



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 04:19 AM UTC

PDB ID : 9JPM / pdb_00009jpm
EMDB ID : EMD-61706
Title : Structure of the Bacterial Ribosome with human tRNA Lys(mcm5s2U34) and mRNA(AAA)
Authors : Ishiguro, K.; Mo, Y.; Shirouzu, M.; Suzuki, T.
Deposited on : 2024-09-26
Resolution : 2.43 Å(reported)
Based on initial model : 7y7e

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

