N1-C6-N6	-6.78	114.53	118.60
24	X	33	LEU	CA-CB-CG	6.78	130.88	115.30
1	A	1161	C	N1-C2-O2	6.76	122.96	118.90
1	A	2410	U	C6-N1-C1'	-6.75	111.75	121.20
1	A	2812	U	N3-C2-O2	-6.74	117.48	122.20
1	A	1589	C	C5-C6-N1	6.73	124.36	121.00
9	I	138	LEU	CA-CB-CG	6.72	130.76	115.30
1	A	1766	U	C4-C5-C6	6.72	123.73	119.70
1	A	1053	G	C2-N3-C4	6.71	115.26	111.90
1	A	1672	G	C8-N9-C4	-6.71	103.72	106.40
1	A	119	A	C4-C5-C6	-6.71	113.65	117.00
1	A	501	C	C6-N1-C2	-6.71	117.62	120.30
2	B	37	C	C5-C6-N1	6.71	124.35	121.00
1	A	964	A	O4'-C1'-N9	6.70	113.56	108.20
1	A	1149	C	C6-N1-C2	-6.70	117.62	120.30
1	A	519	A	C5-C6-N1	-6.70	114.35	117.70
1	A	2118	U	C2-N1-C1'	6.70	125.73	117.70
1	A	2739	C	N3-C2-O2	-6.68	117.22	121.90
2	B	42	C	C5-C6-N1	6.68	124.34	121.00
1	A	359	U	N3-C2-O2	-6.67	117.53	122.20
1	A	1292	C	N3-C2-O2	-6.66	117.23	121.90
1	A	1981	C	C6-N1-C2	-6.65	117.64	120.30
1	A	2199	A	C8-N9-C4	-6.65	103.14	105.80
2	B	67	U	N3-C2-O2	-6.65	117.54	122.20
1	A	1793	C	C6-N1-C2	-6.65	117.64	120.30
1	A	2454	C	N3-C2-O2	-6.65	117.25	121.90
1	A	2889	C	N1-C2-O2	6.64	122.89	118.90
1	A	66	C	C2-N1-C1'	6.64	126.11	118.80
1	A	1572	C	C2-N1-C1'	6.64	126.11	118.80
1	A	825	C	N3-C4-C5	6.64	124.56	121.90
1	A	981	C	C6-N1-C2	-6.64	117.64	120.30
1	A	802	C	C6-N1-C2	-6.63	117.65	120.30
1	A	1594	C	C5-C6-N1	6.63	124.31	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1616	G	N7-C8-N9	6.62	116.41	113.10
1	A	1958	U	C2-N1-C1'	6.62	125.65	117.70
1	A	1913	U	C2-N1-C1'	6.62	125.64	117.70
1	A	1671	G	O4'-C1'-N9	6.61	113.49	108.20
1	A	2317	G	C8-N9-C4	-6.60	103.76	106.40
1	A	1747	C	C5-C6-N1	6.60	124.30	121.00
1	A	1875	G	C8-N9-C4	-6.60	103.76	106.40
1	A	908	U	N1-C2-O2	6.59	127.42	122.80
1	A	942	G	N1-C6-O6	-6.59	115.94	119.90
1	A	2636	C	C5-C6-N1	6.58	124.29	121.00
1	A	1953	A	C5-N7-C8	-6.57	100.61	103.90
1	A	859	U	N3-C2-O2	-6.57	117.60	122.20
1	A	1293	C	N1-C2-O2	6.57	122.84	118.90
1	A	655	U	N3-C2-O2	-6.56	117.61	122.20
1	A	2308	G	N3-C4-C5	-6.55	125.32	128.60
1	A	1424	C	N1-C2-O2	6.55	122.83	118.90
1	A	79	C	N1-C2-O2	6.55	122.83	118.90
1	A	989	U	N3-C2-O2	-6.54	117.62	122.20
1	A	2254	A	C8-N9-C1'	6.54	139.47	127.70
1	A	2739	C	C6-N1-C2	-6.54	117.69	120.30
1	A	2459	G	C8-N9-C4	-6.54	103.78	106.40
1	A	1857	C	N3-C2-O2	-6.54	117.33	121.90
1	A	501	C	C2-N1-C1'	6.53	125.99	118.80
1	A	116	U	N3-C2-O2	-6.53	117.63	122.20
1	A	1616	G	C6-C5-N7	-6.53	126.48	130.40
1	A	1076	A	C2-N3-C4	6.52	113.86	110.60
1	A	2288	C	N3-C2-O2	-6.52	117.34	121.90
1	A	475	C	C5-C6-N1	6.52	124.26	121.00
1	A	348	U	C2-N1-C1'	6.52	125.52	117.70
2	B	88	C	N1-C2-O2	6.51	122.80	118.90
1	A	2742	C	C6-N1-C2	-6.50	117.70	120.30
1	A	2259	U	C6-N1-C2	-6.50	117.10	121.00
1	A	116	U	N1-C2-O2	6.49	127.35	122.80
1	A	1010	A	O4'-C1'-N9	6.49	113.39	108.20
1	A	1124	A	P-O3'-C3'	6.49	127.49	119.70
1	A	1104	C	N1-C2-O2	6.49	122.79	118.90
1	A	1766	U	C5-C6-N1	-6.49	119.46	122.70
1	A	1708	U	N3-C2-O2	-6.48	117.66	122.20
1	A	115	C	C5-C6-N1	6.46	124.23	121.00
1	A	1350	U	N3-C2-O2	-6.46	117.68	122.20
1	A	1671	G	C8-N9-C4	-6.46	103.82	106.40
1	A	2021	U	C6-N1-C1'	-6.46	112.16	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	35	U	N3-C2-O2	-6.45	117.68	122.20
1	A	1777	C	C6-N1-C2	-6.45	117.72	120.30
1	A	2042	C	N3-C2-O2	-6.45	117.39	121.90
1	A	2756	U	N1-C2-O2	6.45	127.31	122.80
1	A	1434	U	N3-C2-O2	-6.44	117.69	122.20
1	A	151	C	C6-N1-C2	-6.44	117.72	120.30
1	A	1366	U	C5-C6-N1	6.44	125.92	122.70
1	A	2153	U	C2-N1-C1'	6.44	125.42	117.70
1	A	2230	U	N3-C2-O2	-6.44	117.69	122.20
1	A	1790	A	C5-N7-C8	-6.43	100.69	103.90
1	A	1073	U	C2-N1-C1'	6.42	125.41	117.70
1	A	2213	C	C6-N1-C2	-6.41	117.73	120.30
1	A	2389	U	P-O3'-C3'	6.41	127.40	119.70
1	A	1370	A	C5-N7-C8	-6.41	100.70	103.90
1	A	1616	G	C2-N3-C4	-6.40	108.70	111.90
1	A	2140	C	N1-C2-O2	6.40	122.74	118.90
1	A	773	A	C5-N7-C8	-6.39	100.70	103.90
1	A	766	G	C5-N7-C8	-6.39	101.11	104.30
1	A	859	U	N1-C2-O2	6.39	127.27	122.80
1	A	449	G	O4'-C1'-N9	6.38	113.30	108.20
1	A	574	C	C5-C6-N1	6.38	124.19	121.00
1	A	793	U	C5-C6-N1	6.38	125.89	122.70
1	A	2054	G	N3-C4-C5	-6.37	125.41	128.60
1	A	195	A	N1-C6-N6	-6.37	114.78	118.60
1	A	1881	C	C6-N1-C2	-6.37	117.75	120.30
1	A	393	A	O4'-C1'-N9	6.37	113.29	108.20
1	A	862	C	P-O3'-C3'	-6.36	112.06	119.70
1	A	974	A	C8-N9-C4	-6.36	103.26	105.80
1	A	2028	U	N1-C2-O2	6.36	127.25	122.80
1	A	2153	U	N1-C2-O2	6.36	127.25	122.80
1	A	782	A	N9-C4-C5	-6.36	103.26	105.80
1	A	828	C	N3-C2-O2	-6.36	117.45	121.90
1	A	2153	U	N3-C2-O2	-6.35	117.75	122.20
1	A	2194	C	C2-N1-C1'	6.35	125.78	118.80
1	A	64	G	C4-N9-C1'	6.35	134.75	126.50
1	A	839	C	C6-N1-C2	-6.34	117.76	120.30
1	A	2007	A	N1-C2-N3	-6.34	126.13	129.30
1	A	2041	A	C2-N3-C4	6.34	113.77	110.60
1	A	1978	U	N3-C2-O2	-6.34	117.76	122.20
1	A	2060	C	C6-N1-C2	-6.34	117.76	120.30
2	B	71	C	C2-N1-C1'	6.34	125.77	118.80
1	A	863	G	OP1-P-OP2	6.34	129.11	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1873	U	N1-C2-O2	6.33	127.23	122.80
1	A	973	A	N7-C8-N9	6.33	116.97	113.80
1	A	805	C	C6-N1-C2	-6.33	117.77	120.30
1	A	1301	C	N1-C2-O2	6.33	122.69	118.90
1	A	1133	A	N3-C4-N9	-6.32	122.34	127.40
1	A	2259	U	N1-C2-O2	6.32	127.22	122.80
1	A	411	C	C6-N1-C2	-6.32	117.77	120.30
1	A	1762	U	N1-C2-O2	6.31	127.22	122.80
1	A	1801	G	C5-C6-O6	6.31	132.39	128.60
1	A	1002	U	N3-C4-O4	-6.29	114.99	119.40
1	A	2308	G	C8-N9-C4	-6.29	103.88	106.40
1	A	1107	C	C6-N1-C2	-6.28	117.79	120.30
1	A	1596	C	O4'-C1'-N1	6.28	113.22	108.20
1	A	1873	U	C2-N1-C1'	6.28	125.23	117.70
1	A	1275	A	O4'-C1'-N9	6.27	113.22	108.20
1	A	1739	C	C5-C6-N1	6.27	124.14	121.00
1	A	164	C	N1-C2-O2	6.27	122.66	118.90
1	A	1477	A	C2-N3-C4	6.26	113.73	110.60
1	A	1616	G	N3-C2-N2	6.26	124.28	119.90
1	A	1792	A	C2-N3-C4	6.26	113.73	110.60
1	A	1191	A	C2-N3-C4	-6.25	107.47	110.60
1	A	1881	C	N1-C2-O2	6.25	122.65	118.90
1	A	1220	C	C6-N1-C2	-6.24	117.80	120.30
1	A	1382	A	O4'-C1'-N9	6.24	113.19	108.20
1	A	2274	A	P-O3'-C3'	6.24	127.18	119.70
1	A	105	C	C6-N1-C2	-6.23	117.81	120.30
1	A	1572	C	N1-C2-O2	6.23	122.64	118.90
1	A	2773	U	N3-C2-O2	-6.23	117.84	122.20
1	A	1379	A	C8-N9-C4	-6.23	103.31	105.80
1	A	348	U	O4'-C1'-N1	6.23	113.18	108.20
1	A	954	C	C6-N1-C2	-6.22	117.81	120.30
1	A	1775	C	N1-C2-O2	6.22	122.63	118.90
1	A	2742	C	C6-N1-C1'	-6.22	113.34	120.80
1	A	393	A	C8-N9-C4	-6.21	103.31	105.80
1	A	933	A	O4'-C1'-N9	6.21	113.17	108.20
1	A	2287	A	C5-C6-N6	-6.21	118.73	123.70
1	A	472	G	O4'-C1'-N9	6.21	113.17	108.20
1	A	2694	U	N3-C2-O2	-6.21	117.85	122.20
1	A	1774	A	N9-C4-C5	-6.21	103.32	105.80
1	A	2329	C	C6-N1-C2	-6.21	117.82	120.30
1	A	234	U	N3-C2-O2	-6.20	117.86	122.20
1	A	2319	C	C5-C6-N1	6.20	124.10	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	444	A	C8-N9-C4	-6.20	103.32	105.80
1	A	1500	C	N1-C2-O2	6.20	122.62	118.90
1	A	1958	U	N1-C2-O2	6.19	127.13	122.80
1	A	1820	C	C6-N1-C2	-6.18	117.83	120.30
1	A	2623	U	C2-N1-C1'	6.18	125.12	117.70
1	A	2639	C	C6-N1-C2	-6.18	117.83	120.30
1	A	2812	U	N1-C2-O2	6.17	127.12	122.80
1	A	2257	A	N7-C8-N9	6.17	116.88	113.80
1	A	2606	C	C6-N1-C2	-6.17	117.83	120.30
1	A	2293	C	N3-C2-O2	-6.17	117.58	121.90
1	A	357	A	N7-C8-N9	6.16	116.88	113.80
1	A	774	G	C5-N7-C8	-6.16	101.22	104.30
1	A	322	U	C5-C6-N1	6.16	125.78	122.70
1	A	1745	U	C2-N1-C1'	6.16	125.09	117.70
1	A	1761	C	C5-C6-N1	6.16	124.08	121.00
1	A	503	G	C4-N9-C1'	-6.15	118.50	126.50
1	A	2546	C	C6-N1-C2	-6.15	117.84	120.30
1	A	1070	C	C2-N3-C4	6.15	122.98	119.90
1	A	1161	C	C5-C6-N1	6.15	124.07	121.00
1	A	27	G	N3-C4-N9	-6.14	122.31	126.00
1	A	1156	U	N3-C2-O2	-6.14	117.90	122.20
1	A	2293	C	C6-N1-C1'	-6.14	113.44	120.80
1	A	2623	U	N1-C2-O2	6.14	127.10	122.80
1	A	397	G	C4-C5-N7	6.13	113.25	110.80
15	O	59	LEU	CA-CB-CG	6.13	129.41	115.30
1	A	1608	A	N7-C8-N9	6.13	116.86	113.80
1	A	69	C	C6-N1-C2	-6.13	117.85	120.30
1	A	1468	U	C2-N1-C1'	6.13	125.05	117.70
1	A	1249	A	N1-C6-N6	-6.12	114.92	118.60
1	A	817	U	O5'-P-OP1	-6.12	100.19	105.70
1	A	1923	A	N1-C2-N3	6.12	132.36	129.30
1	A	1292	C	N1-C2-O2	6.12	122.57	118.90
1	A	393	A	C5-N7-C8	-6.11	100.84	103.90
1	A	2302	G	O4'-C1'-N9	6.11	113.09	108.20
1	A	1313	U	N1-C2-O2	6.11	127.08	122.80
1	A	1064	G	C4-N9-C1'	6.10	134.43	126.50
1	A	998	A	O4'-C1'-N9	6.10	113.08	108.20
1	A	699	U	N3-C2-O2	-6.09	117.93	122.20
1	A	1339	U	N3-C2-O2	-6.09	117.94	122.20
1	A	2636	C	N1-C2-O2	6.09	122.55	118.90
1	A	374	C	N1-C2-O2	6.09	122.55	118.90
1	A	1619	U	N1-C2-N3	6.09	118.55	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1934	C	C6-N1-C2	-6.08	117.87	120.30
1	A	2817	C	C6-N1-C2	-6.08	117.87	120.30
1	A	463	A	C5-N7-C8	-6.08	100.86	103.90
1	A	2037	C	N3-C4-N4	-6.07	113.75	118.00
1	A	1373	C	O4'-C1'-N1	6.07	113.06	108.20
1	A	64	G	C5-N7-C8	-6.07	101.27	104.30
1	A	2059	C	C6-N1-C2	-6.07	117.87	120.30
1	A	2152	C	N3-C2-O2	-6.05	117.66	121.90
1	A	1369	G	O4'-C1'-N9	6.05	113.04	108.20
1	A	1993	C	C5-C6-N1	6.05	124.03	121.00
1	A	2251	C	C6-N1-C2	-6.05	117.88	120.30
1	A	1320	C	N1-C2-O2	6.05	122.53	118.90
1	A	323	G	C5-C6-O6	-6.05	124.97	128.60
1	A	836	U	N1-C2-O2	6.05	127.03	122.80
1	A	1646	C	N1-C2-O2	6.04	122.53	118.90
1	A	1385	C	N1-C2-O2	6.02	122.51	118.90
1	A	1987	C	C5-C6-N1	6.02	124.01	121.00
1	A	116	U	C2-N1-C1'	6.02	124.92	117.70
4	D	100	LEU	CA-CB-CG	6.02	129.14	115.30
1	A	1107	C	C6-N1-C1'	-6.01	113.58	120.80
1	A	1622	A	O4'-C1'-N9	6.01	113.01	108.20
1	A	1187	C	C6-N1-C2	-6.00	117.90	120.30
1	A	664	G	O5'-P-OP2	-6.00	100.30	105.70
1	A	538	G	C4-N9-C1'	6.00	134.30	126.50
1	A	1494	C	N3-C2-O2	-6.00	117.70	121.90
1	A	2337	C	N1-C2-O2	6.00	122.50	118.90
1	A	574	C	C6-N1-C2	-6.00	117.90	120.30
1	A	836	U	C6-N1-C1'	-5.99	112.81	121.20
1	A	933	A	C4-C5-N7	5.99	113.69	110.70
1	A	62	U	OP2-P-O3'	5.99	118.38	105.20
1	A	1756	U	N1-C2-O2	5.99	126.99	122.80
1	A	2284	C	N3-C2-O2	-5.99	117.71	121.90
1	A	463	A	O4'-C1'-N9	5.98	112.98	108.20
1	A	1958	U	N3-C2-O2	-5.98	118.02	122.20
1	A	1671	G	N1-C6-O6	5.97	123.48	119.90
1	A	538	G	C5-C6-O6	-5.97	125.02	128.60
1	A	2717	C	C6-N1-C2	-5.96	117.91	120.30
1	A	2707	U	N3-C2-O2	-5.96	118.03	122.20
1	A	2329	C	C5-C6-N1	5.96	123.98	121.00
1	A	2030	U	C5-C6-N1	5.96	125.68	122.70
1	A	208	C	C2-N1-C1'	5.96	125.35	118.80
1	A	2752	A	C2-N3-C4	5.96	113.58	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	733	C	C6-N1-C2	-5.95	117.92	120.30
1	A	78	U	N1-C2-O2	5.95	126.96	122.80
1	A	1325	G	N1-C6-O6	-5.95	116.33	119.90
1	A	2254	A	C4-N9-C1'	-5.94	115.60	126.30
1	A	865	C	N1-C2-O2	5.94	122.46	118.90
1	A	1094	C	N1-C2-O2	5.94	122.47	118.90
1	A	2643	U	N1-C2-O2	5.94	126.96	122.80
1	A	1128	G	N1-C6-O6	-5.93	116.34	119.90
1	A	2595	G	C4-C5-N7	5.93	113.17	110.80
1	A	397	G	C5-N7-C8	-5.93	101.33	104.30
1	A	1191	A	C5-C6-N1	-5.92	114.74	117.70
1	A	1672	G	N3-C4-C5	-5.92	125.64	128.60
1	A	2836	U	C2-N1-C1'	5.92	124.81	117.70
1	A	1814	U	N3-C2-O2	-5.92	118.06	122.20
1	A	1564	C	C6-N1-C2	-5.92	117.93	120.30
1	A	1790	A	O4'-C1'-N9	5.92	112.93	108.20
1	A	1660	C	C5-C6-N1	5.92	123.96	121.00
1	A	172	C	C2-N1-C1'	5.92	125.31	118.80
1	A	1642	A	P-O3'-C3'	5.91	126.79	119.70
1	A	348	U	N1-C2-O2	5.91	126.94	122.80
1	A	1739	C	C6-N1-C2	-5.91	117.94	120.30
1	A	2266	G	N3-C4-C5	-5.91	125.64	128.60
1	A	2410	U	C6-N1-C2	-5.91	117.45	121.00
1	A	974	A	C2-N3-C4	5.90	113.55	110.60
1	A	1211	A	O4'-C1'-N9	5.90	112.92	108.20
1	A	2174	C	C6-N1-C2	-5.89	117.94	120.30
1	A	503	G	C8-N9-C1'	5.89	134.66	127.00
1	A	227	A	P-O3'-C3'	5.89	126.77	119.70
1	A	2152	C	N1-C2-O2	5.89	122.43	118.90
1	A	540	U	P-O3'-C3'	5.88	126.76	119.70
1	A	1627	A	C2'-C3'-O3'	5.88	123.11	113.70
1	A	2050	C	N1-C2-O2	5.88	122.43	118.90
1	A	2058	A	N1-C2-N3	-5.88	126.36	129.30
19	S	84	ARG	CG-CD-NE	-5.88	99.46	111.80
1	A	2461	U	N3-C2-O2	-5.87	118.09	122.20
2	B	71	C	N1-C2-O2	5.87	122.42	118.90
1	A	2526	C	C2-N1-C1'	5.87	125.25	118.80
1	A	2623	U	N3-C2-O2	-5.87	118.09	122.20
1	A	1640	A	C4-C5-C6	-5.87	114.07	117.00
1	A	1873	U	N3-C2-O2	-5.86	118.10	122.20
1	A	2771	U	N3-C2-O2	-5.86	118.10	122.20
1	A	2823	U	N3-C2-O2	-5.86	118.10	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2124	C	C5-C6-N1	5.86	123.93	121.00
1	A	1966	C	C6-N1-C2	-5.86	117.96	120.30
1	A	2603	C	C6-N1-C2	-5.85	117.96	120.30
23	W	40	LEU	CB-CG-CD1	-5.85	101.05	111.00
1	A	2459	G	N7-C8-N9	5.85	116.03	113.10
1	A	1289	A	N7-C8-N9	5.85	116.72	113.80
1	A	1011	A	C5-N7-C8	-5.85	100.97	103.90
1	A	2174	C	C5-C6-N1	5.85	123.92	121.00
15	O	16	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	1362	U	O4'-C1'-N1	5.84	112.87	108.20
1	A	1748	C	C6-N1-C2	-5.84	117.96	120.30
1	A	2732	C	N1-C2-O2	5.84	122.40	118.90
1	A	1327	U	N3-C2-O2	-5.84	118.11	122.20
1	A	2724	G	C8-N9-C4	-5.83	104.07	106.40
1	A	2194	C	C5-C6-N1	5.83	123.92	121.00
1	A	807	C	C6-N1-C2	-5.83	117.97	120.30
1	A	1589	C	C6-N1-C2	-5.82	117.97	120.30
1	A	2082	A	O4'-C1'-N9	5.82	112.86	108.20
1	A	2248	C	C6-N1-C2	-5.82	117.97	120.30
1	A	2889	C	N3-C2-O2	-5.82	117.83	121.90
1	A	1930	U	N1-C2-O2	5.82	126.87	122.80
1	A	119	A	C6-C5-N7	5.81	136.37	132.30
1	A	1077	G	N1-C2-N2	5.81	121.43	116.20
1	A	2308	G	N1-C6-O6	-5.81	116.41	119.90
1	A	698	G	C4-N9-C1'	5.81	134.05	126.50
1	A	1665	C	N1-C2-O2	5.81	122.39	118.90
1	A	1988	C	N1-C2-O2	5.81	122.39	118.90
1	A	800	U	C5-C6-N1	5.81	125.60	122.70
1	A	1972	C	C6-N1-C2	-5.81	117.98	120.30
1	A	383	C	N1-C2-O2	5.80	122.38	118.90
1	A	824	G	C8-N9-C4	-5.80	104.08	106.40
1	A	1790	A	N7-C8-N9	5.80	116.70	113.80
1	A	306	G	N3-C4-N9	5.80	129.48	126.00
1	A	1977	C	C6-N1-C2	-5.80	117.98	120.30
2	B	111	C	N3-C2-O2	-5.80	117.84	121.90
1	A	933	A	N7-C8-N9	5.80	116.70	113.80
1	A	2079	U	N3-C2-O2	-5.80	118.14	122.20
1	A	538	G	C8-N9-C1'	-5.79	119.47	127.00
1	A	694	G	O4'-C1'-N9	5.79	112.83	108.20
1	A	2549	U	N1-C2-O2	5.79	126.86	122.80
1	A	2366	G	C4-N9-C1'	5.79	134.03	126.50
1	A	920	C	OP2-P-O3'	5.79	117.93	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2382	C	C6-N1-C1'	-5.79	113.86	120.80
1	A	519	A	C8-N9-C1'	5.78	138.10	127.70
1	A	773	A	C8-N9-C4	-5.78	103.49	105.80
1	A	1076	A	N3-C4-C5	-5.78	122.76	126.80
1	A	1875	G	C5-N7-C8	-5.78	101.41	104.30
14	N	33	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	1698	C	N1-C2-O2	5.78	122.37	118.90
1	A	192	C	C5-C6-N1	5.77	123.88	121.00
1	A	1289	A	C4-C5-N7	5.76	113.58	110.70
1	A	686	A	N9-C1'-C2'	-5.76	105.66	112.00
1	A	2445	G	C4-N9-C1'	5.76	133.99	126.50
11	K	91	GLN	C-N-CA	5.76	136.11	121.70
1	A	863	G	N7-C8-N9	5.76	115.98	113.10
1	A	1659	A	C4-N9-C1'	5.75	136.65	126.30
1	A	1564	C	N3-C2-O2	-5.75	117.88	121.90
1	A	1009	U	O4'-C1'-N1	5.75	112.80	108.20
1	A	938	C	C6-N1-C2	-5.75	118.00	120.30
1	A	1161	C	C6-N1-C2	-5.75	118.00	120.30
1	A	2445	G	O4'-C1'-N9	5.75	112.80	108.20
1	A	257	C	C6-N1-C2	-5.74	118.00	120.30
1	A	640	C	C6-N1-C2	-5.74	118.00	120.30
1	A	288	A	O4'-C1'-N9	5.74	112.79	108.20
1	A	1156	U	C6-N1-C2	-5.74	117.56	121.00
1	A	1191	A	N3-C4-C5	5.74	130.82	126.80
1	A	2776	C	C6-N1-C2	-5.74	118.00	120.30
1	A	699	U	N1-C2-O2	5.74	126.82	122.80
1	A	2410	U	C5-C6-N1	5.74	125.57	122.70
1	A	1607	C	C6-N1-C2	-5.74	118.01	120.30
1	A	964	A	C4-C5-N7	5.73	113.56	110.70
1	A	2331	U	C5-C6-N1	5.73	125.57	122.70
1	A	538	G	N3-C4-N9	5.73	129.44	126.00
1	A	1261	A	N7-C8-N9	5.72	116.66	113.80
1	A	2454	C	C6-N1-C2	-5.72	118.01	120.30
1	A	519	A	C6-N1-C2	5.72	122.03	118.60
1	A	1595	C	N1-C2-O2	5.72	122.33	118.90
1	A	787	C	C6-N1-C2	-5.71	118.02	120.30
1	A	799	G	N1-C6-O6	-5.71	116.47	119.90
1	A	1293	C	N3-C2-O2	-5.71	117.91	121.90
1	A	2732	C	C2-N1-C1'	5.70	125.08	118.80
1	A	68	G	N3-C4-N9	5.70	129.42	126.00
1	A	243	U	P-O3'-C3'	5.70	126.54	119.70
1	A	923	A	O4'-C1'-N9	5.70	112.76	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2257	A	C5-N7-C8	-5.70	101.05	103.90
1	A	971	A	O4'-C1'-N9	5.70	112.76	108.20
1	A	376	C	C6-N1-C2	-5.69	118.02	120.30
1	A	1300	U	C6-N1-C1'	-5.69	113.24	121.20
1	A	2124	C	C6-N1-C2	-5.69	118.03	120.30
1	A	2653	C	C6-N1-C1'	-5.69	113.98	120.80
1	A	25	U	N3-C2-O2	-5.69	118.22	122.20
1	A	1301	C	N3-C2-O2	-5.68	117.92	121.90
1	A	463	A	N7-C8-N9	5.68	116.64	113.80
1	A	1993	C	C6-N1-C2	-5.68	118.03	120.30
1	A	1101	A	N3-C4-N9	5.67	131.94	127.40
1	A	1661	U	C5-C6-N1	5.67	125.54	122.70
1	A	1802	A	C8-N9-C4	5.67	108.07	105.80
1	A	901	C	C2-N1-C1'	5.67	125.03	118.80
1	A	1254	U	N1-C2-O2	5.67	126.77	122.80
1	A	1660	C	N1-C2-O2	5.67	122.30	118.90
1	A	1772	A	N1-C6-N6	-5.66	115.20	118.60
1	A	2334	C	C2-N1-C1'	5.66	125.03	118.80
1	A	2467	C	C2-N1-C1'	5.66	125.03	118.80
1	A	2874	C	C6-N1-C2	-5.66	118.04	120.30
1	A	1741	A	O4'-C1'-N9	5.66	112.73	108.20
2	B	3	C	C5-C6-N1	5.66	123.83	121.00
1	A	434	A	OP2-P-O3'	5.65	117.64	105.20
1	A	726	C	C6-N1-C2	-5.65	118.04	120.30
1	A	2042	C	C6-N1-C2	-5.65	118.04	120.30
1	A	2835	G	O4'-C1'-N9	5.65	112.72	108.20
1	A	571	C	C6-N1-C2	-5.65	118.04	120.30
1	A	377	G	N3-C4-C5	5.65	131.42	128.60
1	A	359	U	C2-N1-C1'	5.64	124.47	117.70
1	A	411	C	C2-N1-C1'	5.64	125.01	118.80
1	A	773	A	N7-C8-N9	5.64	116.62	113.80
1	A	1092	C	C6-N1-C1'	-5.64	114.03	120.80
1	A	2454	C	N1-C2-O2	5.64	122.29	118.90
1	A	1211	A	C5-N7-C8	-5.64	101.08	103.90
1	A	1453	U	N1-C2-O2	5.64	126.75	122.80
1	A	2302	G	N1-C6-O6	-5.64	116.52	119.90
1	A	2237	G	C5-N7-C8	-5.64	101.48	104.30
1	A	1254	U	N3-C2-O2	-5.64	118.25	122.20
26	Z	12	LEU	CA-CB-CG	5.64	128.26	115.30
1	A	422	U	N1-C2-O2	5.63	126.74	122.80
1	A	150	U	C6-N1-C2	-5.63	117.62	121.00
1	A	1787	C	N1-C2-O2	5.63	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1156	U	C5-C6-N1	5.62	125.51	122.70
1	A	400	G	N7-C8-N9	5.62	115.91	113.10
1	A	1046	G	C8-N9-C4	-5.62	104.15	106.40
1	A	209	C	C6-N1-C2	-5.61	118.06	120.30
1	A	1211	A	N7-C8-N9	5.61	116.60	113.80
20	T	40	LEU	CA-CB-CG	5.61	128.19	115.30
1	A	1784	C	C5-C6-N1	5.60	123.80	121.00
1	A	2287	A	N9-C4-C5	-5.60	103.56	105.80
1	A	2366	G	N3-C4-N9	5.60	129.36	126.00
1	A	2593	C	C6-N1-C2	-5.60	118.06	120.30
1	A	1993	C	N1-C2-O2	5.60	122.26	118.90
1	A	2041	A	N1-C2-N3	-5.60	126.50	129.30
1	A	251	A	C4-C5-N7	5.60	113.50	110.70
1	A	2422	A	N1-C6-N6	-5.60	115.24	118.60
2	B	35	U	O4'-C1'-N1	5.60	112.68	108.20
1	A	1244	C	C6-N1-C2	-5.59	118.06	120.30
1	A	1484	U	N3-C2-O2	-5.59	118.28	122.20
1	A	333	U	C6-N1-C2	-5.59	117.65	121.00
1	A	642	U	C5-C6-N1	5.59	125.49	122.70
1	A	192	C	C6-N1-C2	-5.58	118.07	120.30
1	A	397	G	N7-C8-N9	5.58	115.89	113.10
1	A	1801	G	N1-C2-N3	5.58	127.25	123.90
1	A	2028	U	N3-C2-O2	-5.58	118.29	122.20
1	A	172	C	C5-C6-N1	5.58	123.79	121.00
1	A	518	C	N3-C4-N4	-5.58	114.10	118.00
1	A	1601	C	C2-N1-C1'	5.58	124.94	118.80
1	A	2607	C	C6-N1-C2	-5.58	118.07	120.30
1	A	787	C	C5-C6-N1	5.57	123.79	121.00
1	A	2443	C	C5-C6-N1	5.57	123.79	121.00
1	A	2382	C	C6-N1-C2	-5.57	118.07	120.30
1	A	1197	G	N3-C4-C5	5.57	131.38	128.60
1	A	879	C	N1-C2-O2	5.56	122.24	118.90
1	A	2252	U	C2-N1-C1'	5.56	124.38	117.70
1	A	995	C	C2-N1-C1'	5.56	124.91	118.80
1	A	123	G	N1-C6-O6	-5.55	116.57	119.90
1	A	428	U	N3-C2-O2	-5.55	118.31	122.20
1	A	2632	G	C5-N7-C8	-5.55	101.52	104.30
2	B	111	C	C6-N1-C2	-5.55	118.08	120.30
2	B	111	C	N1-C2-O2	5.55	122.23	118.90
1	A	1053	G	C8-N9-C1'	-5.55	119.79	127.00
1	A	1708	U	N1-C2-O2	5.55	126.68	122.80
1	A	208	C	C5-C6-N1	5.55	123.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2042	C	N1-C2-O2	5.54	122.22	118.90
1	A	1077	G	N3-C2-N2	-5.54	116.02	119.90
1	A	2378	G	O4'-C1'-N9	5.54	112.63	108.20
1	A	2675	G	C5-N7-C8	-5.54	101.53	104.30
1	A	264	U	O4'-C1'-N1	5.54	112.63	108.20
1	A	2467	C	C6-N1-C2	-5.54	118.09	120.30
1	A	507	C	N1-C2-O2	5.53	122.22	118.90
1	A	1649	G	N1-C6-O6	-5.53	116.58	119.90
1	A	995	C	C5-C6-N1	5.53	123.77	121.00
1	A	1802	A	N9-C4-C5	-5.53	103.59	105.80
1	A	1992	A	N1-C6-N6	-5.53	115.28	118.60
1	A	408	C	C2-N1-C1'	5.52	124.87	118.80
1	A	784	G	C8-N9-C1'	-5.52	119.82	127.00
1	A	1171	G	N3-C4-C5	-5.52	125.84	128.60
1	A	1500	C	C2-N1-C1'	5.51	124.86	118.80
1	A	2537	G	O5'-P-OP1	-5.51	100.74	105.70
1	A	1967	G	N3-C4-N9	5.51	129.31	126.00
1	A	1600	A	N7-C8-N9	5.51	116.55	113.80
1	A	518	C	C2-N1-C1'	5.50	124.85	118.80
1	A	1616	G	C8-N9-C4	-5.50	104.20	106.40
1	A	440	A	O5'-P-OP1	-5.50	100.75	105.70
1	A	1481	A	O4'-C1'-N9	5.50	112.60	108.20
1	A	2304	C	C6-N1-C2	-5.50	118.10	120.30
1	A	2337	C	N3-C2-O2	-5.50	118.05	121.90
12	L	112	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	422	U	N3-C2-O2	-5.49	118.36	122.20
1	A	2788	U	C5-C4-O4	-5.49	122.61	125.90
1	A	741	A	N7-C8-N9	5.49	116.55	113.80
1	A	2403	C	C5-C6-N1	5.49	123.75	121.00
1	A	2124	C	C2-N1-C1'	5.49	124.84	118.80
1	A	2638	C	C6-N1-C1'	-5.49	114.22	120.80
1	A	1320	C	C5-C6-N1	5.49	123.74	121.00
1	A	428	U	N1-C2-O2	5.48	126.64	122.80
1	A	64	G	C8-N9-C4	-5.48	104.21	106.40
1	A	2022	G	O4'-C1'-N9	5.48	112.58	108.20
1	A	836	U	O4'-C1'-N1	5.48	112.58	108.20
1	A	1300	U	C6-N1-C2	-5.48	117.71	121.00
1	A	1599	A	C4-C5-N7	5.47	113.44	110.70
1	A	1851	U	N3-C2-O2	-5.47	118.37	122.20
1	A	2050	C	C2-N1-C1'	5.47	124.82	118.80
1	A	27	G	N9-C4-C5	5.47	107.59	105.40
1	A	1442	G	N7-C8-N9	5.47	115.84	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	U	N3-C2-O2	-5.47	118.37	122.20
1	A	2417	A	C2-N3-C4	5.47	113.33	110.60
1	A	299	C	C6-N1-C2	-5.47	118.11	120.30
1	A	1077	G	N1-C6-O6	5.47	123.18	119.90
1	A	475	C	C6-N1-C2	-5.46	118.12	120.30
1	A	293	A	C4-C5-N7	5.45	113.43	110.70
1	A	1171	G	C2-N3-C4	5.45	114.63	111.90
1	A	1763	G	C5-C6-N1	5.45	114.23	111.50
1	A	2546	C	C5-C6-N1	5.45	123.72	121.00
1	A	1094	C	N3-C2-O2	-5.45	118.09	121.90
1	A	2669	U	N1-C2-O2	5.45	126.61	122.80
1	A	31	C	C6-N1-C2	-5.44	118.12	120.30
1	A	113	C	C6-N1-C1'	-5.44	114.27	120.80
1	A	2655	G	C4-N9-C1'	5.44	133.58	126.50
1	A	802	C	N1-C2-O2	5.44	122.17	118.90
1	A	2788	U	C5-C6-N1	5.44	125.42	122.70
1	A	164	C	N3-C2-O2	-5.44	118.09	121.90
1	A	1616	G	C5-N7-C8	-5.44	101.58	104.30
1	A	69	C	C2-N1-C1'	5.44	124.78	118.80
1	A	545	G	O4'-C1'-N9	5.44	112.55	108.20
1	A	550	C	N1-C2-O2	5.44	122.16	118.90
1	A	2270	U	N3-C2-O2	-5.44	118.39	122.20
1	A	2124	C	N1-C2-O2	5.44	122.16	118.90
1	A	119	A	N3-C4-N9	-5.43	123.05	127.40
1	A	1990	A	C4-C5-C6	-5.43	114.28	117.00
1	A	2057	A	C5-C6-N1	5.43	120.42	117.70
1	A	2560	C	N1-C2-O2	5.43	122.16	118.90
1	A	234	U	N1-C2-O2	5.43	126.60	122.80
1	A	2521	C	N1-C2-O2	5.43	122.16	118.90
1	A	374	C	N3-C2-O2	-5.43	118.10	121.90
1	A	1801	G	N1-C6-O6	-5.42	116.65	119.90
1	A	2052	C	C2-N1-C1'	5.42	124.76	118.80
1	A	2237	G	N7-C8-N9	5.42	115.81	113.10
1	A	2060	C	N1-C2-O2	5.42	122.15	118.90
1	A	2724	G	N9-C4-C5	5.42	107.57	105.40
1	A	1300	U	C5-C6-N1	5.42	125.41	122.70
1	A	1741	A	C4-C5-N7	5.42	113.41	110.70
1	A	784	G	C4-N9-C1'	5.41	133.53	126.50
1	A	1881	C	C6-N1-C1'	-5.41	114.31	120.80
1	A	846	G	N7-C8-N9	5.41	115.81	113.10
1	A	862	C	O3'-P-O5'	5.41	114.27	104.00
1	A	16	C	N1-C2-O2	5.40	122.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1370	A	C8-N9-C4	-5.40	103.64	105.80
9	I	80	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	1232	G	C8-N9-C4	-5.40	104.24	106.40
1	A	1076	A	N3-C4-N9	5.40	131.72	127.40
1	A	2302	G	C5-C6-O6	5.40	131.84	128.60
1	A	526	G	N9-C4-C5	-5.40	103.24	105.40
1	A	1191	A	O4'-C1'-N9	5.40	112.52	108.20
1	A	922	G	N3-C4-N9	5.39	129.24	126.00
1	A	2382	C	C5-C6-N1	5.39	123.70	121.00
1	A	510	U	C5-C6-N1	5.39	125.40	122.70
1	A	2875	C	C6-N1-C2	-5.39	118.14	120.30
1	A	1149	C	C2-N1-C1'	5.39	124.73	118.80
1	A	2739	C	C5-C6-N1	5.39	123.69	121.00
1	A	727	C	C6-N1-C2	-5.38	118.15	120.30
1	A	1741	A	C5-N7-C8	-5.38	101.21	103.90
1	A	2156	A	C2-N3-C4	5.38	113.29	110.60
1	A	1672	G	P-O3'-C3'	5.38	126.16	119.70
1	A	591	C	C6-N1-C2	-5.38	118.15	120.30
1	A	865	C	N3-C2-O2	-5.37	118.14	121.90
1	A	1218	U	N3-C2-O2	-5.37	118.44	122.20
1	A	625	C	C6-N1-C2	-5.37	118.15	120.30
1	A	1407	U	C6-N1-C2	-5.37	117.78	121.00
1	A	363	G	O4'-C1'-N9	5.37	112.49	108.20
1	A	865	C	C2-N1-C1'	5.37	124.70	118.80
2	B	31	C	C6-N1-C2	-5.36	118.16	120.30
1	A	2068	U	N1-C2-O2	5.36	126.55	122.80
1	A	126	A	C4-C5-N7	5.36	113.38	110.70
1	A	972	C	N1-C2-O2	5.36	122.11	118.90
1	A	1559	A	C4-C5-C6	-5.36	114.32	117.00
1	A	114	U	C6-N1-C2	-5.36	117.78	121.00
1	A	1762	U	N3-C2-O2	-5.36	118.45	122.20
1	A	535	C	C6-N1-C2	-5.35	118.16	120.30
1	A	2382	C	N1-C2-O2	5.35	122.11	118.90
1	A	1913	U	O4'-C1'-N1	5.35	112.48	108.20
1	A	408	C	N1-C2-O2	5.35	122.11	118.90
1	A	748	G	N3-C4-C5	-5.34	125.93	128.60
1	A	863	G	C8-N9-C4	-5.34	104.26	106.40
1	A	1608	A	O4'-C1'-N9	5.34	112.47	108.20
1	A	1149	C	N3-C2-O2	-5.34	118.16	121.90
1	A	2634	U	N3-C2-O2	-5.34	118.46	122.20
1	A	2118	U	N1-C2-O2	5.34	126.53	122.80
1	A	519	A	N9-C4-C5	5.33	107.93	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1191	A	C5-N7-C8	-5.33	101.23	103.90
1	A	321	G	O4'-C1'-N9	5.33	112.46	108.20
1	A	1144	C	C6-N1-C2	-5.33	118.17	120.30
1	A	967	G	N3-C2-N2	-5.33	116.17	119.90
1	A	1484	U	N1-C2-O2	5.32	126.53	122.80
2	B	31	C	N3-C2-O2	-5.32	118.17	121.90
1	A	972	C	C2-N1-C1'	5.32	124.65	118.80
1	A	1628	C	N3-C4-C5	5.32	124.03	121.90
1	A	1749	A	N7-C8-N9	5.32	116.46	113.80
1	A	2014	G	C4-C5-N7	5.32	112.93	110.80
1	A	1500	C	C6-N1-C2	-5.32	118.17	120.30
1	A	1801	G	N3-C2-N2	5.32	123.62	119.90
1	A	2037	C	C5-C4-N4	5.32	123.92	120.20
1	A	1191	A	C4-C5-N7	5.32	113.36	110.70
1	A	2697	C	C6-N1-C2	-5.32	118.17	120.30
1	A	538	G	N1-C6-O6	5.31	123.09	119.90
12	L	6	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	285	U	N1-C2-O2	5.31	126.52	122.80
1	A	404	C	N1-C2-O2	5.31	122.08	118.90
1	A	427	C	C6-N1-C2	-5.30	118.18	120.30
1	A	737	U	O4'-C1'-N1	5.30	112.44	108.20
1	A	2771	U	N1-C2-O2	5.30	126.51	122.80
1	A	1801	G	C8-N9-C4	-5.30	104.28	106.40
1	A	1972	C	N3-C2-O2	-5.30	118.19	121.90
1	A	400	G	C6-C5-N7	-5.30	127.22	130.40
1	A	862	C	OP2-P-O3'	5.30	116.86	105.20
2	B	67	U	C2-N1-C1'	5.30	124.06	117.70
1	A	408	C	C5-C6-N1	5.30	123.65	121.00
1	A	983	G	C4-C5-N7	5.30	112.92	110.80
1	A	824	G	N7-C8-N9	5.30	115.75	113.10
1	A	2479	U	O4'-C1'-N1	5.29	112.44	108.20
1	A	1445	U	C2-N1-C1'	5.29	124.05	117.70
1	A	535	C	C2-N1-C1'	5.29	124.61	118.80
1	A	1011	A	C8-N9-C1'	5.29	137.22	127.70
1	A	2052	C	C6-N1-C2	-5.29	118.19	120.30
1	A	2874	C	C5-C6-N1	5.29	123.64	121.00
1	A	904	C	C2-N1-C1'	5.28	124.61	118.80
1	A	2703	C	C5-C6-N1	5.28	123.64	121.00
1	A	904	C	N1-C2-O2	5.28	122.07	118.90
1	A	1010	A	C5-N7-C8	-5.28	101.26	103.90
1	A	766	G	C4-C5-N7	5.28	112.91	110.80
1	A	2348	C	N3-C2-O2	-5.28	118.21	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	774	G	N7-C8-N9	5.28	115.74	113.10
1	A	1016	U	P-O3'-C3'	5.28	126.03	119.70
1	A	2543	C	N1-C2-O2	5.28	122.06	118.90
6	F	156	LEU	CA-CB-CG	5.28	127.43	115.30
29	3	4	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	2583	U	O4'-C1'-N1	5.27	112.42	108.20
1	A	1091	U	N1-C2-O2	5.27	126.49	122.80
1	A	1968	A	C4-N9-C1'	5.27	135.79	126.30
1	A	1966	C	N3-C2-O2	-5.27	118.21	121.90
17	Q	117	LEU	CA-CB-CG	5.27	127.41	115.30
1	A	2483	C	N1-C2-O2	5.26	122.06	118.90
1	A	243	U	N3-C2-O2	-5.26	118.52	122.20
1	A	478	C	C6-N1-C2	-5.26	118.19	120.30
1	A	1424	C	N3-C2-O2	-5.26	118.22	121.90
1	A	1341	A	C4-C5-N7	5.26	113.33	110.70
1	A	2366	G	C8-N9-C1'	-5.26	120.17	127.00
1	A	1282	C	N3-C2-O2	-5.25	118.22	121.90
1	A	1385	C	C6-N1-C2	-5.25	118.20	120.30
1	A	2563	G	N7-C8-N9	5.25	115.73	113.10
1	A	698	G	C8-N9-C1'	-5.25	120.17	127.00
1	A	1532	C	N1-C2-O2	5.25	122.05	118.90
1	A	937	A	N1-C2-N3	-5.25	126.67	129.30
1	A	1363	C	N3-C2-O2	-5.25	118.22	121.90
1	A	852	A	C4-C5-N7	5.25	113.32	110.70
1	A	114	U	P-O3'-C3'	5.25	126.00	119.70
1	A	813	C	C6-N1-C2	-5.25	118.20	120.30
1	A	2237	G	C4-C5-N7	5.25	112.90	110.80
1	A	450	U	C2-N1-C1'	5.24	123.99	117.70
1	A	1500	C	N3-C2-O2	-5.24	118.23	121.90
1	A	2445	G	C6-C5-N7	-5.24	127.26	130.40
1	A	1869	U	N3-C2-O2	-5.24	118.53	122.20
1	A	2549	U	C2-N1-C1'	5.24	123.98	117.70
1	A	1276	C	C5-C6-N1	5.24	123.62	121.00
1	A	807	C	N3-C2-O2	-5.23	118.24	121.90
1	A	418	U	N3-C2-O2	-5.23	118.54	122.20
1	A	1002	U	C5-C4-O4	5.23	129.04	125.90
1	A	2876	C	C6-N1-C2	-5.23	118.21	120.30
1	A	995	C	N3-C4-C5	-5.22	119.81	121.90
1	A	1327	U	OP2-P-O3'	5.22	116.69	105.20
1	A	1185	U	N3-C2-O2	-5.22	118.54	122.20
1	A	444	A	P-O3'-C3'	5.22	125.97	119.70
1	A	172	C	C6-N1-C2	-5.22	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	G	O4'-C1'-N9	5.22	112.37	108.20
1	A	2809	G	C5-C6-O6	-5.22	125.47	128.60
1	A	1370	A	O4'-C1'-N9	5.21	112.37	108.20
1	A	2308	G	P-O3'-C3'	5.21	125.96	119.70
1	A	802	C	C5-C6-N1	5.21	123.61	121.00
1	A	2809	G	C4-C5-N7	5.21	112.89	110.80
1	A	2117	U	C2-N1-C1'	5.21	123.95	117.70
1	A	864	G	C4-N9-C1'	5.21	133.27	126.50
1	A	2287	A	C4-C5-N7	5.21	113.30	110.70
1	A	35	G	N3-C4-N9	5.21	129.12	126.00
2	B	88	C	N3-C2-O2	-5.21	118.26	121.90
1	A	1572	C	C6-N1-C1'	-5.20	114.56	120.80
1	A	2003	U	C6-N1-C1'	-5.20	113.91	121.20
1	A	2187	C	C6-N1-C2	-5.20	118.22	120.30
1	A	938	C	C5-C6-N1	5.20	123.60	121.00
1	A	1221	U	N3-C2-O2	-5.20	118.56	122.20
1	A	2308	G	C8-N9-C1'	-5.20	120.24	127.00
1	A	2403	C	C6-N1-C2	-5.20	118.22	120.30
1	A	972	C	N3-C4-N4	-5.19	114.36	118.00
1	A	2812	U	O4'-C1'-N1	5.19	112.36	108.20
1	A	1634	C	C6-N1-C2	-5.19	118.22	120.30
1	A	2612	A	C2-N3-C4	5.19	113.19	110.60
1	A	2308	G	C5-C6-O6	5.19	131.71	128.60
1	A	183	C	C6-N1-C2	-5.19	118.22	120.30
1	A	922	G	C2-N3-C4	5.19	114.49	111.90
1	A	1659	A	C8-N9-C1'	-5.19	118.36	127.70
1	A	1918	U	C2-N1-C1'	5.19	123.93	117.70
1	A	1756	U	C6-N1-C2	-5.18	117.89	121.00
1	A	2638	C	N3-C2-O2	-5.18	118.27	121.90
1	A	1616	G	C4-C5-N7	5.18	112.87	110.80
1	A	2818	G	C8-N9-C4	5.18	108.47	106.40
1	A	741	A	C5-N7-C8	-5.18	101.31	103.90
1	A	1896	C	N3-C2-O2	-5.18	118.28	121.90
1	A	2812	U	C6-N1-C1'	-5.18	113.95	121.20
1	A	293	A	C6-C5-N7	-5.18	128.68	132.30
1	A	1099	C	N1-C2-O2	5.18	122.01	118.90
1	A	243	U	N1-C2-O2	5.17	126.42	122.80
1	A	2461	U	N1-C2-O2	5.17	126.42	122.80
1	A	518	C	C5-C4-N4	5.17	123.82	120.20
19	S	84	ARG	CB-CG-CD	5.17	125.04	111.60
1	A	1887	A	N7-C8-N9	5.17	116.39	113.80
1	A	2579	G	N3-C4-C5	-5.17	126.02	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1063	A	P-O3'-C3'	5.17	125.90	119.70
1	A	1176	A	O5'-P-OP1	-5.17	101.05	105.70
1	A	1197	G	C4-C5-N7	5.17	112.87	110.80
1	A	2284	C	N1-C2-O2	5.17	122.00	118.90
4	D	165	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	227	A	OP1-P-O3'	5.17	116.56	105.20
1	A	1453	U	N3-C2-O2	-5.17	118.58	122.20
1	A	1918	U	N1-C2-O2	5.17	126.42	122.80
1	A	680	U	C5-C6-N1	5.16	125.28	122.70
1	A	852	A	N9-C4-C5	-5.16	103.74	105.80
1	A	1293	C	C6-N1-C2	-5.16	118.24	120.30
1	A	1775	C	N3-C2-O2	-5.16	118.29	121.90
1	A	2267	G	N1-C6-O6	-5.16	116.81	119.90
1	A	630	C	C5-C6-N1	5.15	123.58	121.00
1	A	2361	C	C2-N1-C1'	5.15	124.47	118.80
1	A	2578	C	C6-N1-C2	-5.15	118.24	120.30
1	A	1232	G	C5-C6-O6	5.15	131.69	128.60
1	A	2174	C	C2-N1-C1'	5.15	124.47	118.80
1	A	37	C	N3-C2-O2	-5.15	118.30	121.90
1	A	62	U	P-O3'-C3'	5.15	125.88	119.70
1	A	1179	G	C8-N9-C4	-5.15	104.34	106.40
2	B	95	U	C6-N1-C2	-5.15	117.91	121.00
1	A	2502	C	C6-N1-C2	-5.15	118.24	120.30
1	A	1790	A	N3-C4-C5	5.15	130.40	126.80
1	A	2637	U	C2-N1-C1'	5.15	123.88	117.70
1	A	1076	A	C4-N9-C1'	5.14	135.56	126.30
1	A	2335	U	N3-C2-O2	-5.14	118.60	122.20
1	A	733	C	C5-C6-N1	5.14	123.57	121.00
1	A	1881	C	C5-C6-N1	5.14	123.57	121.00
20	T	22	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	A	114	U	C5-C6-N1	5.14	125.27	122.70
1	A	408	C	C6-N1-C2	-5.14	118.25	120.30
1	A	411	C	N3-C2-O2	-5.14	118.30	121.90
1	A	886	C	C2-N1-C1'	5.14	124.45	118.80
1	A	1170	C	C5-C6-N1	5.13	123.57	121.00
1	A	1366	U	C2-N1-C1'	5.13	123.86	117.70
1	A	251	A	C5-N7-C8	-5.13	101.33	103.90
1	A	2636	C	C2-N1-C1'	5.13	124.44	118.80
1	A	1981	C	C5-C6-N1	5.13	123.56	121.00
1	A	374	C	C6-N1-C2	-5.12	118.25	120.30
1	A	774	G	C4-C5-N7	5.12	112.85	110.80
1	A	974	A	O4'-C1'-N9	5.12	112.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1092	C	C4-C5-C6	5.12	119.96	117.40
1	A	807	C	N1-C2-O2	5.12	121.97	118.90
1	A	475	C	C2-N1-C1'	5.11	124.42	118.80
1	A	1708	U	C2-N1-C1'	5.11	123.83	117.70
2	B	31	C	C6-N1-C1'	-5.11	114.67	120.80
1	A	2569	G	N3-C4-N9	5.10	129.06	126.00
1	A	960	U	C5-C6-N1	5.10	125.25	122.70
1	A	1599	A	C5-N7-C8	-5.10	101.35	103.90
1	A	2247	C	C6-N1-C2	-5.10	118.26	120.30
1	A	964	A	N9-C1'-C2'	5.10	120.62	114.00
1	A	1880	C	N1-C2-O2	5.09	121.96	118.90
1	A	2686	C	C6-N1-C2	-5.09	118.26	120.30
1	A	1448	C	C6-N1-C2	-5.09	118.26	120.30
1	A	2054	G	C8-N9-C4	-5.09	104.36	106.40
1	A	2432	G	C5-C6-N1	5.09	114.04	111.50
1	A	2681	G	N9-C4-C5	-5.08	103.37	105.40
1	A	1407	U	C2-N1-C1'	5.08	123.80	117.70
1	A	357	A	C5-N7-C8	-5.08	101.36	103.90
1	A	802	C	N3-C2-O2	-5.08	118.35	121.90
1	A	2638	C	C5-C6-N1	5.08	123.54	121.00
1	A	1968	A	O5'-P-OP1	5.07	116.79	110.70
1	A	2669	U	N3-C2-O2	-5.07	118.65	122.20
1	A	2403	C	N1-C2-O2	5.07	121.94	118.90
1	A	2315	A	N1-C2-N3	-5.07	126.77	129.30
1	A	2039	A	N1-C2-N3	-5.07	126.77	129.30
9	I	7	ALA	C-N-CA	5.07	134.37	121.70
1	A	1445	U	N1-C2-O2	5.07	126.35	122.80
1	A	1752	C	C6-N1-C2	-5.07	118.27	120.30
1	A	2008	A	C4-C5-N7	5.07	113.23	110.70
2	B	60	C	C5-C6-N1	5.07	123.53	121.00
1	A	1843	U	N3-C2-O2	-5.07	118.66	122.20
23	W	40	LEU	CA-CB-CG	5.07	126.95	115.30
2	B	34	A	P-O3'-C3'	5.06	125.78	119.70
1	A	1262	A	OP1-P-O3'	5.06	116.34	105.20
1	A	2228	A	N1-C6-N6	-5.06	115.56	118.60
1	A	2546	C	C2-N1-C1'	5.06	124.37	118.80
1	A	2505	A	C2-N3-C4	5.06	113.13	110.60
1	A	76	C	C5-C6-N1	5.06	123.53	121.00
1	A	1064	G	C8-N9-C1'	-5.05	120.43	127.00
2	B	70	C	C6-N1-C2	-5.05	118.28	120.30
1	A	2808	A	O5'-P-OP1	-5.05	101.15	105.70
1	A	1179	G	N9-C4-C5	5.05	107.42	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1851	U	N1-C2-O2	5.05	126.33	122.80
1	A	2445	G	C8-N9-C1'	-5.05	120.44	127.00
1	A	533	U	C2-N1-C1'	5.05	123.76	117.70
1	A	2235	C	N1-C2-O2	5.05	121.93	118.90
1	A	964	A	C4-N9-C1'	5.04	135.38	126.30
1	A	290	C	C5-C6-N1	5.04	123.52	121.00
1	A	1011	A	C8-N9-C4	-5.04	103.78	105.80
1	A	1101	A	C4-N9-C1'	5.04	135.37	126.30
1	A	1987	C	N3-C2-O2	-5.04	118.37	121.90
1	A	2010	C	C6-N1-C2	-5.04	118.28	120.30
1	A	2117	U	N3-C2-O2	-5.04	118.67	122.20
1	A	2366	G	N3-C4-C5	-5.04	126.08	128.60
1	A	2493	U	N1-C2-O2	5.04	126.33	122.80
1	A	79	C	N3-C2-O2	-5.04	118.37	121.90
1	A	466	C	C6-N1-C2	-5.04	118.28	120.30
1	A	1169	A	P-O3'-C3'	5.04	125.74	119.70
1	A	2229	G	N7-C8-N9	5.04	115.62	113.10
1	A	196	A	C2-N3-C4	5.03	113.12	110.60
1	A	1218	U	C5-C6-N1	5.03	125.22	122.70
1	A	1951	G	O4'-C1'-N9	-5.03	104.17	108.20
1	A	538	G	C6-C5-N7	-5.03	127.38	130.40
1	A	904	C	N3-C2-O2	-5.03	118.38	121.90
1	A	726	C	C5-C6-N1	5.03	123.52	121.00
1	A	1325	G	C5-C6-N1	5.03	114.02	111.50
1	A	2636	C	N3-C2-O2	-5.03	118.38	121.90
1	A	1091	U	C2-N1-C1'	5.03	123.73	117.70
1	A	438	A	N1-C2-N3	-5.03	126.79	129.30
1	A	2003	U	O4'-C1'-N1	5.03	112.22	108.20
1	A	1276	C	C6-N1-C2	-5.02	118.29	120.30
1	A	1981	C	N1-C2-O2	5.02	121.91	118.90
1	A	2254	A	N9-C4-C5	5.02	107.81	105.80
1	A	377	G	C5-N7-C8	-5.01	101.79	104.30
1	A	1284	C	N1-C2-O2	5.01	121.91	118.90
1	A	104	U	N3-C2-O2	-5.01	118.69	122.20
1	A	1671	G	C8-N9-C1'	-5.01	120.49	127.00
1	A	1913	U	N3-C2-O2	-5.01	118.69	122.20
1	A	2005	G	N1-C2-N2	5.01	120.71	116.20
1	A	2850	C	C6-N1-C2	-5.01	118.30	120.30
1	A	1185	U	N1-C2-O2	5.01	126.31	122.80
1	A	113	C	O4'-C1'-N1	5.01	112.20	108.20
1	A	1826	G	N3-C4-N9	5.01	129.00	126.00
1	A	1923	A	C4-C5-N7	5.00	113.20	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1966	C	N1-C2-O2	5.00	121.90	118.90
1	A	1327	U	N1-C2-O2	5.00	126.30	122.80
1	A	201	C	N3-C2-O2	-5.00	118.40	121.90
1	A	1197	G	C5-N7-C8	-5.00	101.80	104.30

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	1	13	GLU	Peptide
27	1	15	THR	Peptide
27	1	20	ASN	Peptide
27	1	24	THR	Peptide
27	1	25	ARG	Peptide
27	1	26	SER	Peptide
27	1	28	LEU	Peptide
32	6	35	GLN	Peptide
3	C	232	HIS	Peptide
4	D	53	ALA	Peptide
4	D	75	ALA	Peptide
6	F	25	VAL	Peptide
6	F	34	ILE	Peptide
6	F	4	LEU	Peptide
9	I	22	PRO	Peptide
9	I	56	PRO	Peptide
9	I	58	ILE	Peptide
9	I	66	SER	Peptide
9	I	86	ILE	Peptide
11	K	90	LYS	Peptide
14	N	106	ASP	Peptide
14	N	70	THR	Peptide
16	P	17	GLU	Peptide
18	R	51	LEU	Peptide
18	R	69	HIS	Peptide
20	T	89	GLY	Peptide
22	V	110	HIS	Peptide
22	V	111	PHE	Peptide
22	V	78	LYS	Peptide
22	V	89	VAL	Peptide
22	V	90	MET	Peptide
23	W	11	ARG	Peptide
23	W	13	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61899	0	31128	440	0
2	B	2495	0	1263	18	0
3	C	2048	0	2097	36	0
4	D	1549	0	1560	20	0
5	E	1509	0	1563	21	0
6	F	1278	0	1245	40	0
7	G	1264	0	1314	17	0
8	H	577	0	606	6	0
9	I	1026	0	1063	68	0
10	J	1122	0	1148	14	0
11	K	922	0	992	27	0
12	L	1055	0	1096	15	0
13	M	1069	0	1139	20	0
14	N	945	0	989	15	0
15	O	881	0	920	15	0
16	P	891	0	950	13	0
17	Q	936	0	1025	16	0
18	R	801	0	830	9	0
19	S	825	0	885	6	0
20	T	701	0	741	6	0
21	U	801	0	864	13	0
22	V	1397	0	1417	14	0
23	W	574	0	601	11	0
24	X	626	0	649	5	0
25	Y	468	0	489	3	0
26	Z	445	0	472	4	0
27	1	232	0	238	17	0
28	2	423	0	420	7	0
29	3	418	0	445	4	0
30	4	376	0	421	9	0
31	5	506	0	569	11	0
32	6	303	0	341	4	0
All	All	90362	0	59480	721	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (721) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:C:C5	1:A:1092:C:C6	2.24	1.26
1:A:1092:C:C5	1:A:1092:C:C4	2.35	1.13
1:A:1461:G:H21	1:A:1504:A:H62	0.98	0.97
1:A:1092:C:C4	1:A:1092:C:N3	2.32	0.97
1:A:1092:C:C4	9:I:8:TYR:HA	2.00	0.96
1:A:1092:C:N3	1:A:1092:C:C2	2.34	0.95
1:A:1461:G:N2	1:A:1504:A:H62	1.64	0.95
1:A:1092:C:C6	1:A:1092:C:N1	2.35	0.94
1:A:2493:U:H3	1:A:2570:G:H1	1.16	0.93
1:A:2087:G:H1	1:A:2176:U:H3	1.17	0.93
1:A:2084:U:H3	1:A:2179:G:H1	1.15	0.92
1:A:1092:C:N3	9:I:8:TYR:HA	1.85	0.90
1:A:1092:C:C2	1:A:1092:C:N1	2.45	0.84
1:A:1461:G:H21	1:A:1504:A:N6	1.75	0.83
1:A:2644:A:H62	1:A:2651:G:H21	1.28	0.80
1:A:1239:G:H1	17:Q:37:GLN:HE21	1.29	0.78
1:A:1092:C:C2	9:I:8:TYR:CB	2.67	0.77
1:A:766:G:H1	1:A:783:A:HO2'	1.31	0.76
1:A:1029:A:H61	1:A:1106:G:H1	1.33	0.76
1:A:1092:C:N1	9:I:8:TYR:HB3	2.00	0.75
1:A:575:G:N7	17:Q:6:ARG:NH1	2.35	0.75
1:A:1288:A:H2	1:A:1616:G:H21	1.35	0.73
4:D:34:ARG:HH22	4:D:54:GLY:HA2	1.54	0.71
1:A:244:A:H5"	12:L:67:VAL:HG21	1.72	0.71
1:A:1092:C:H3'	9:I:7:ALA:H	1.55	0.69
1:A:1092:C:C2	9:I:8:TYR:HB2	2.28	0.68
1:A:2670:C:O2	11:K:70:ARG:NH2	2.27	0.68
1:A:1092:C:C4	9:I:8:TYR:CB	2.78	0.67
1:A:362:A:H62	1:A:393:A:H2	1.43	0.67
14:N:2:ARG:HA	14:N:5:LYS:HD3	1.78	0.66
1:A:1081:G:N3	9:I:8:TYR:OH	2.27	0.66
1:A:27:G:N2	1:A:503:G:O2'	2.25	0.66
1:A:1519:G:H1	1:A:1529:U:H3	1.43	0.66
1:A:1047:A:N1	9:I:72:LYS:NZ	2.44	0.66
30:4:24:THR:HG23	30:4:27:GLY:H	1.61	0.65
1:A:1092:C:N1	9:I:8:TYR:CB	2.60	0.65
1:A:1092:C:C4	9:I:8:TYR:CA	2.80	0.65
1:A:1092:C:C2	9:I:8:TYR:CA	2.80	0.65
1:A:2131:G:N2	1:A:2135:G:N7	2.44	0.65
5:E:5:VAL:HG12	5:E:7:GLY:H	1.61	0.65
1:A:1052:G:H1	9:I:76:ALA:HA	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2462:C:H42	1:A:2516:G:H22	1.44	0.64
1:A:1092:C:N3	9:I:8:TYR:HB2	2.13	0.64
1:A:2346:C:H5"	31:5:50:ASN:HD21	1.63	0.64
6:F:4:LEU:O	6:F:9:ARG:NH1	2.30	0.64
6:F:90:THR:OG1	27:1:30:LYS:N	2.28	0.64
1:A:2122:A:OP2	1:A:2140:C:N4	2.30	0.64
4:D:118:PHE:HA	4:D:164:HIS:H	1.62	0.64
1:A:1116:A:H4'	1:A:1117:A:H5"	1.79	0.64
1:A:870:G:N7	1:A:881:A:N6	2.46	0.63
1:A:862:C:O2'	13:M:65:TRP:NE1	2.30	0.63
1:A:1284:C:O2'	1:A:1289:A:N6	2.31	0.63
1:A:265:A:N6	1:A:418:U:O2'	2.30	0.63
2:B:43:C:O2'	6:F:92:ARG:NH1	2.32	0.63
1:A:1092:C:C6	9:I:8:TYR:CB	2.81	0.63
1:A:1092:C:N3	9:I:8:TYR:CB	2.62	0.63
9:I:81:LYS:NZ	9:I:136:MET:SD	2.71	0.63
1:A:1237:G:N7	12:L:18:ARG:NH2	2.45	0.62
1:A:2707:U:OP1	16:P:54:ARG:NH1	2.33	0.62
1:A:2226:G:OP1	3:C:243:ARG:NH2	2.30	0.62
7:G:74:ASN:HA	7:G:77:VAL:HG12	1.81	0.62
1:A:553:A:OP2	18:R:79:ARG:NH2	2.31	0.62
6:F:92:ARG:NH1	27:1:32:ILE:O	2.33	0.62
1:A:2266:G:N7	23:W:14:ARG:NH2	2.47	0.62
6:F:20:LEU:HD13	6:F:165:GLU:HG2	1.82	0.62
1:A:357:A:H2	1:A:415:G:H21	1.44	0.62
3:C:81:VAL:HG21	3:C:110:VAL:HB	1.82	0.61
10:J:17:VAL:HG23	10:J:137:PRO:HB2	1.81	0.61
1:A:293:A:H8	1:A:313:C:HO2'	1.48	0.61
3:C:152:ALA:O	3:C:156:ARG:NH1	2.33	0.61
1:A:2302:G:HO2'	27:1:24:THR:HG1	1.42	0.61
9:I:107:GLU:HA	9:I:110:ALA:HB3	1.81	0.61
1:A:1253:G:OP1	28:2:16:ARG:NH2	2.33	0.61
1:A:1309:A:O3'	19:S:84:ARG:NH2	2.33	0.61
1:A:2245:C:O2'	1:A:2414:C:OP2	2.19	0.60
1:A:2644:A:H62	1:A:2651:G:N2	1.97	0.60
1:A:303:A:N3	1:A:323:G:O2'	2.33	0.60
21:U:11:ILE:HD11	21:U:79:ALA:HB2	1.83	0.60
1:A:314:A:N3	5:E:162:ASN:ND2	2.50	0.60
1:A:1058:G:H5"	9:I:86:ILE:HB	1.84	0.60
1:A:1199:G:O2'	1:A:1224:A:N6	2.35	0.60
4:D:110:THR:HG23	4:D:202:ILE:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:5:ASP:O	12:L:7:ARG:NH1	2.35	0.60
5:E:175:ASP:OD1	5:E:175:ASP:N	2.33	0.60
9:I:131:GLY:HA2	9:I:134:ARG:HD3	1.84	0.60
1:A:2392:G:O2'	1:A:2398:A:N6	2.35	0.60
1:A:2292:U:H3	6:F:133:LYS:HE2	1.67	0.60
21:U:3:LYS:HD2	21:U:82:VAL:HG23	1.84	0.60
1:A:971:A:H8	1:A:2014:G:H21	1.48	0.59
13:M:12:GLN:O	13:M:87:LYS:NZ	2.34	0.59
20:T:5:ARG:NH2	20:T:36:ASP:O	2.35	0.59
21:U:11:ILE:HG22	21:U:21:ARG:HG2	1.84	0.59
1:A:1594:C:O2'	1:A:1600:A:N6	2.35	0.59
1:A:1643:G:H3'	14:N:2:ARG:HG2	1.85	0.59
1:A:2513:G:O2'	32:6:1:MET:N	2.35	0.59
6:F:134:GLU:HG2	6:F:136:ILE:H	1.66	0.59
21:U:40:LEU:HD12	21:U:59:GLU:HG2	1.83	0.59
1:A:1251:G:OP1	28:2:16:ARG:NH1	2.25	0.59
1:A:1070:C:N4	9:I:114:GLN:OE1	2.36	0.59
1:A:1327:U:OP1	20:T:83:TYR:OH	2.18	0.59
1:A:2670:C:OP1	16:P:52:ARG:NH2	2.34	0.59
11:K:78:ARG:NH2	16:P:72:GLU:OE1	2.35	0.59
13:M:39:ARG:HB3	13:M:99:PRO:HD3	1.84	0.59
6:F:157:THR:HA	27:1:19:GLY:HA2	1.85	0.58
1:A:1030:A:H61	1:A:1105:G:H1	1.51	0.58
4:D:52:THR:HG21	4:D:76:ALA:HB1	1.85	0.58
1:A:626:G:H5"	12:L:128:THR:HB	1.85	0.58
1:A:1853:A:N6	1:A:1862:G:O2'	2.36	0.58
2:B:30:C:H1'	2:B:57:A:H61	1.68	0.58
22:V:11:ARG:HD3	22:V:42:SER:HB3	1.86	0.58
1:A:1856:G:O2'	1:A:1859:A:N6	2.36	0.58
9:I:81:LYS:HE2	9:I:89:GLY:HA2	1.86	0.58
1:A:1253:G:OP2	28:2:17:ARG:NH2	2.37	0.58
1:A:1660:C:O2	4:D:134:HIS:NE2	2.36	0.58
1:A:1063:A:N6	9:I:99:GLY:O	2.36	0.58
1:A:1313:U:HO2'	1:A:1997:G:HO2'	1.44	0.58
1:A:748:G:H21	1:A:1968:A:H62	1.50	0.58
1:A:964:A:H8	1:A:980:A:H62	1.52	0.57
1:A:1426:A:H62	1:A:1542:G:H8	1.51	0.57
1:A:2330:U:HO2'	1:A:2360:A:HO2'	1.45	0.57
12:L:84:LYS:HD2	12:L:100:LEU:HD21	1.86	0.57
17:Q:112:LYS:HD2	18:R:49:ILE:HD11	1.85	0.57
1:A:301:G:N1	1:A:304:A:OP2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:G:OP1	31:5:64:ARG:NH1	2.38	0.57
1:A:2102:G:N1	1:A:2106:A:OP2	2.36	0.57
3:C:119:GLY:O	3:C:134:ASN:ND2	2.37	0.57
12:L:58:HIS:O	31:5:13:ARG:NH1	2.37	0.57
1:A:374:C:N4	1:A:377:G:OP2	2.32	0.57
1:A:2337:C:OP2	31:5:44:ARG:NH1	2.38	0.57
1:A:2671:U:OP2	16:P:52:ARG:NH1	2.37	0.57
15:O:61:GLU:HG3	15:O:63:ALA:H	1.69	0.57
21:U:17:ASP:HB3	21:U:20:LYS:HD3	1.85	0.57
2:B:41:C:N4	6:F:67:VAL:O	2.36	0.57
14:N:101:GLY:H	28:2:41:HIS:HD2	1.52	0.57
1:A:1034:U:O3'	1:A:1101:A:N6	2.37	0.56
1:A:91:A:H4'	1:A:92:A:H5'	1.86	0.56
1:A:2392:G:O2'	1:A:2399:A:N6	2.39	0.56
2:B:9:G:OP1	15:O:20:ARG:NH1	2.37	0.56
5:E:115:ASP:O	5:E:184:LYS:NZ	2.38	0.56
1:A:2459:G:N2	1:A:2465:A:H62	2.04	0.56
1:A:889:A:OP2	1:A:890:A:N6	2.38	0.56
1:A:1017:A:O2'	1:A:1116:A:N6	2.34	0.56
1:A:1098:U:O2	9:I:4:LYS:NZ	2.38	0.56
3:C:161:SER:HB3	3:C:194:GLU:HG2	1.87	0.56
6:F:35:THR:HG22	6:F:37:ASN:H	1.70	0.56
13:M:67:ARG:NH1	13:M:105:GLU:OE2	2.38	0.56
1:A:1092:C:C5	9:I:8:TYR:CB	2.88	0.56
11:K:1:MET:HG3	11:K:82:ASN:HB3	1.88	0.56
24:X:18:ILE:HG13	24:X:24:LYS:HG2	1.88	0.56
23:W:11:ARG:O	23:W:14:ARG:NH1	2.39	0.56
22:V:33:VAL:HG22	22:V:94:PHE:HE2	1.72	0.55
7:G:15:VAL:HG21	7:G:76:VAL:HG13	1.89	0.55
1:A:1263:U:OP2	1:A:1635:G:O2'	2.24	0.55
16:P:4:LYS:N	16:P:7:GLN:OE1	2.40	0.55
1:A:459:G:N7	30:4:39:ARG:NH2	2.54	0.55
1:A:1089:G:H5'	9:I:24:VAL:HG12	1.88	0.55
1:A:1784:C:HO2'	3:C:258:THR:HG1	1.54	0.55
1:A:2644:A:N6	1:A:2651:G:H21	2.02	0.55
7:G:89:LEU:O	7:G:125:THR:OG1	2.23	0.55
1:A:1092:C:N3	9:I:8:TYR:CA	2.67	0.55
1:A:2237:G:O2'	1:A:2483:C:OP1	2.25	0.55
1:A:2808:A:OP2	4:D:115:GLY:N	2.39	0.55
6:F:11:GLU:HG2	6:F:15:LYS:HE3	1.89	0.55
10:J:98:GLU:HB2	10:J:124:VAL:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:35:ILE:HD12	11:K:69:VAL:HB	1.88	0.55
1:A:654:G:N2	31:5:64:ARG:O	2.39	0.55
1:A:1028:G:H1	1:A:1107:C:H5	1.55	0.55
11:K:104:ARG:HH11	16:P:35:GLU:HB2	1.71	0.55
1:A:2519:G:N2	1:A:2650:G:O2'	2.40	0.55
3:C:261:ASN:ND2	3:C:264:THR:OG1	2.39	0.55
27:1:27:THR:HG22	27:1:28:LEU:HG	1.89	0.55
12:L:70:LYS:O	12:L:107:ARG:NH2	2.40	0.55
2:B:40:U:O2'	2:B:42:C:O2	2.25	0.55
5:E:148:VAL:HB	5:E:187:VAL:HG12	1.87	0.55
1:A:294:A:OP2	21:U:81:ARG:NH2	2.40	0.54
11:K:98:ILE:HD13	11:K:114:ILE:HG23	1.88	0.54
1:A:1067:A:N6	1:A:1080:A:OP2	2.41	0.54
5:E:172:GLN:HE22	5:E:198:LEU:HD21	1.72	0.54
1:A:859:U:H3	1:A:896:G:H1	1.54	0.54
7:G:117:ILE:HG12	7:G:140:VAL:HG21	1.90	0.54
22:V:83:HIS:HD2	22:V:86:LYS:H	1.54	0.54
1:A:83:G:H21	1:A:103:A:H2	1.55	0.54
1:A:96:G:H4'	25:Y:39:GLN:HA	1.89	0.54
1:A:508:C:O2'	19:S:18:ARG:NH2	2.41	0.54
2:B:24:G:H4'	2:B:25:A:H8	1.72	0.54
1:A:664:G:O2'	5:E:61:GLN:NE2	2.40	0.54
1:A:1352:A:OP2	24:X:2:SER:OG	2.26	0.54
2:B:76:G:OP1	22:V:11:ARG:NH1	2.41	0.54
11:K:80:ASP:OD2	16:P:63:ARG:NH2	2.40	0.54
1:A:2835:G:O2'	1:A:2854:G:N2	2.35	0.54
3:C:163:GLN:OE1	3:C:175:ARG:NH1	2.40	0.54
22:V:128:SER:HB3	22:V:186:ASN:HB3	1.90	0.54
1:A:883:U:O2'	1:A:885:A:N1	2.41	0.54
1:A:1067:A:OP1	9:I:127:ARG:NH2	2.41	0.54
1:A:1894:G:N2	1:A:1910:U:O2	2.35	0.54
2:B:52:A:N6	15:O:34:GLN:OE1	2.40	0.54
1:A:1845:A:N6	1:A:1871:G:O2'	2.41	0.53
1:A:1852:U:H6	1:A:1863:A:H62	1.55	0.53
13:M:78:PRO:HG2	13:M:81:VAL:HG21	1.90	0.53
1:A:405:C:H2'	1:A:406:A:C8	2.44	0.53
2:B:8:C:H5"	15:O:16:ARG:HH22	1.73	0.53
27:1:12:ILE:HG23	27:1:13:GLU:HG3	1.91	0.53
3:C:164:LEU:HD12	3:C:174:LEU:HB3	1.91	0.53
1:A:2638:C:H42	1:A:2656:G:H1	1.55	0.53
5:E:17:THR:OG1	5:E:200:GLY:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:44:VAL:HG22	6:F:82:GLY:HA3	1.90	0.53
1:A:393:A:H8	1:A:397:G:HO2'	1.56	0.53
9:I:134:ARG:HA	9:I:138:LEU:HD12	1.90	0.53
1:A:1049:G:H5"	9:I:51:PRO:HD3	1.90	0.53
1:A:2378:G:O2'	1:A:2411:C:N4	2.41	0.53
14:N:79:LEU:HD23	14:N:83:LEU:HB2	1.90	0.53
16:P:52:ARG:HH21	16:P:54:ARG:HG2	1.73	0.53
18:R:68:ARG:O	18:R:90:ARG:NH2	2.42	0.53
1:A:567:G:O2'	1:A:1241:A:OP1	2.27	0.53
5:E:105:ARG:NH1	5:E:199:LEU:O	2.39	0.53
1:A:617:A:N7	12:L:113:SER:OG	2.42	0.53
1:A:2074:U:H2'	1:A:2075:G:H8	1.73	0.53
1:A:2238:G:OP1	13:M:82:ARG:NH1	2.42	0.53
1:A:356:A:OP1	1:A:416:G:O2'	2.25	0.52
1:A:1018:A:H61	1:A:1115:G:H2'	1.74	0.52
1:A:1785:U:OP2	3:C:272:ARG:NH2	2.42	0.52
11:K:10:VAL:HG21	11:K:16:ALA:HB3	1.90	0.52
1:A:461:A:OP1	5:E:73:ARG:NH1	2.41	0.52
1:A:896:G:OP1	13:M:24:GLY:N	2.43	0.52
1:A:1080:A:H61	9:I:8:TYR:HB2	1.74	0.52
1:A:1841:A:H62	1:A:1875:G:H8	1.58	0.52
6:F:8:TYR:HA	6:F:12:ILE:HB	1.89	0.52
1:A:1233:A:H4'	5:E:39:ARG:HH22	1.74	0.52
1:A:107:G:H21	1:A:340:A:H62	1.56	0.52
1:A:718:G:H4'	3:C:13:ARG:HD3	1.91	0.52
1:A:269:C:H42	1:A:361:A:H61	1.56	0.52
22:V:63:VAL:HG13	22:V:74:THR:HG23	1.92	0.52
1:A:83:G:OP1	21:U:91:LYS:NZ	2.36	0.52
6:F:92:ARG:O	6:F:96:MET:N	2.43	0.52
1:A:92:A:O2'	1:A:93:A:O5'	2.28	0.52
1:A:1341:A:OP1	3:C:36:LYS:NZ	2.42	0.52
1:A:1477:A:O2'	3:C:98:ASP:OD2	2.24	0.52
1:A:2733:U:H5"	7:G:134:LYS:HG2	1.91	0.52
6:F:127:ASN:HA	27:1:18:CYS:HA	1.92	0.52
7:G:58:ASP:HB2	7:G:61:THR:HG22	1.91	0.52
1:A:1370:A:H8	1:A:1392:U:HO2'	1.58	0.52
1:A:1621:G:N1	1:A:1624:A:OP2	2.35	0.52
1:A:1642:A:OP1	14:N:8:ARG:NH1	2.43	0.52
15:O:65:GLY:HA2	15:O:101:ARG:HH12	1.74	0.52
1:A:899:A:C8	13:M:13:MET:HG2	2.45	0.52
1:A:2290:G:H21	27:1:11:ALA:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:11:GLU:O	6:F:15:LYS:N	2.42	0.52
31:5:41:ARG:HG3	31:5:44:ARG:HH12	1.74	0.52
1:A:664:G:H4'	5:E:68:ARG:HG2	1.92	0.51
1:A:1052:G:H1'	9:I:109:ILE:HG21	1.91	0.51
3:C:53:HIS:HA	3:C:217:ARG:HB3	1.92	0.51
14:N:2:ARG:NH2	14:N:5:LYS:O	2.43	0.51
4:D:74:VAL:HG12	4:D:76:ALA:HB2	1.92	0.51
11:K:25:LEU:HD12	11:K:38:ILE:HG22	1.92	0.51
11:K:87:LEU:HD13	11:K:91:GLN:HB3	1.92	0.51
1:A:1034:U:O2'	1:A:1101:A:N1	2.41	0.51
1:A:1782:C:O2	3:C:254:LYS:NZ	2.44	0.51
1:A:2278:U:H2'	1:A:2279:G:C8	2.45	0.51
23:W:52:GLY:HA2	23:W:62:LYS:HE2	1.92	0.51
13:M:48:GLU:OE2	13:M:51:ARG:NH1	2.37	0.51
21:U:32:ARG:NH2	21:U:63:PRO:O	2.44	0.51
1:A:391:G:N7	24:X:57:ARG:NH1	2.59	0.51
1:A:1373:C:H2'	1:A:1374:A:C8	2.45	0.51
1:A:1671:G:C8	1:A:1749:A:H2'	2.46	0.51
1:A:1046:G:H21	9:I:11:LEU:HA	1.74	0.51
1:A:2776:C:H3'	1:A:2880:A:H62	1.75	0.51
1:A:1092:C:C6	9:I:8:TYR:CA	2.94	0.51
1:A:1892:C:H4'	1:A:1916:G:H8	1.74	0.51
1:A:2462:C:N4	1:A:2516:G:H22	2.08	0.51
14:N:37:THR:HG22	14:N:39:PRO:HD2	1.92	0.51
1:A:288:A:O2'	1:A:289:G:O4'	2.28	0.51
1:A:719:G:C6	3:C:207:LYS:HB2	2.45	0.51
1:A:845:G:H2'	1:A:846:G:C8	2.46	0.51
1:A:1203:G:OP1	17:Q:11:ARG:NH1	2.42	0.51
1:A:2633:C:OP2	1:A:2719:G:O2'	2.28	0.51
22:V:137:SER:HB3	22:V:172:GLU:HB3	1.93	0.51
1:A:1070:C:N3	9:I:73:SER:OG	2.40	0.51
1:A:1092:C:N1	9:I:8:TYR:CA	2.74	0.51
1:A:1804:G:OP2	3:C:156:ARG:NH2	2.44	0.51
15:O:97:LYS:HD3	15:O:99:HIS:HB2	1.93	0.51
1:A:1092:C:H5"	9:I:6:GLN:HB2	1.92	0.50
2:B:37:C:H2'	15:O:99:HIS:HE1	1.76	0.50
1:A:1063:A:C4	9:I:137:GLY:HA2	2.46	0.50
6:F:33:LYS:H	27:1:27:THR:H	1.59	0.50
1:A:263:U:O2'	1:A:420:A:N3	2.44	0.50
1:A:491:G:N1	1:A:494:A:OP2	2.40	0.50
6:F:89:VAL:HA	27:1:30:LYS:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2562:C:H5'	4:D:149:CYS:HB2	1.93	0.50
6:F:158:THR:HG22	6:F:166:GLY:HA3	1.94	0.50
17:Q:88:ILE:HG23	17:Q:90:ILE:H	1.76	0.50
1:A:1052:G:H21	9:I:80:LEU:HB3	1.76	0.50
1:A:1053:G:H1'	9:I:106:LEU:HD23	1.93	0.50
1:A:1699:C:O2'	1:A:2846:G:N3	2.42	0.50
1:A:2128:G:O6	1:A:2137:U:O4	2.28	0.50
5:E:111:LEU:HB3	5:E:117:LEU:HB2	1.92	0.50
22:V:142:ASP:OD1	22:V:142:ASP:N	2.40	0.50
32:6:4:ARG:O	32:6:37:GLN:NE2	2.45	0.50
1:A:911:C:O2'	23:W:29:GLN:NE2	2.43	0.50
1:A:1403:G:H1	1:A:1572:C:H5	1.58	0.50
14:N:33:LEU:HD23	14:N:114:GLU:HB2	1.92	0.50
32:6:17:ILE:HD13	32:6:26:ILE:HD12	1.93	0.50
1:A:729:A:H1'	1:A:730:C:H5	1.76	0.50
1:A:1012:G:N2	1:A:1013:U:O4	2.43	0.50
20:T:66:THR:HG21	20:T:73:LEU:HD12	1.94	0.50
12:L:91:SER:H	12:L:94:THR:HB	1.77	0.49
14:N:107:ASN:HD21	19:S:40:SER:HB3	1.77	0.49
1:A:1184:G:O2'	17:Q:12:ARG:NH2	2.45	0.49
1:A:2125:G:H22	1:A:2140:C:H1'	1.77	0.49
1:A:2228:A:H2'	1:A:2229:G:C8	2.47	0.49
1:A:2286:G:H2'	1:A:2287:A:C8	2.48	0.49
1:A:2568:G:OP2	1:A:2568:G:N2	2.40	0.49
3:C:25:HIS:CG	3:C:80:ARG:HD2	2.47	0.49
7:G:3:ARG:HD3	7:G:5:ALA:H	1.77	0.49
1:A:571:C:H2'	1:A:572:A:C8	2.48	0.49
1:A:977:C:O2'	1:A:990:A:N3	2.39	0.49
1:A:1434:U:O2'	1:A:1534:A:N3	2.40	0.49
7:G:17:ILE:HD13	7:G:50:LEU:HD11	1.95	0.49
8:H:2:GLU:N	8:H:19:VAL:O	2.45	0.49
17:Q:58:ARG:HE	17:Q:62:ILE:HD11	1.78	0.49
1:A:1081:G:H21	1:A:1082:C:H5	1.60	0.49
1:A:2743:U:H4'	1:A:2744:A:H5'	1.94	0.49
4:D:122:ILE:HD12	4:D:141:ARG:HG3	1.95	0.49
1:A:1065:C:H1'	9:I:141:GLU:HG3	1.94	0.49
1:A:1329:A:O2'	1:A:1331:U:OP1	2.28	0.49
25:Y:32:LYS:HD2	25:Y:43:LEU:HD21	1.95	0.49
1:A:1804:G:OP1	3:C:87:ARG:NH2	2.45	0.49
13:M:51:ARG:HH21	13:M:55:THR:HG21	1.77	0.49
26:Z:4:VAL:HG23	26:Z:58:GLY:HA2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:60:ALA:HB2	11:K:86:LEU:HD23	1.94	0.49
1:A:160:A:N3	1:A:2195:C:O2'	2.41	0.49
1:A:823:A:H2'	1:A:824:G:C8	2.48	0.49
1:A:2126:U:N3	1:A:2141:G:OP1	2.46	0.49
6:F:22:LEU:HD13	6:F:27:GLU:HG2	1.94	0.49
11:K:2:ILE:O	11:K:32:TYR:HA	2.13	0.49
1:A:1587:A:H5"	1:A:1588:A:H5'	1.95	0.49
18:R:38:VAL:HG21	18:R:57:ALA:HB3	1.95	0.49
28:2:43:SER:HB3	28:2:47:PHE:H	1.78	0.49
1:A:1063:A:O2'	9:I:94:ASN:ND2	2.38	0.48
1:A:1402:U:O2	1:A:1578:G:N1	2.46	0.48
18:R:71:LYS:HA	18:R:89:HIS:O	2.13	0.48
1:A:766:G:N2	1:A:783:A:HO2'	2.12	0.48
1:A:1276:C:H2'	1:A:1277:A:H8	1.78	0.48
23:W:40:LEU:HD11	23:W:44:LYS:HB2	1.94	0.48
1:A:1092:C:C5	9:I:8:TYR:CA	2.96	0.48
10:J:16:PHE:HB3	10:J:140:LEU:HD22	1.95	0.48
1:A:2302:G:C2	27:1:23:LYS:HG2	2.48	0.48
1:A:952:G:H21	1:A:2237:G:H1	1.59	0.48
1:A:1967:G:H3'	1:A:1968:A:H5"	1.95	0.48
6:F:36:LEU:HD23	6:F:152:LEU:HA	1.94	0.48
22:V:77:ILE:HA	22:V:94:PHE:HB3	1.94	0.48
29:3:8:VAL:HG12	29:3:47:GLU:HB2	1.96	0.48
1:A:1276:C:H2'	1:A:1277:A:C8	2.49	0.48
1:A:1455:U:O2	1:A:1511:G:O6	2.30	0.48
1:A:2462:C:H42	1:A:2516:G:N2	2.10	0.48
2:B:43:C:H1'	27:1:32:ILE:HB	1.95	0.48
4:D:15:ILE:HD13	4:D:25:VAL:HG21	1.94	0.48
1:A:2465:A:OP2	32:6:2:LYS:NZ	2.40	0.48
6:F:16:LEU:HG	6:F:169:LEU:HD23	1.96	0.48
12:L:30:THR:HG22	12:L:33:ARG:HB2	1.96	0.48
1:A:1048:G:H2'	9:I:49:GLN:HE21	1.78	0.48
1:A:1061:G:H21	1:A:1079:A:H61	1.62	0.48
10:J:49:ASP:OD1	10:J:49:ASP:N	2.45	0.48
13:M:65:TRP:HB2	13:M:105:GLU:HB2	1.96	0.48
1:A:847:G:N2	1:A:2256:G:OP2	2.45	0.48
1:A:69:C:O2	1:A:73:A:O2'	2.30	0.48
1:A:2038:U:H3'	1:A:2565:G:H5"	1.96	0.48
14:N:51:LEU:HD21	14:N:69:ARG:HG3	1.95	0.48
22:V:33:VAL:HG12	22:V:96:ARG:HD2	1.96	0.48
1:A:1018:A:H2'	1:A:1019:A:C8	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:A:H3'	9:I:28:LEU:HD12	1.95	0.47
1:A:1514:G:N1	1:A:1534:A:OP2	2.41	0.47
1:A:1778:A:N6	1:A:1815:G:O2'	2.42	0.47
27:1:30:LYS:HB2	27:1:32:ILE:HG12	1.96	0.47
1:A:1787:C:H5	1:A:1804:G:H22	1.62	0.47
3:C:145:GLU:HB2	3:C:188:CYS:HB2	1.96	0.47
10:J:18:VAL:HB	10:J:56:VAL:HG22	1.96	0.47
1:A:683:A:O2'	1:A:1340:A:N3	2.44	0.47
1:A:1502:A:H3'	1:A:1503:G:H8	1.79	0.47
1:A:1770:A:HO2'	1:A:2594:G:HO2'	1.58	0.47
1:A:2490:A:O2'	1:A:2492:G:OP2	2.27	0.47
1:A:2623:U:HO2'	4:D:46:TYR:HH	1.61	0.47
2:B:51:G:OP2	15:O:66:ASN:ND2	2.43	0.47
1:A:1035:U:H6	1:A:1037:G:H21	1.62	0.47
1:A:1776:A:OP2	3:C:221:ARG:NH1	2.47	0.47
1:A:2094:C:O2'	1:A:2095:U:O4'	2.32	0.47
6:F:46:ASP:OD1	6:F:46:ASP:N	2.43	0.47
18:R:5:ILE:HG22	18:R:38:VAL:HG12	1.97	0.47
1:A:988:C:OP1	17:Q:84:LYS:NZ	2.42	0.47
11:K:64:ARG:NH2	11:K:99:PHE:O	2.46	0.47
1:A:1359:U:HO2'	1:A:2199:A:H8	1.62	0.47
6:F:3:ARG:N	6:F:97:TYR:O	2.48	0.47
1:A:743:G:H2'	1:A:744:G:H8	1.80	0.47
1:A:889:A:H3'	1:A:890:A:C8	2.50	0.47
1:A:896:G:H5'	13:M:23:ARG:HB3	1.97	0.47
1:A:1020:C:H5	1:A:1114:G:H1	1.63	0.47
1:A:1048:G:H4'	9:I:46:THR:HA	1.96	0.47
1:A:1092:C:C2	9:I:8:TYR:N	2.82	0.47
1:A:2566:C:O2'	4:D:136:ASN:OD1	2.33	0.47
15:O:38:ALA:HB2	15:O:105:LEU:HD21	1.95	0.47
1:A:471:A:OP2	21:U:43:ARG:NH1	2.48	0.47
1:A:822:U:H2'	1:A:823:A:C8	2.50	0.47
1:A:1070:C:H6	9:I:116:ASP:HB3	1.79	0.47
1:A:1270:G:H22	1:A:1273:A:H5"	1.79	0.47
1:A:2628:A:H5"	10:J:78:SER:HB2	1.97	0.47
10:J:92:LEU:HD11	10:J:99:ARG:HD2	1.96	0.47
31:5:58:GLU:HG3	31:5:64:ARG:HG2	1.96	0.47
1:A:705:A:N7	1:A:706:A:N6	2.63	0.47
5:E:6:ASN:HD22	5:E:120:VAL:HG12	1.80	0.47
6:F:33:LYS:N	27:1:27:THR:H	2.13	0.47
22:V:23:ARG:HH11	22:V:90:MET:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:A:H5"	9:I:38:PHE:HZ	1.79	0.47
2:B:42:C:O2'	6:F:64:LYS:O	2.24	0.47
22:V:62:HIS:ND1	22:V:63:VAL:O	2.38	0.47
1:A:797:U:O2'	1:A:2047:A:N1	2.47	0.46
1:A:1328:U:OP2	1:A:1381:U:O2'	2.25	0.46
9:I:103:ARG:HB2	9:I:140:VAL:HG22	1.97	0.46
1:A:822:U:H2'	1:A:823:A:H8	1.81	0.46
1:A:1065:C:H2'	9:I:139:ASN:HB3	1.97	0.46
1:A:2459:G:H21	1:A:2465:A:H62	1.64	0.46
1:A:1059:A:H61	9:I:98:VAL:HG13	1.80	0.46
1:A:1144:C:OP1	17:Q:92:ARG:NH2	2.38	0.46
1:A:1350:U:O2'	1:A:1796:A:N3	2.41	0.46
1:A:2409:C:O2'	1:A:2410:U:O2	2.30	0.46
7:G:71:LEU:O	7:G:75:MET:HB2	2.15	0.46
8:H:8:LYS:HB3	8:H:15:LEU:HD23	1.97	0.46
1:A:1352:A:OP1	24:X:3:ARG:NH2	2.39	0.46
1:A:1641:G:H5'	14:N:39:PRO:HG2	1.97	0.46
1:A:2262:C:O2'	13:M:84:GLY:O	2.33	0.46
1:A:2301:G:N2	6:F:155:THR:OG1	2.48	0.46
1:A:2315:A:H2'	1:A:2316:A:C8	2.51	0.46
11:K:27:GLY:H	11:K:30:ARG:HG3	1.80	0.46
14:N:8:ARG:HG3	14:N:10:LEU:HG	1.98	0.46
1:A:2017:A:N3	1:A:2486:C:H5"	2.30	0.46
6:F:60:ILE:HG13	6:F:61:THR:HG23	1.98	0.46
7:G:52:PHE:CE2	7:G:72:VAL:HG21	2.51	0.46
9:I:21:SER:O	9:I:25:GLY:N	2.41	0.46
23:W:32:LYS:H	23:W:35:ASN:ND2	2.13	0.46
1:A:2115:G:H5"	1:A:2116:C:H5	1.80	0.46
5:E:2:GLN:HB3	5:E:13:VAL:HG22	1.98	0.46
8:H:31:LEU:HD21	8:H:38:VAL:HG23	1.98	0.46
1:A:2026:U:H2'	1:A:2027:G:H8	1.80	0.45
1:A:786:U:H2'	1:A:787:C:C6	2.52	0.45
1:A:1012:G:O6	10:J:68:LYS:NZ	2.49	0.45
1:A:2493:U:O2	1:A:2570:G:N2	2.44	0.45
11:K:76:ILE:HD12	11:K:78:ARG:HD3	1.98	0.45
1:A:59:U:O2'	1:A:74:A:OP2	2.27	0.45
1:A:472:G:O2'	1:A:498:A:N1	2.46	0.45
1:A:2101:A:O2'	1:A:2154:U:O2'	2.30	0.45
1:A:2644:A:O2'	7:G:156:LYS:NZ	2.45	0.45
1:A:1478:G:O2'	3:C:100:GLU:OE1	2.34	0.45
1:A:92:A:O2'	1:A:93:A:O4'	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:C:H42	1:A:898:A:H2	1.64	0.45
1:A:982:C:OP1	17:Q:47:TYR:OH	2.23	0.45
1:A:1469:G:H2'	1:A:1470:A:C8	2.51	0.45
11:K:24:VAL:HG13	11:K:33:ALA:HB2	1.99	0.45
1:A:950:A:H61	13:M:83:MET:HE1	1.82	0.45
1:A:2120:G:O2'	1:A:2122:A:OP1	2.29	0.45
1:A:2317:G:H21	23:W:42:GLY:HA3	1.82	0.45
8:H:44:VAL:HA	8:H:47:PHE:HD2	1.81	0.45
9:I:8:TYR:CB	9:I:8:TYR:CA	2.95	0.45
3:C:67:PHE:HB3	3:C:152:ALA:H	1.82	0.45
10:J:56:VAL:HB	10:J:124:VAL:HG12	1.98	0.45
1:A:1018:A:N6	1:A:1115:G:H2'	2.31	0.45
1:A:2254:A:H62	1:A:2259:U:H5	1.64	0.45
1:A:2301:G:OP1	6:F:35:THR:OG1	2.31	0.44
1:A:579:U:H2'	1:A:580:A:C8	2.52	0.44
1:A:2806:G:H2'	1:A:2808:A:N7	2.32	0.44
6:F:35:THR:HG23	6:F:88:LYS:HG3	1.98	0.44
10:J:45:THR:HB	10:J:48:VAL:HG12	1.98	0.44
13:M:34:LEU:HD13	13:M:118:PHE:HB3	2.00	0.44
20:T:36:ASP:OD1	20:T:36:ASP:N	2.49	0.44
1:A:559:U:H5'	1:A:936:C:H1'	1.99	0.44
1:A:1070:C:C4	9:I:117:LEU:HD12	2.53	0.44
1:A:1799:U:H2'	1:A:1800:G:H8	1.82	0.44
1:A:2455:A:O2'	1:A:2468:G:N2	2.50	0.44
6:F:4:LEU:H	6:F:97:TYR:HD1	1.66	0.44
1:A:2026:U:H2'	1:A:2027:G:C8	2.52	0.44
2:B:25:A:O2'	2:B:26:A:O5'	2.32	0.44
7:G:18:LYS:HB3	7:G:25:SER:HB3	1.99	0.44
1:A:518:C:N4	1:A:2766:U:OP2	2.49	0.44
1:A:1783:U:H2'	1:A:1784:C:C6	2.52	0.44
1:A:1939:A:N3	1:A:2547:A:O2'	2.40	0.44
1:A:2321:A:N6	15:O:21:GLU:OE1	2.48	0.44
6:F:33:LYS:O	27:1:26:SER:N	2.51	0.44
17:Q:43:GLY:HA3	18:R:75:ILE:HD13	1.98	0.44
18:R:14:VAL:HG13	18:R:98:ILE:HG13	2.00	0.44
1:A:862:C:HO2'	13:M:65:TRP:HE1	1.45	0.44
1:A:1766:U:H5	1:A:1771:A:N7	2.16	0.44
11:K:9:ASP:OD1	11:K:18:ARG:NH1	2.45	0.44
1:A:1245:U:H2'	1:A:1246:G:C8	2.53	0.44
21:U:41:ILE:HD13	21:U:41:ILE:HA	1.89	0.44
1:A:899:A:N3	1:A:2251:C:O2'	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2152:C:N4	1:A:2159:U:O4	2.50	0.44
3:C:96:TYR:HB2	3:C:100:GLU:HB3	2.00	0.44
13:M:57:HIS:HE1	13:M:116:GLU:HG3	1.83	0.44
16:P:23:PRO:HD3	16:P:51:LYS:HD3	2.00	0.44
17:Q:27:ALA:HB1	17:Q:31:VAL:HG22	1.99	0.44
18:R:7:THR:OG1	18:R:8:GLY:N	2.50	0.44
1:A:1781:A:H2'	1:A:1782:C:H6	1.83	0.44
6:F:91:LEU:HA	6:F:95:ARG:HE	1.82	0.44
10:J:36:LEU:HD11	10:J:122:LEU:HB2	1.99	0.44
13:M:42:LEU:HD22	13:M:125:LEU:HD22	2.00	0.44
1:A:1058:G:H4'	9:I:88:SER:HB2	2.00	0.43
1:A:2117:U:N3	1:A:2120:G:OP1	2.51	0.43
1:A:2414:C:H5'	1:A:2416:G:H5'	2.00	0.43
1:A:2445:G:O2'	1:A:2447:U:O4	2.30	0.43
6:F:99:PHE:HD1	6:F:102:ARG:HH11	1.66	0.43
7:G:64:MET:HA	7:G:67:THR:HG22	2.00	0.43
7:G:102:SER:HB2	7:G:108:PRO:HB3	2.00	0.43
1:A:664:G:H2'	1:A:794:A:H61	1.82	0.43
1:A:742:A:OP1	30:4:3:ARG:NH1	2.46	0.43
1:A:1017:A:C2	1:A:2475:G:H5'	2.53	0.43
1:A:1035:U:H5	1:A:1101:A:H5"	1.83	0.43
1:A:351:A:H2'	1:A:352:A:C8	2.52	0.43
1:A:702:G:H3'	1:A:703:G:H8	1.81	0.43
1:A:1046:G:H2'	9:I:13:VAL:HG12	1.99	0.43
1:A:2125:G:H1	1:A:2140:C:H1'	1.82	0.43
21:U:4:ILE:HG12	21:U:71:ILE:HD11	1.99	0.43
1:A:361:A:O2'	1:A:415:G:OP1	2.30	0.43
1:A:523:A:H5'	17:Q:28:ARG:HH12	1.84	0.43
1:A:1020:C:H5	1:A:1114:G:H22	1.65	0.43
1:A:1488:G:OP1	3:C:101:ARG:NH2	2.52	0.43
1:A:1796:A:H2'	1:A:1797:A:C8	2.53	0.43
4:D:6:VAL:H	4:D:33:ASN:ND2	2.16	0.43
1:A:357:A:H2'	1:A:358:A:H4'	2.00	0.43
1:A:399:G:O2'	1:A:400:G:H8	2.01	0.43
1:A:1421:A:H62	1:A:1548:A:H61	1.66	0.43
1:A:1469:G:H2'	1:A:1470:A:H8	1.84	0.43
1:A:1781:A:H2'	1:A:1782:C:C6	2.53	0.43
3:C:133:ARG:O	3:C:167:ARG:NH2	2.51	0.43
4:D:5:VAL:HG22	4:D:33:ASN:HD22	1.83	0.43
1:A:1470:A:H2'	1:A:1471:A:C8	2.52	0.43
1:A:1471:A:H2'	1:A:1472:A:H8	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:A:HO2'	1:A:1546:C:HO2'	1.59	0.43
3:C:44:ASN:HD22	3:C:44:ASN:HA	1.55	0.43
6:F:125:ARG:HB3	27:1:19:GLY:HA3	2.00	0.43
1:A:28:A:N6	1:A:503:G:H1'	2.33	0.43
1:A:126:A:H5'	30:4:19:ARG:HG3	2.01	0.43
1:A:1083:G:N2	1:A:1090:C:N3	2.66	0.43
1:A:1431:A:H2'	1:A:1432:G:H8	1.84	0.43
1:A:2493:U:O4	1:A:2570:G:O6	2.37	0.43
7:G:47:SER:OG	7:G:49:GLU:O	2.26	0.43
26:Z:29:ARG:HB2	26:Z:30:ARG:HH11	1.82	0.43
1:A:1143:C:H2'	1:A:1144:C:H6	1.83	0.43
1:A:1529:U:H2'	1:A:1530:G:C8	2.53	0.43
1:A:2186:A:OP1	24:X:37:ARG:NH1	2.51	0.43
1:A:2260:A:H2'	1:A:2261:A:C8	2.54	0.43
1:A:2278:U:O2'	1:A:2361:C:O2	2.33	0.43
1:A:629:U:H2'	1:A:630:C:C6	2.53	0.43
29:3:4:LEU:HA	29:3:20:ASP:HA	2.00	0.43
30:4:3:ARG:HA	30:4:3:ARG:HD3	1.84	0.43
1:A:548:U:OP1	10:J:112:ASN:HB3	2.19	0.43
1:A:1060:A:C2	9:I:81:LYS:HG2	2.53	0.43
1:A:1147:A:C8	17:Q:51:ARG:HG2	2.54	0.43
1:A:1406:A:H61	1:A:1481:A:H62	1.66	0.43
1:A:2172:U:H2'	1:A:2173:G:C4	2.54	0.43
1:A:1766:U:OP2	1:A:1771:A:N6	2.46	0.42
1:A:2366:G:H4'	15:O:22:LEU:HD11	1.99	0.42
3:C:53:HIS:CE1	3:C:219:THR:HG23	2.54	0.42
5:E:147:ILE:HG23	5:E:186:LEU:HD22	2.00	0.42
9:I:115:ALA:HA	9:I:118:THR:HG22	2.00	0.42
10:J:109:LEU:O	10:J:111:LYS:NZ	2.50	0.42
1:A:1075:A:C4	9:I:59:ILE:HD11	2.53	0.42
1:A:1783:U:H2'	1:A:1784:C:H6	1.83	0.42
1:A:1786:G:C2	3:C:154:ILE:HG23	2.55	0.42
1:A:2113:A:H4'	1:A:2114:G:H4'	2.01	0.42
1:A:2128:G:N2	1:A:2137:U:O2	2.52	0.42
5:E:158:LEU:HD23	5:E:158:LEU:HA	1.88	0.42
14:N:66:ALA:O	14:N:70:THR:HG22	2.18	0.42
21:U:39:ASN:HB3	21:U:62:ALA:HB3	2.01	0.42
29:3:6:ARG:HB2	29:3:50:ILE:HG22	2.00	0.42
1:A:669:C:H2'	1:A:670:G:H8	1.84	0.42
1:A:1059:A:H5'	9:I:81:LYS:HE3	2.00	0.42
1:A:1558:G:OP1	3:C:63:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1648:C:H2'	1:A:1649:G:C8	2.54	0.42
1:A:1657:G:O2'	1:A:1978:U:O4	2.28	0.42
1:A:1786:G:OP1	3:C:259:ARG:NH1	2.43	0.42
1:A:2248:C:OP1	23:W:19:LYS:NZ	2.41	0.42
1:A:2775:A:O2'	1:A:2796:A:N3	2.39	0.42
30:4:3:ARG:O	30:4:6:GLN:NE2	2.44	0.42
1:A:264:U:H4'	1:A:419:A:H2	1.84	0.42
1:A:456:G:H5'	30:4:44:VAL:HB	2.01	0.42
1:A:2001:A:H2'	1:A:2002:A:C8	2.54	0.42
15:O:5:LYS:HA	15:O:8:ARG:HG2	2.00	0.42
20:T:69:THR:OG1	20:T:70:ALA:N	2.53	0.42
1:A:688:C:O2'	1:A:724:A:N6	2.53	0.42
1:A:704:U:N3	1:A:707:C:OP2	2.50	0.42
1:A:950:A:H2'	1:A:952:G:H5'	2.01	0.42
1:A:1063:A:H3'	9:I:139:ASN:HD21	1.85	0.42
1:A:1781:A:H1'	1:A:1887:A:C8	2.54	0.42
1:A:1790:A:H8	1:A:1809:G:H21	1.66	0.42
4:D:15:ILE:HG13	16:P:13:GLN:HE22	1.85	0.42
4:D:34:ARG:HH21	4:D:76:ALA:HA	1.85	0.42
6:F:5:LYS:O	6:F:8:TYR:N	2.52	0.42
10:J:28:LEU:HD23	10:J:101:ILE:HD11	2.00	0.42
11:K:77:ILE:HG13	16:P:73:ARG:HD3	2.01	0.42
12:L:144:ASP:OD1	12:L:144:ASP:N	2.51	0.42
1:A:1057:A:H5'	1:A:1058:G:N7	2.34	0.42
1:A:2724:G:H2'	1:A:2725:A:C8	2.55	0.42
4:D:179:ARG:HB3	4:D:188:LEU:HB2	2.01	0.42
5:E:3:LEU:HD23	5:E:119:VAL:HG21	2.02	0.42
6:F:151:GLY:HA3	27:1:9:TYR:CZ	2.55	0.42
11:K:113:LYS:HE3	11:K:117:LEU:HD11	2.01	0.42
13:M:75:THR:HG21	13:M:87:LYS:HE2	2.02	0.42
1:A:1795:A:H3'	1:A:1796:A:C8	2.54	0.42
28:2:35:GLU:OE2	28:2:43:SER:OG	2.27	0.42
1:A:1242:U:H5"	1:A:1243:G:H5"	2.01	0.42
1:A:1471:A:H2'	1:A:1472:A:C8	2.54	0.42
1:A:1958:U:C6	3:C:240:SER:HB3	2.53	0.42
1:A:2104:A:N1	1:A:2159:U:N3	2.67	0.42
1:A:2787:A:H2'	1:A:2788:U:C6	2.55	0.42
3:C:147:LYS:HA	3:C:148:PRO:HD3	1.92	0.42
1:A:1084:U:H5	1:A:1087:U:H5"	1.84	0.42
1:A:2286:G:H2'	1:A:2287:A:H8	1.84	0.42
2:B:75:G:H21	22:V:91:HIS:CE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:133:THR:O	4:D:135:GLY:N	2.53	0.42
7:G:11:LEU:HD12	7:G:15:VAL:HB	2.01	0.42
14:N:107:ASN:ND2	19:S:40:SER:HB3	2.35	0.42
1:A:517:A:O2'	1:A:2030:U:O2	2.38	0.42
1:A:2155:G:N1	1:A:2158:A:OP2	2.52	0.42
1:A:2695:G:H5'	14:N:68:ASP:HB2	2.01	0.42
2:B:45:A:H62	6:F:90:THR:HG21	1.85	0.42
8:H:65:ALA:HA	8:H:68:ARG:HB3	2.02	0.42
1:A:249:C:O2	31:5:12:LYS:NZ	2.43	0.41
1:A:866:U:H2'	1:A:867:A:H8	1.85	0.41
1:A:1725:A:H2'	1:A:1726:A:H8	1.85	0.41
1:A:2233:G:H2'	1:A:2234:A:C8	2.55	0.41
2:B:34:A:N6	2:B:44:G:O2'	2.53	0.41
3:C:235:GLY:HA3	3:C:239:THR:HG21	2.01	0.41
9:I:130:ALA:HA	9:I:140:VAL:HG21	2.02	0.41
11:K:19:VAL:HB	11:K:41:VAL:HB	2.01	0.41
15:O:35:HIS:CE1	15:O:55:LEU:HD23	2.55	0.41
23:W:36:ILE:HG21	23:W:39:ARG:HE	1.85	0.41
1:A:583:U:O2'	31:5:64:ARG:OXT	2.35	0.41
1:A:840:U:H5"	26:Z:49:LYS:HG3	2.01	0.41
1:A:2330:U:O2'	1:A:2360:A:O2'	2.21	0.41
11:K:38:ILE:HD11	11:K:111:PHE:HZ	1.84	0.41
25:Y:49:ASP:OD1	25:Y:52:ARG:NH1	2.44	0.41
1:A:946:G:H2'	1:A:947:C:H2'	2.02	0.41
1:A:1045:G:H3'	1:A:1046:G:C8	2.54	0.41
1:A:1092:C:C5	9:I:8:TYR:CG	3.08	0.41
4:D:32:PRO:HB2	4:D:95:GLN:HE21	1.85	0.41
1:A:155:U:H2'	1:A:156:A:H8	1.85	0.41
1:A:583:U:H2'	1:A:584:U:C6	2.55	0.41
1:A:2128:G:N1	1:A:2137:U:N3	2.52	0.41
1:A:2140:C:OP1	1:A:2143:G:N2	2.54	0.41
1:A:2176:U:H2'	1:A:2177:G:H8	1.85	0.41
1:A:2502:C:H2'	1:A:2503:A:H8	1.86	0.41
11:K:40:LYS:HE2	11:K:40:LYS:HB2	1.90	0.41
21:U:6:ARG:O	21:U:8:ASP:N	2.54	0.41
1:A:1303:U:H2'	1:A:1304:G:H8	1.85	0.41
1:A:1589:C:H5'	20:T:38:THR:HG22	2.02	0.41
1:A:2871:U:O4'	28:2:49:ARG:NH2	2.53	0.41
1:A:2087:G:H2'	1:A:2088:A:C8	2.55	0.41
9:I:134:ARG:HD2	9:I:140:VAL:HG23	2.02	0.41
15:O:35:HIS:HB3	15:O:64:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:U:H2'	12:L:21:ARG:HA	2.03	0.41
1:A:835:A:N1	1:A:922:G:N1	2.58	0.41
1:A:1892:C:H2'	1:A:1917:G:C8	2.55	0.41
5:E:11:ILE:HD12	5:E:189:VAL:HG22	2.02	0.41
9:I:3:LYS:HB3	9:I:4:LYS:H	1.65	0.41
30:4:22:MET:HG3	30:4:28:ARG:HG2	2.02	0.41
1:A:1048:G:N3	9:I:49:GLN:NE2	2.69	0.41
1:A:1053:G:O2'	9:I:105:GLN:O	2.37	0.41
1:A:1673:C:H2'	1:A:1674:A:C8	2.56	0.41
11:K:70:ARG:HH11	11:K:76:ILE:HG23	1.86	0.41
1:A:161:A:OP2	1:A:162:U:O2'	2.34	0.41
1:A:523:A:H5"	17:Q:28:ARG:HH22	1.86	0.41
1:A:766:G:N1	1:A:783:A:O2'	2.37	0.41
1:A:1373:C:H2'	1:A:1374:A:H8	1.86	0.41
1:A:1712:G:H2'	1:A:1713:G:C8	2.55	0.41
1:A:2084:U:O4	1:A:2179:G:O6	2.38	0.41
4:D:71:LYS:HE2	4:D:71:LYS:HB3	1.90	0.41
11:K:71:ARG:NE	11:K:77:ILE:HD11	2.35	0.41
12:L:82:LEU:HD11	12:L:110:VAL:HG11	2.02	0.41
13:M:57:HIS:CE1	13:M:116:GLU:HG3	2.55	0.41
29:3:17:TYR:HD2	29:3:34:LYS:HD3	1.86	0.41
30:4:34:ARG:HE	30:4:42:LEU:HA	1.86	0.41
1:A:2126:U:N3	1:A:2139:G:C6	2.89	0.41
7:G:83:PHE:CE1	7:G:134:LYS:HD3	2.56	0.41
15:O:8:ARG:HA	15:O:11:ARG:HE	1.86	0.41
1:A:62:U:H3	1:A:93:A:H61	1.68	0.40
1:A:358:A:O2'	1:A:359:U:O2	2.27	0.40
1:A:770:G:H21	1:A:773:A:H62	1.68	0.40
1:A:857:U:H3	1:A:898:A:H62	1.69	0.40
1:A:2694:U:H2'	1:A:2695:G:C8	2.56	0.40
5:E:74:SER:HB3	5:E:77:TRP:CD1	2.56	0.40
8:H:23:GLY:O	8:H:27:ARG:HB2	2.21	0.40
19:S:82:LEU:HD23	19:S:84:ARG:NH2	2.36	0.40
31:5:28:LYS:HE2	31:5:28:LYS:HB3	1.77	0.40
31:5:35:MET:HG2	31:5:39:ARG:NH2	2.37	0.40
1:A:191:A:H2'	1:A:192:C:C6	2.57	0.40
1:A:1143:C:H2'	1:A:1144:C:C6	2.56	0.40
1:A:1515:A:C5	1:A:1516:G:H1'	2.57	0.40
1:A:1777:C:H2'	1:A:1778:A:C5	2.56	0.40
1:A:2074:U:H2'	1:A:2075:G:C8	2.55	0.40
1:A:2318:G:O2'	23:W:42:GLY:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:G:H21	6:F:26:MET:HE1	1.87	0.40
22:V:149:VAL:HG22	22:V:165:LEU:HD13	2.02	0.40
1:A:155:U:H2'	1:A:156:A:C8	2.57	0.40
1:A:952:G:N2	1:A:2237:G:H1	2.18	0.40
1:A:1020:C:H41	1:A:1114:G:H1	1.69	0.40
1:A:1405:G:H1'	1:A:1570:A:H61	1.86	0.40
1:A:1659:A:H5"	1:A:2537:G:OP1	2.21	0.40
26:Z:16:LEU:HB2	26:Z:19:HIS:HD2	1.86	0.40
1:A:18:C:OP1	17:Q:30:ARG:NH2	2.54	0.40
1:A:624:G:N7	12:L:74:ARG:NH1	2.69	0.40
1:A:2082:A:H2'	1:A:2083:C:C6	2.57	0.40
1:A:2661:G:H4'	11:K:30:ARG:HG2	2.04	0.40
3:C:135:ILE:HD11	3:C:164:LEU:HD22	2.04	0.40
11:K:104:ARG:HH22	16:P:33:VAL:HB	1.85	0.40
12:L:123:LYS:HE2	12:L:123:LYS:HB2	1.90	0.40
16:P:93:VAL:HB	16:P:98:LEU:HD21	2.04	0.40
19:S:80:ARG:HH11	19:S:80:ARG:HD2	1.74	0.40
1:A:1392:U:H2'	1:A:1393:U:C6	2.56	0.40
1:A:1488:G:H5"	3:C:95:LYS:HD2	2.04	0.40
1:A:1656:G:HO2'	11:K:6:SER:HG	1.67	0.40
1:A:2373:U:H4'	23:W:56:ASP:HA	2.04	0.40
1:A:2834:U:H2'	1:A:2835:G:O4'	2.21	0.40
5:E:20:GLY:O	5:E:113:ARG:NH2	2.39	0.40
6:F:121:SER:O	6:F:127:ASN:ND2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	269/271 (99%)	247 (92%)	21 (8%)	1 (0%)	34 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	205/207 (99%)	175 (85%)	30 (15%)	0	100	100
5	E	197/199 (99%)	190 (96%)	7 (4%)	0	100	100
6	F	172/174 (99%)	122 (71%)	50 (29%)	0	100	100
7	G	167/169 (99%)	149 (89%)	18 (11%)	0	100	100
8	H	76/78 (97%)	71 (93%)	5 (7%)	0	100	100
9	I	138/140 (99%)	86 (62%)	52 (38%)	0	100	100
10	J	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
11	K	118/120 (98%)	107 (91%)	11 (9%)	0	100	100
12	L	141/144 (98%)	127 (90%)	14 (10%)	0	100	100
13	M	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
14	N	116/120 (97%)	105 (90%)	10 (9%)	1 (1%)	17	44
15	O	113/115 (98%)	104 (92%)	9 (8%)	0	100	100
16	P	111/115 (96%)	96 (86%)	15 (14%)	0	100	100
17	Q	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
18	R	100/102 (98%)	90 (90%)	10 (10%)	0	100	100
19	S	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
20	T	90/94 (96%)	83 (92%)	7 (8%)	0	100	100
21	U	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
22	V	186/188 (99%)	162 (87%)	24 (13%)	0	100	100
23	W	74/76 (97%)	56 (76%)	18 (24%)	0	100	100
24	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
25	Y	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
26	Z	55/57 (96%)	52 (94%)	3 (6%)	0	100	100
27	1	29/31 (94%)	19 (66%)	10 (34%)	0	100	100
28	2	51/53 (96%)	45 (88%)	6 (12%)	0	100	100
29	3	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
30	4	43/44 (98%)	40 (93%)	3 (7%)	0	100	100
31	5	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
32	6	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
All	All	3324/3392 (98%)	2945 (89%)	377 (11%)	2 (0%)	54	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	112	ALA
14	N	71	ARG

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
3	C	206/212 (97%)	202 (98%)	4 (2%)	57 84
4	D	157/159 (99%)	150 (96%)	7 (4%)	27 59
5	E	155/157 (99%)	152 (98%)	3 (2%)	57 84
6	F	122/147 (83%)	119 (98%)	3 (2%)	47 78
7	G	131/135 (97%)	130 (99%)	1 (1%)	81 94
8	H	55/55 (100%)	55 (100%)	0	100 100
9	I	108/108 (100%)	106 (98%)	2 (2%)	57 84
10	J	118/118 (100%)	116 (98%)	2 (2%)	60 86
11	K	100/100 (100%)	98 (98%)	2 (2%)	55 83
12	L	104/106 (98%)	101 (97%)	3 (3%)	42 74
13	M	108/109 (99%)	107 (99%)	1 (1%)	78 93
14	N	97/99 (98%)	95 (98%)	2 (2%)	53 82
15	O	86/86 (100%)	84 (98%)	2 (2%)	50 80
16	P	94/97 (97%)	93 (99%)	1 (1%)	73 91
17	Q	87/87 (100%)	86 (99%)	1 (1%)	73 91
18	R	82/86 (95%)	80 (98%)	2 (2%)	49 80
19	S	86/87 (99%)	86 (100%)	0	100 100
20	T	73/77 (95%)	72 (99%)	1 (1%)	67 89
21	U	88/88 (100%)	88 (100%)	0	100 100
22	V	144/153 (94%)	142 (99%)	2 (1%)	67 89
23	W	56/56 (100%)	56 (100%)	0	100 100
24	X	65/66 (98%)	64 (98%)	1 (2%)	65 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	Y	51/53 (96%)	50 (98%)	1 (2%)	55 83
26	Z	48/48 (100%)	47 (98%)	1 (2%)	53 82
27	1	27/27 (100%)	27 (100%)	0	100 100
28	2	46/46 (100%)	46 (100%)	0	100 100
29	3	46/46 (100%)	46 (100%)	0	100 100
30	4	38/37 (103%)	36 (95%)	2 (5%)	22 52
31	5	54/54 (100%)	54 (100%)	0	100 100
32	6	33/34 (97%)	33 (100%)	0	100 100
All	All	2665/2733 (98%)	2621 (98%)	44 (2%)	64 86

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	21	ASN
3	C	44	ASN
3	C	180	GLU
3	C	217	ARG
4	D	5	VAL
4	D	27	VAL
4	D	47	ARG
4	D	110	THR
4	D	154	ARG
4	D	184	ARG
4	D	204	ARG
5	E	16	ARG
5	E	23	ASN
5	E	161	ARG
6	F	9	ARG
6	F	48	LYS
6	F	118	ASN
7	G	3	ARG
9	I	82	LYS
9	I	101	VAL
10	J	116	ARG
10	J	123	LYS
11	K	49	ARG
11	K	89	ASN
12	L	4	ASN
12	L	7	ARG

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Mol	Chain	Res	Type
12	L	78	ARG
13	M	6	ARG
14	N	2	ARG
14	N	17	ARG
15	O	57	LYS
15	O	76	LEU
16	P	97	LYS
17	Q	4	VAL
18	R	43	ASN
18	R	58	LYS
20	T	83	TYR
22	V	91	HIS
22	V	186	ASN
24	X	27	ARG
25	Y	21	LEU
26	Z	30	ARG
30	4	41[A]	ARG
30	4	41[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	21	ASN
3	C	44	ASN
3	C	53	HIS
3	C	142	HIS
3	C	244	HIS
3	C	261	ASN
4	D	33	ASN
4	D	37	GLN
4	D	68	HIS
4	D	105	GLN
5	E	6	ASN
5	E	23	ASN
5	E	172	GLN
6	F	52	ASN
6	F	118	ASN
7	G	59	GLN
9	I	49	GLN
10	J	58	ASN
10	J	77	HIS
10	J	135	GLN

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Mol	Chain	Res	Type
11	K	89	ASN
12	L	58	HIS
13	M	57	HIS
14	N	9	HIS
15	O	35	HIS
15	O	99	HIS
16	P	76	GLN
17	Q	37	GLN
18	R	43	ASN
18	R	66	HIS
18	R	82	HIS
19	S	61	ASN
19	S	102	HIS
22	V	178	HIS
22	V	186	ASN
23	W	46	HIS
26	Z	19	HIS
26	Z	33	HIS
28	2	41	HIS
31	5	50	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2883/2888 (99%)	823 (28%)	42 (1%)
2	B	116/117 (99%)	29 (25%)	5 (4%)
All	All	2999/3005 (99%)	852 (28%)	47 (1%)

All (852) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	14	A
1	A	15	G
1	A	17	G
1	A	27	G
1	A	28	A
1	A	34	U
1	A	35	G
1	A	44	A
1	A	46	G

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Mol	Chain	Res	Type
1	A	50	U
1	A	55	G
1	A	58	G
1	A	60	G
1	A	62	U
1	A	63	A
1	A	64	G
1	A	69	C
1	A	70	G
1	A	71	A
1	A	74	A
1	A	75	G
1	A	79	C
1	A	82	G
1	A	83	G
1	A	85	G
1	A	92	A
1	A	93	A
1	A	97	A
1	A	100	U
1	A	102	G
1	A	103	A
1	A	110	G
1	A	114	U
1	A	115	C
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	G
1	A	131	A
1	A	139	U
1	A	140	A
1	A	141	A
1	A	142	C
1	A	144	U
1	A	147	G
1	A	160	A
1	A	163	C
1	A	166	U
1	A	170	U
1	A	173	A
1	A	181	A

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Mol	Chain	Res	Type
1	A	196	A
1	A	199	A
1	A	205	G
1	A	206	U
1	A	212	G
1	A	215	G
1	A	216	A
1	A	220	G
1	A	222	A
1	A	223	A
1	A	224	U
1	A	227	A
1	A	228	C
1	A	229	C
1	A	230	G
1	A	232	G
1	A	233	A
1	A	240	U
1	A	241	A
1	A	242	G
1	A	243	U
1	A	244	A
1	A	248	G
1	A	249	C
1	A	250	G
1	A	252	G
1	A	255	A
1	A	261	G
1	A	265	A
1	A	266	G
1	A	267	C
1	A	268	C
1	A	271	U
1	A	276	U
1	A	281	U
1	A	282	G
1	A	289	G
1	A	294	A
1	A	296	G
1	A	304	A
1	A	305	A
1	A	315	U

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Mol	Chain	Res	Type
1	A	316	A
1	A	318	U
1	A	319	G
1	A	322	U
1	A	323	G
1	A	324	A
1	A	325	U
1	A	336	G
1	A	339	A
1	A	341	A
1	A	342	G
1	A	348	U
1	A	349	U
1	A	350	G
1	A	353	G
1	A	357	A
1	A	358	A
1	A	359	U
1	A	361	A
1	A	377	G
1	A	378	A
1	A	380	A
1	A	385	U
1	A	386	U
1	A	387	G
1	A	395	A
1	A	397	G
1	A	399	G
1	A	400	G
1	A	403	A
1	A	435	C
1	A	439	U
1	A	445	A
1	A	447	C
1	A	454	G
1	A	461	A
1	A	464	G
1	A	466	C
1	A	471	A
1	A	472	G
1	A	482	G
1	A	485	G

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Mol	Chain	Res	Type
1	A	487	G
1	A	492	A
1	A	495	U
1	A	496	A
1	A	499	A
1	A	516	U
1	A	519	A
1	A	520	A
1	A	521	G
1	A	523	A
1	A	526	G
1	A	534	A
1	A	535	C
1	A	536	U
1	A	537	U
1	A	538	G
1	A	539	U
1	A	540	U
1	A	541	A
1	A	544	U
1	A	553	A
1	A	558	U
1	A	561	U
1	A	563	U
1	A	564	A
1	A	565	A
1	A	573	G
1	A	576	A
1	A	593	A
1	A	594	G
1	A	599	A
1	A	604	A
1	A	605	U
1	A	622	A
1	A	624	G
1	A	627	A
1	A	633	A
1	A	634	A
1	A	635	U
1	A	643	U
1	A	645	A
1	A	647	U

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Mol	Chain	Res	Type
1	A	649	G
1	A	659	G
1	A	660	A
1	A	667	A
1	A	674	G
1	A	675	A
1	A	676	U
1	A	679	A
1	A	687	G
1	A	689	A
1	A	698	G
1	A	699	U
1	A	701	A
1	A	702	G
1	A	703	G
1	A	704	U
1	A	705	A
1	A	706	A
1	A	708	A
1	A	711	G
1	A	716	G
1	A	720	A
1	A	722	C
1	A	724	A
1	A	725	A
1	A	737	U
1	A	738	G
1	A	742	A
1	A	743	G
1	A	745	U
1	A	747	G
1	A	753	G
1	A	754	A
1	A	755	C
1	A	765	G
1	A	766	G
1	A	767	A
1	A	771	A
1	A	772	A
1	A	773	A
1	A	774	G
1	A	775	G

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Mol	Chain	Res	Type
1	A	778	A
1	A	779	A
1	A	781	C
1	A	782	A
1	A	783	A
1	A	784	G
1	A	795	G
1	A	801	U
1	A	802	C
1	A	818	U
1	A	836	U
1	A	838	A
1	A	839	C
1	A	844	G
1	A	846	G
1	A	848	G
1	A	855	A
1	A	859	U
1	A	860	U
1	A	862	C
1	A	863	G
1	A	864	G
1	A	865	C
1	A	866	U
1	A	868	G
1	A	870	G
1	A	872	G
1	A	875	A
1	A	877	C
1	A	878	C
1	A	881	A
1	A	882	C
1	A	884	U
1	A	886	C
1	A	889	A
1	A	890	A
1	A	898	A
1	A	899	A
1	A	908	U
1	A	921	C
1	A	922	G
1	A	931	A

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Mol	Chain	Res	Type
1	A	935	A
1	A	936	C
1	A	949	A
1	A	951	C
1	A	952	G
1	A	954	C
1	A	963	A
1	A	964	A
1	A	972	C
1	A	973	A
1	A	975	C
1	A	979	G
1	A	986	A
1	A	993	G
1	A	1002	U
1	A	1003	U
1	A	1007	G
1	A	1012	G
1	A	1016	U
1	A	1017	A
1	A	1023	U
1	A	1025	U
1	A	1030	A
1	A	1033	C
1	A	1034	U
1	A	1035	U
1	A	1036	A
1	A	1037	G
1	A	1038	A
1	A	1039	C
1	A	1040	A
1	A	1041	G
1	A	1042	C
1	A	1043	U
1	A	1044	A
1	A	1045	G
1	A	1047	A
1	A	1048	G
1	A	1049	G
1	A	1050	U
1	A	1051	U
1	A	1052	G

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Mol	Chain	Res	Type
1	A	1053	G
1	A	1054	C
1	A	1055	U
1	A	1056	U
1	A	1057	A
1	A	1058	G
1	A	1059	A
1	A	1060	A
1	A	1062	C
1	A	1063	A
1	A	1064	G
1	A	1065	C
1	A	1066	C
1	A	1068	C
1	A	1069	C
1	A	1070	C
1	A	1071	U
1	A	1072	U
1	A	1073	U
1	A	1074	A
1	A	1076	A
1	A	1078	A
1	A	1079	A
1	A	1080	A
1	A	1082	C
1	A	1083	G
1	A	1084	U
1	A	1085	A
1	A	1086	A
1	A	1087	U
1	A	1088	A
1	A	1090	C
1	A	1093	A
1	A	1094	C
1	A	1095	U
1	A	1096	A
1	A	1098	U
1	A	1099	C
1	A	1101	A
1	A	1102	G
1	A	1103	U
1	A	1105	G

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Mol	Chain	Res	Type
1	A	1106	G
1	A	1112	G
1	A	1114	G
1	A	1117	A
1	A	1119	A
1	A	1120	U
1	A	1122	U
1	A	1124	A
1	A	1125	C
1	A	1129	G
1	A	1146	A
1	A	1148	G
1	A	1149	C
1	A	1156	U
1	A	1163	U
1	A	1164	A
1	A	1165	A
1	A	1166	G
1	A	1167	U
1	A	1168	G
1	A	1170	C
1	A	1171	G
1	A	1191	A
1	A	1193	G
1	A	1199	G
1	A	1211	A
1	A	1214	A
1	A	1223	G
1	A	1224	A
1	A	1225	G
1	A	1228	A
1	A	1229	U
1	A	1231	A
1	A	1232	G
1	A	1234	A
1	A	1237	G
1	A	1238	C
1	A	1240	A
1	A	1242	U
1	A	1243	G
1	A	1244	C
1	A	1249	A

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Mol	Chain	Res	Type
1	A	1250	U
1	A	1253	G
1	A	1257	C
1	A	1258	G
1	A	1259	A
1	A	1261	A
1	A	1263	U
1	A	1271	A
1	A	1273	A
1	A	1274	A
1	A	1275	A
1	A	1276	C
1	A	1282	C
1	A	1283	G
1	A	1287	A
1	A	1288	A
1	A	1289	A
1	A	1291	A
1	A	1306	G
1	A	1307	C
1	A	1316	U
1	A	1327	U
1	A	1331	U
1	A	1333	G
1	A	1337	C
1	A	1339	U
1	A	1346	A
1	A	1347	G
1	A	1349	C
1	A	1352	A
1	A	1355	A
1	A	1361	G
1	A	1362	U
1	A	1365	A
1	A	1366	U
1	A	1367	G
1	A	1372	A
1	A	1373	C
1	A	1378	U
1	A	1379	A
1	A	1382	A
1	A	1397	G

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Mol	Chain	Res	Type
1	A	1403	G
1	A	1404	C
1	A	1407	U
1	A	1408	G
1	A	1414	A
1	A	1420	A
1	A	1421	A
1	A	1422	G
1	A	1424	C
1	A	1434	U
1	A	1439	G
1	A	1440	U
1	A	1445	U
1	A	1447	U
1	A	1454	U
1	A	1459	G
1	A	1469	G
1	A	1477	A
1	A	1478	G
1	A	1480	U
1	A	1481	A
1	A	1484	U
1	A	1485	C
1	A	1496	A
1	A	1497	G
1	A	1499	C
1	A	1509	A
1	A	1511	G
1	A	1512	A
1	A	1516	G
1	A	1528	A
1	A	1542	G
1	A	1556	A
1	A	1557	A
1	A	1558	G
1	A	1559	A
1	A	1560	A
1	A	1568	U
1	A	1571	G
1	A	1573	U
1	A	1574	U
1	A	1576	A

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Mol	Chain	Res	Type
1	A	1593	A
1	A	1596	C
1	A	1597	C
1	A	1598	A
1	A	1599	A
1	A	1600	A
1	A	1609	G
1	A	1624	A
1	A	1627	A
1	A	1628	C
1	A	1629	C
1	A	1636	C
1	A	1637	U
1	A	1638	U
1	A	1639	G
1	A	1641	G
1	A	1643	G
1	A	1650	G
1	A	1657	G
1	A	1664	G
1	A	1666	A
1	A	1673	C
1	A	1683	U
1	A	1685	G
1	A	1686	G
1	A	1698	C
1	A	1699	C
1	A	1700	G
1	A	1705	G
1	A	1710	A
1	A	1711	A
1	A	1713	G
1	A	1714	A
1	A	1716	U
1	A	1717	U
1	A	1718	A
1	A	1720	U
1	A	1724	U
1	A	1731	U
1	A	1736	G
1	A	1739	C
1	A	1740	G

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Mol	Chain	Res	Type
1	A	1741	A
1	A	1743	G
1	A	1745	U
1	A	1746	A
1	A	1750	G
1	A	1751	G
1	A	1756	U
1	A	1760	A
1	A	1768	U
1	A	1771	A
1	A	1787	C
1	A	1788	A
1	A	1789	A
1	A	1795	A
1	A	1796	A
1	A	1797	A
1	A	1803	C
1	A	1807	U
1	A	1815	G
1	A	1816	A
1	A	1820	C
1	A	1834	A
1	A	1835	A
1	A	1838	U
1	A	1840	A
1	A	1841	A
1	A	1842	U
1	A	1844	G
1	A	1851	U
1	A	1853	A
1	A	1855	C
1	A	1862	G
1	A	1863	A
1	A	1875	G
1	A	1890	G
1	A	1893	G
1	A	1896	C
1	A	1898	U
1	A	1900	A
1	A	1902	U
1	A	1903	A
1	A	1905	A

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Mol	Chain	Res	Type
1	A	1916	G
1	A	1917	G
1	A	1920	G
1	A	1925	A
1	A	1942	U
1	A	1949	C
1	A	1951	G
1	A	1953	A
1	A	1954	C
1	A	1957	A
1	A	1958	U
1	A	1959	G
1	A	1962	G
1	A	1967	G
1	A	1968	A
1	A	1969	U
1	A	1972	C
1	A	1978	U
1	A	1979	G
1	A	1980	U
1	A	1984	C
1	A	1989	G
1	A	2007	A
1	A	2008	A
1	A	2009	U
1	A	2010	C
1	A	2018	A
1	A	2020	A
1	A	2022	G
1	A	2030	U
1	A	2039	A
1	A	2040	G
1	A	2042	C
1	A	2043	G
1	A	2047	A
1	A	2048	G
1	A	2049	A
1	A	2055	U
1	A	2056	G
1	A	2060	C
1	A	2063	U
1	A	2064	A

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Mol	Chain	Res	Type
1	A	2068	U
1	A	2077	A
1	A	2080	G
1	A	2082	A
1	A	2094	C
1	A	2095	U
1	A	2098	U
1	A	2099	G
1	A	2101	A
1	A	2106	A
1	A	2107	G
1	A	2108	G
1	A	2112	G
1	A	2113	A
1	A	2114	G
1	A	2116	C
1	A	2117	U
1	A	2119	U
1	A	2120	G
1	A	2121	A
1	A	2122	A
1	A	2132	C
1	A	2133	C
1	A	2135	G
1	A	2140	C
1	A	2141	G
1	A	2142	U
1	A	2143	G
1	A	2144	G
1	A	2145	A
1	A	2146	G
1	A	2147	C
1	A	2148	C
1	A	2150	U
1	A	2151	C
1	A	2156	A
1	A	2157	A
1	A	2160	A
1	A	2163	A
1	A	2165	C
1	A	2169	G
1	A	2174	C

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Mol	Chain	Res	Type
1	A	2175	U
1	A	2185	A
1	A	2191	G
1	A	2199	A
1	A	2212	A
1	A	2225	G
1	A	2226	G
1	A	2229	G
1	A	2237	G
1	A	2270	U
1	A	2274	A
1	A	2275	A
1	A	2291	G
1	A	2292	U
1	A	2294	G
1	A	2295	G
1	A	2296	A
1	A	2297	A
1	A	2300	C
1	A	2301	G
1	A	2302	G
1	A	2303	U
1	A	2305	G
1	A	2306	C
1	A	2307	A
1	A	2308	G
1	A	2309	A
1	A	2312	A
1	A	2313	U
1	A	2318	G
1	A	2319	C
1	A	2320	A
1	A	2321	A
1	A	2323	A
1	A	2329	C
1	A	2332	G
1	A	2334	C
1	A	2337	C
1	A	2343	A
1	A	2345	A
1	A	2348	C
1	A	2359	U

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Mol	Chain	Res	Type
1	A	2360	A
1	A	2361	C
1	A	2363	A
1	A	2366	G
1	A	2367	U
1	A	2370	G
1	A	2371	U
1	A	2372	C
1	A	2375	A
1	A	2378	G
1	A	2383	G
1	A	2389	U
1	A	2390	C
1	A	2393	U
1	A	2394	A
1	A	2409	C
1	A	2410	U
1	A	2411	C
1	A	2413	A
1	A	2416	G
1	A	2417	A
1	A	2421	A
1	A	2427	C
1	A	2428	U
1	A	2434	G
1	A	2435	A
1	A	2454	C
1	A	2457	G
1	A	2459	G
1	A	2461	U
1	A	2465	A
1	A	2466	U
1	A	2471	G
1	A	2474	G
1	A	2477	G
1	A	2478	U
1	A	2479	U
1	A	2480	U
1	A	2481	G
1	A	2485	C
1	A	2489	G
1	A	2492	G

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Mol	Chain	Res	Type
1	A	2505	A
1	A	2506	U
1	A	2512	G
1	A	2516	G
1	A	2517	A
1	A	2521	C
1	A	2522	G
1	A	2534	A
1	A	2537	G
1	A	2545	C
1	A	2549	U
1	A	2551	A
1	A	2553	A
1	A	2554	G
1	A	2560	C
1	A	2565	G
1	A	2572	U
1	A	2573	U
1	A	2586	G
1	A	2589	A
1	A	2590	G
1	A	2595	G
1	A	2597	C
1	A	2600	U
1	A	2604	U
1	A	2612	A
1	A	2616	U
1	A	2617	U
1	A	2619	A
1	A	2621	A
1	A	2633	C
1	A	2637	U
1	A	2638	C
1	A	2640	U
1	A	2651	G
1	A	2655	G
1	A	2656	G
1	A	2657	A
1	A	2658	G
1	A	2659	U
1	A	2669	U
1	A	2672	G

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Mol	Chain	Res	Type
1	A	2676	U
1	A	2677	U
1	A	2689	G
1	A	2696	G
1	A	2701	G
1	A	2703	C
1	A	2704	G
1	A	2705	G
1	A	2713	U
1	A	2719	G
1	A	2720	A
1	A	2728	A
1	A	2731	G
1	A	2732	C
1	A	2735	A
1	A	2738	G
1	A	2739	C
1	A	2740	A
1	A	2744	A
1	A	2745	A
1	A	2748	G
1	A	2749	G
1	A	2752	A
1	A	2756	U
1	A	2763	A
1	A	2765	A
1	A	2766	U
1	A	2772	C
1	A	2776	C
1	A	2779	G
1	A	2784	U
1	A	2785	U
1	A	2786	G
1	A	2787	A
1	A	2795	G
1	A	2798	G
1	A	2805	C
1	A	2807	A
1	A	2810	A
1	A	2811	C
1	A	2812	U
1	A	2819	U

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Mol	Chain	Res	Type
1	A	2820	U
1	A	2821	G
1	A	2822	A
1	A	2836	U
1	A	2846	G
1	A	2848	G
1	A	2850	C
1	A	2851	G
1	A	2860	A
1	A	2866	A
1	A	2871	U
1	A	2873	G
1	A	2878	U
1	A	2888	C
1	A	2889	C
2	B	9	G
2	B	24	G
2	B	25	A
2	B	26	A
2	B	35	U
2	B	37	C
2	B	41	C
2	B	42	C
2	B	43	C
2	B	44	G
2	B	45	A
2	B	46	A
2	B	51	G
2	B	52	A
2	B	53	A
2	B	54	G
2	B	56	G
2	B	57	A
2	B	67	U
2	B	73	A
2	B	80	U
2	B	89	U
2	B	90	C
2	B	91	C
2	B	100	G
2	B	109	A
2	B	112	G

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Mol	Chain	Res	Type
2	B	116	A
2	B	117	G

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	62	U
1	A	81	G
1	A	114	U
1	A	227	A
1	A	243	U
1	A	266	G
1	A	314	A
1	A	434	A
1	A	437	G
1	A	444	A
1	A	540	U
1	A	817	U
1	A	920	C
1	A	953	U
1	A	1016	U
1	A	1063	A
1	A	1065	C
1	A	1124	A
1	A	1166	G
1	A	1169	A
1	A	1378	U
1	A	1496	A
1	A	1627	A
1	A	1635	G
1	A	1642	A
1	A	1672	G
1	A	1968	A
1	A	2063	U
1	A	2228	A
1	A	2274	A
1	A	2308	G
1	A	2311	U
1	A	2317	G
1	A	2389	U
1	A	2408	G
1	A	2417	A

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Mol	Chain	Res	Type
1	A	2536	G
1	A	2636	C
1	A	2703	C
1	A	2731	G
1	A	2784	U
1	A	2860	A
2	B	25	A
2	B	34	A
2	B	43	C
2	B	51	G
2	B	66	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1522:U	O3'	1526:A	P	15.24

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Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1908:G	O3'	1909:G	P	1.86

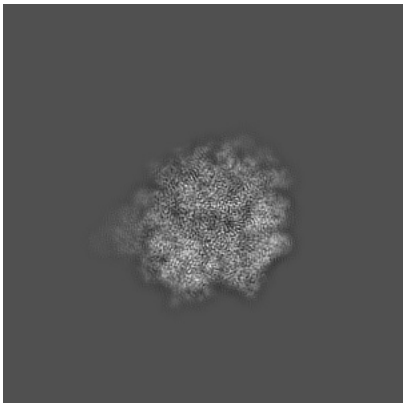
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10280. These allow visual inspection of the internal detail of the map and identification of artifacts.

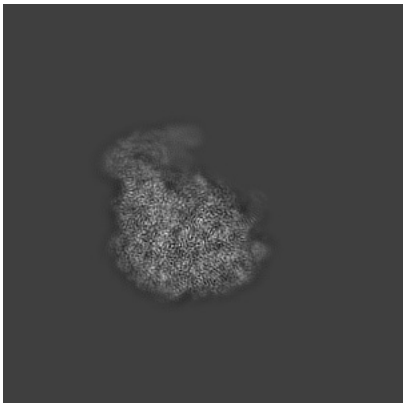
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

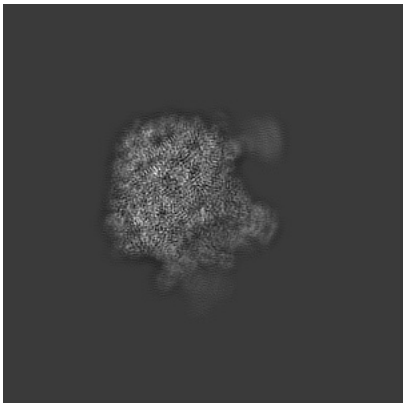
6.1.1 Primary map



X



Y

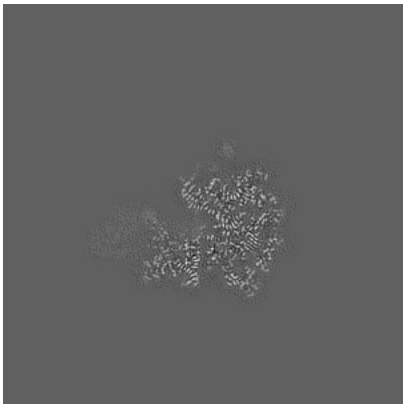


Z

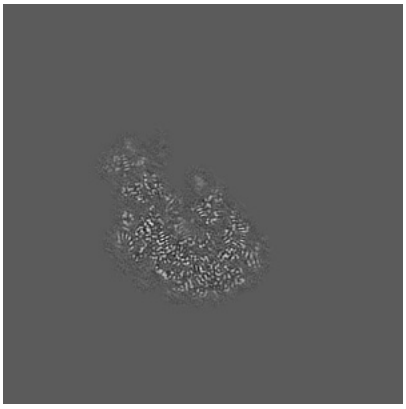
The images above show the map projected in three orthogonal directions.

6.2 Central slices

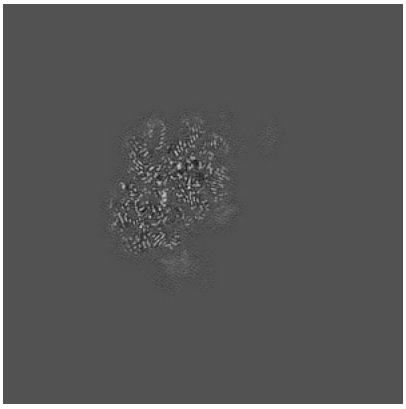
6.2.1 Primary map



X Index: 200



Y Index: 200



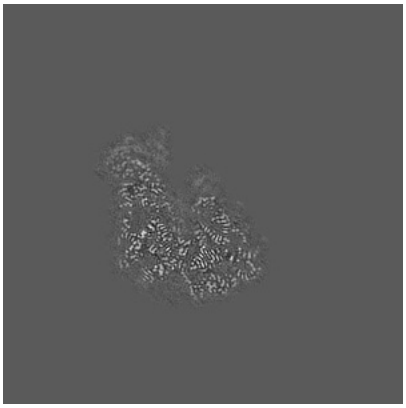
Z Index: 200

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

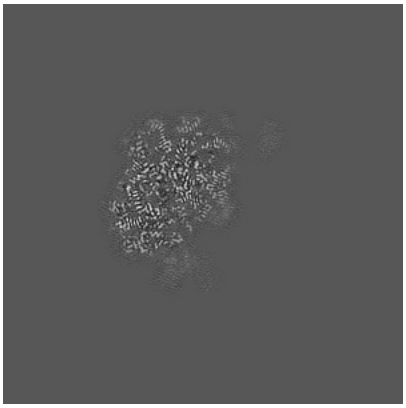
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 152



Y Index: 194

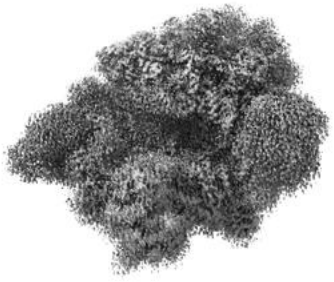


Z Index: 198

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0166. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

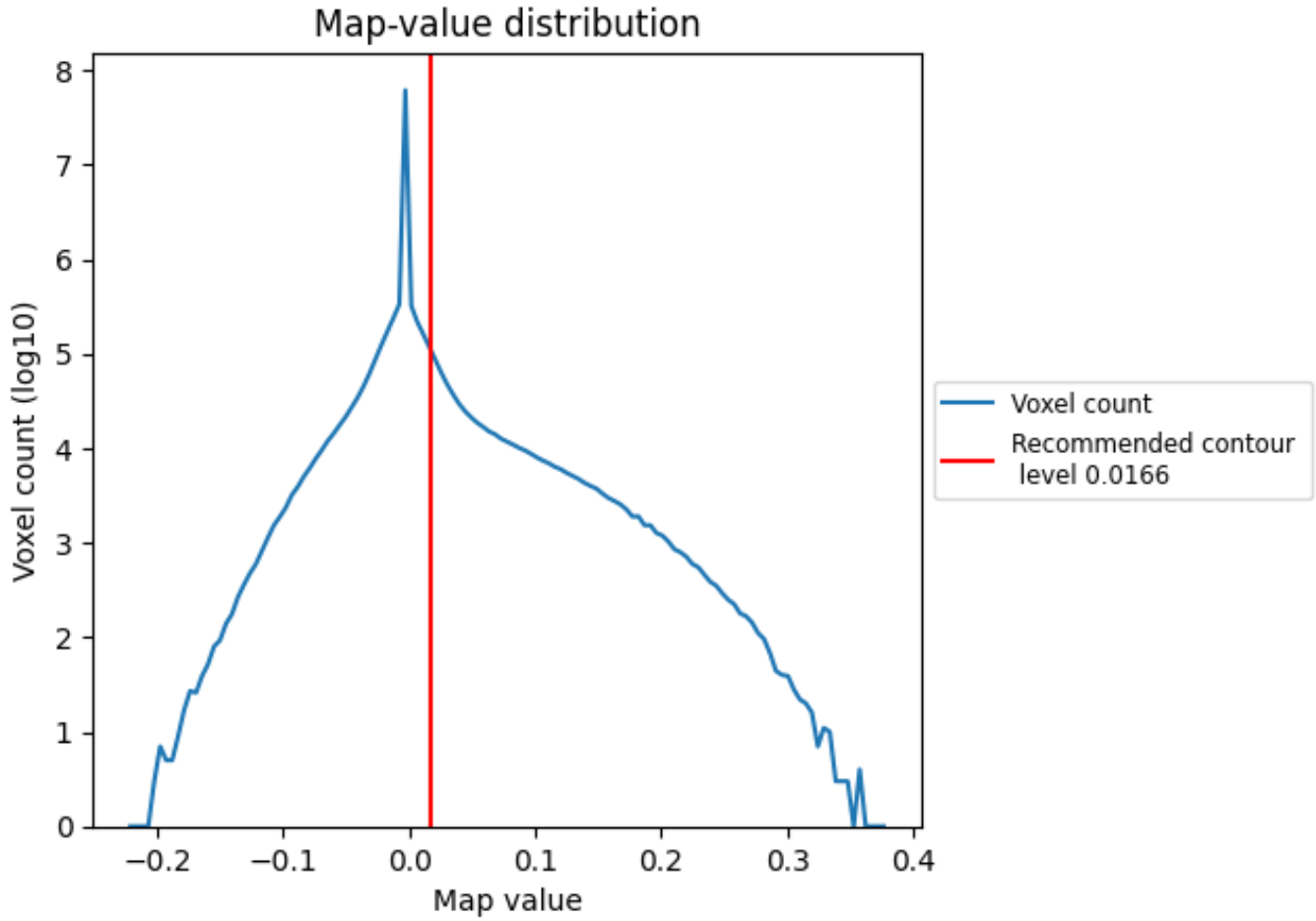
6.5 Mask visualisation (i)

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

7 Map analysis

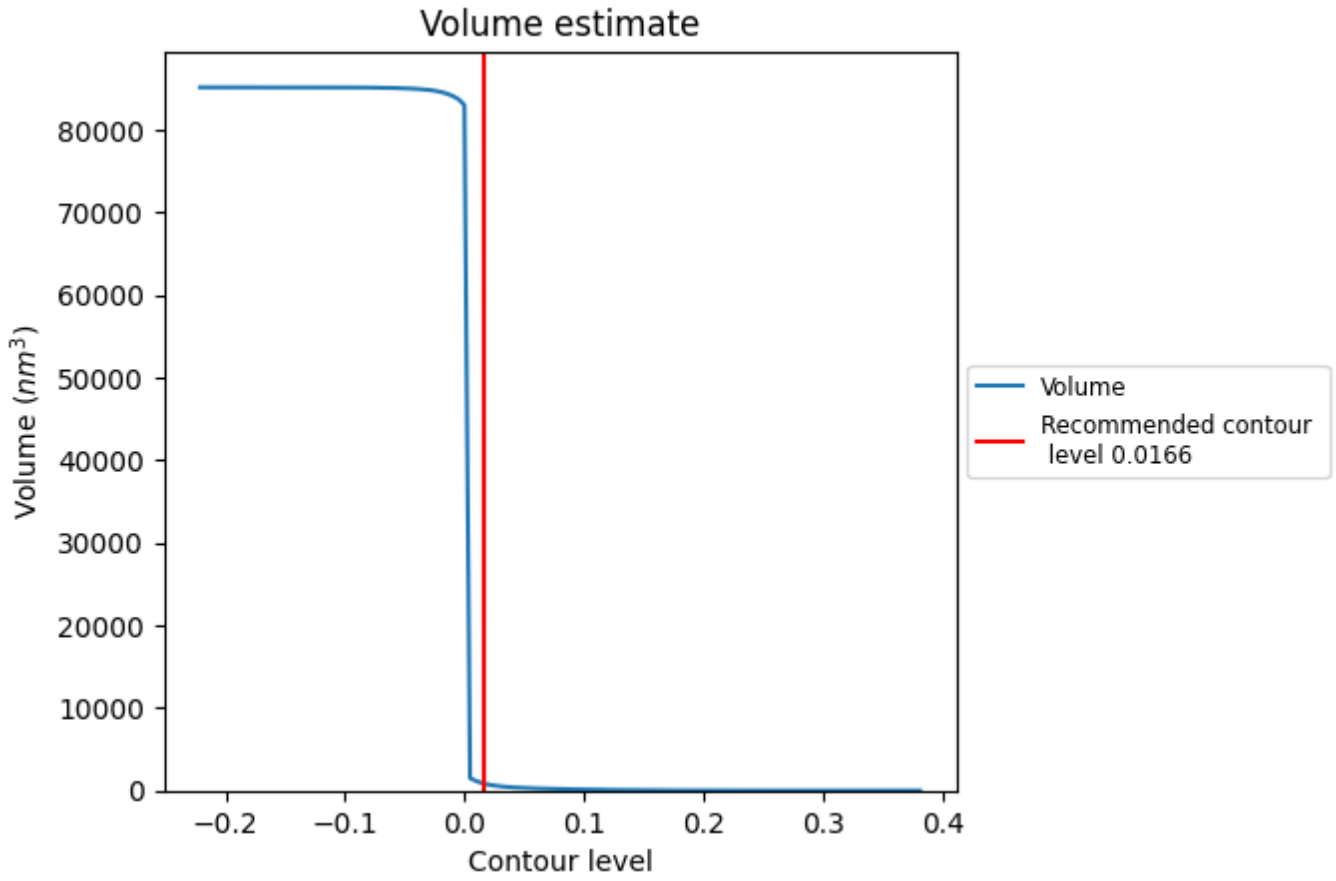
This section contains the results of statistical analysis of the map.

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.

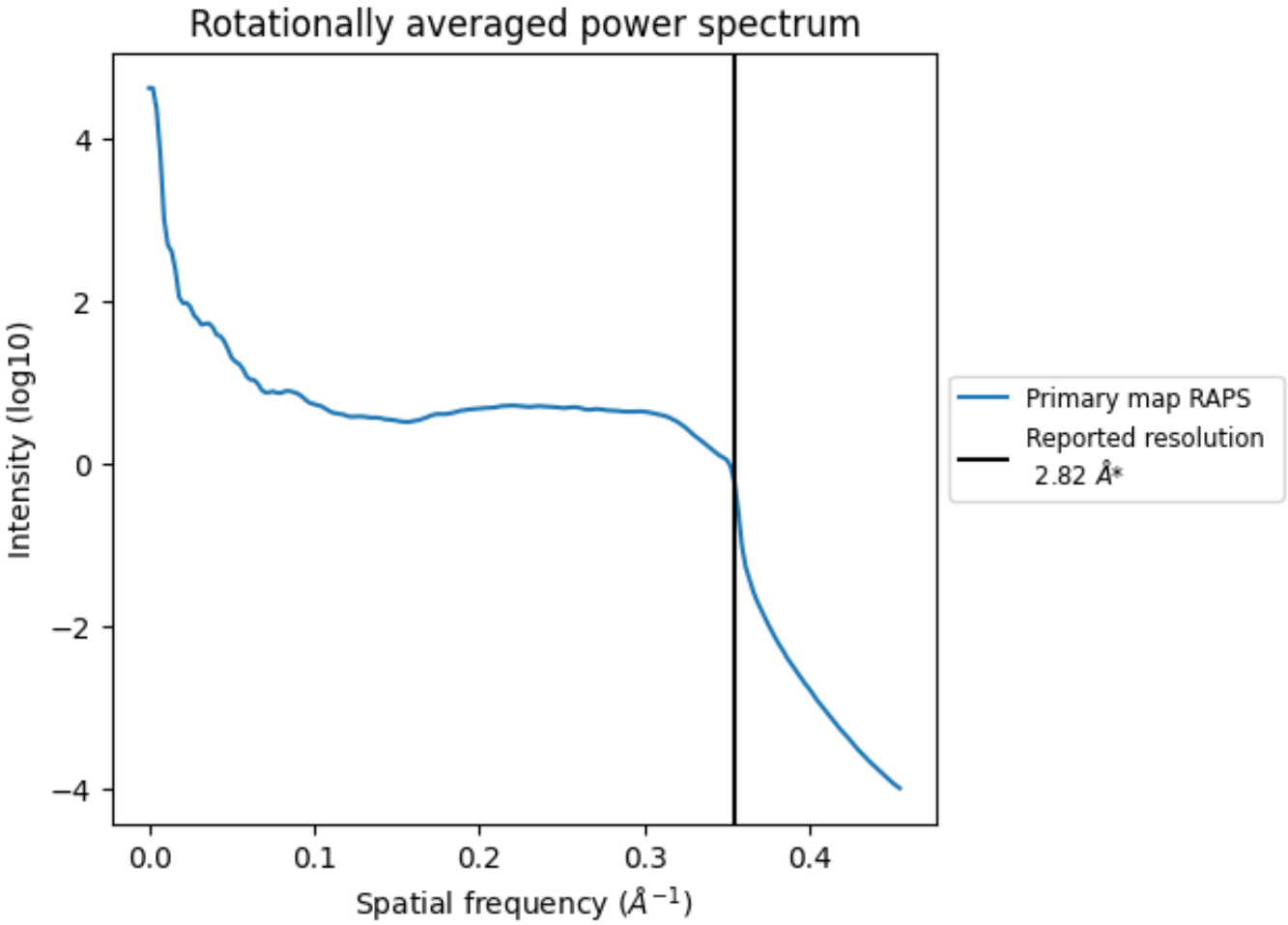
7.2 Volume estimate



The volume at the recommended contour level is 843 nm^3; this corresponds to an approximate mass of 761 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 0.355 $Å^{-1}$

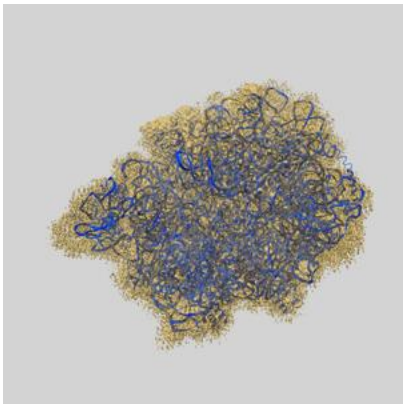
8 Fourier-Shell correlation

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

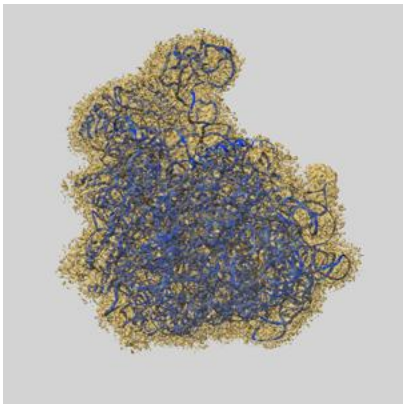
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10280 and PDB model 6SPB. Per-residue inclusion information can be found in section 3 on page 10.

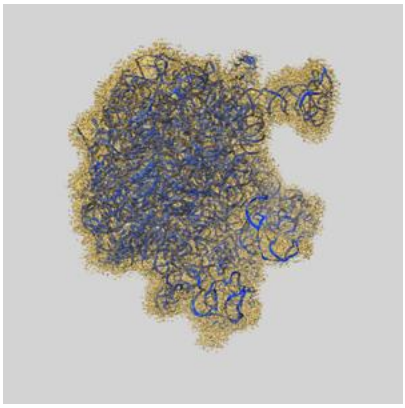
9.1 Map-model overlay



X



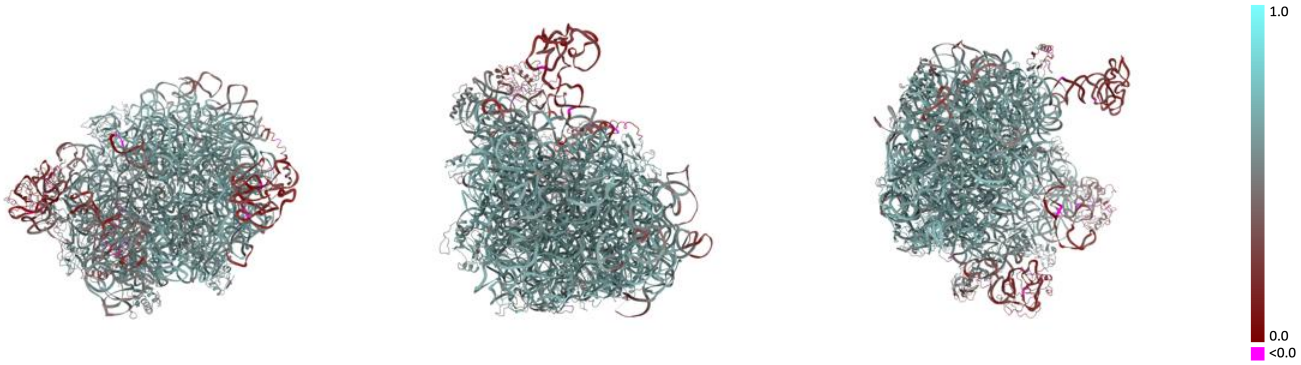
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0166 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.

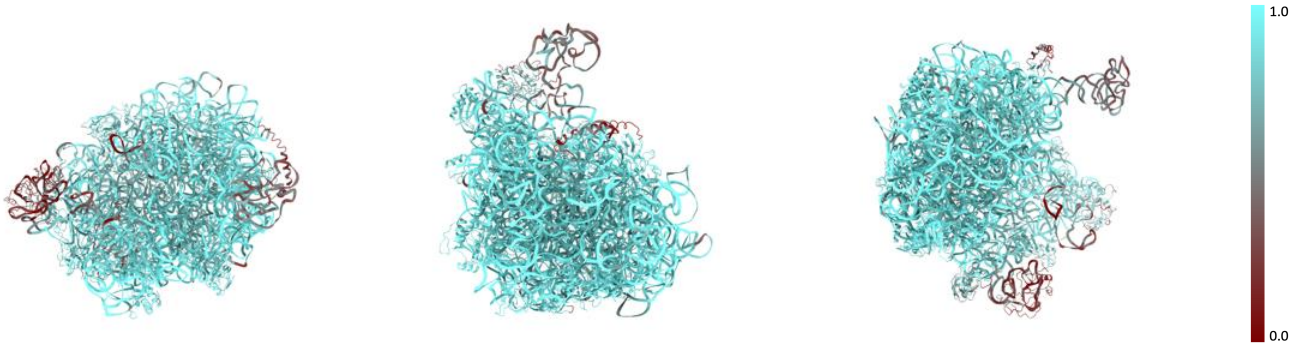
9.2 Q-score mapped to coordinate model (i)



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.

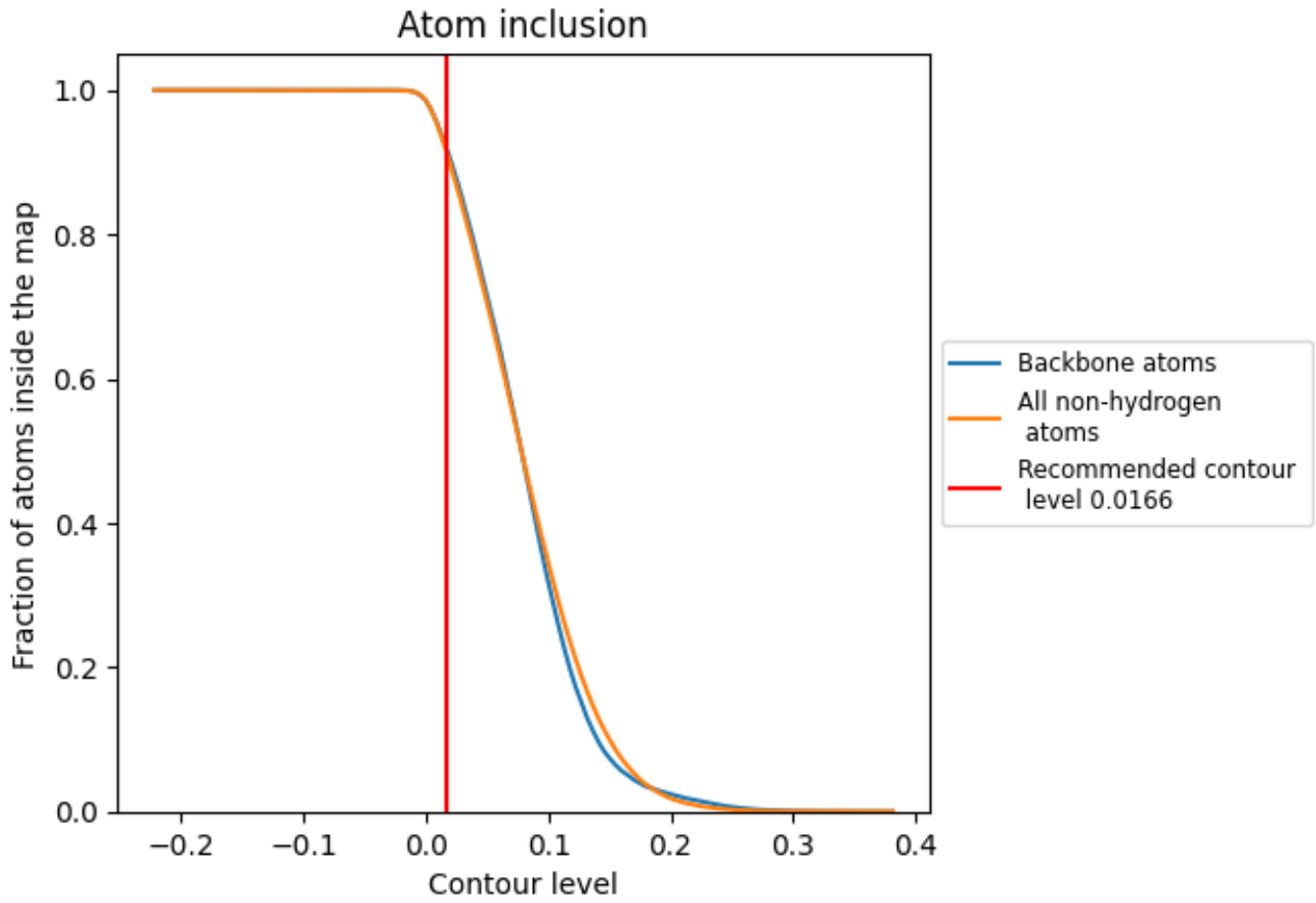
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0166).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.0166) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9169	0.5730
1	0.4891	0.0980
2	0.9314	0.5970
3	0.8256	0.5310
4	0.9738	0.6440
5	0.9367	0.6070
6	0.9343	0.5720
A	0.9354	0.5850
B	0.9695	0.5510
C	0.9586	0.6190
D	0.9543	0.6140
E	0.9579	0.6030
F	0.6456	0.2850
G	0.6392	0.4190
H	0.4701	0.3360
I	0.2189	0.1930
J	0.9672	0.6210
K	0.9253	0.5930
L	0.9464	0.5950
M	0.8926	0.5860
N	0.9758	0.6300
O	0.9096	0.5240
P	0.9284	0.5800
Q	0.9743	0.6300
R	0.9617	0.6110
S	0.9554	0.6230
T	0.9567	0.5980
U	0.8933	0.5320
V	0.8710	0.5240
W	0.9500	0.6010
X	0.9517	0.6190
Y	0.9454	0.5760
Z	0.9700	0.6190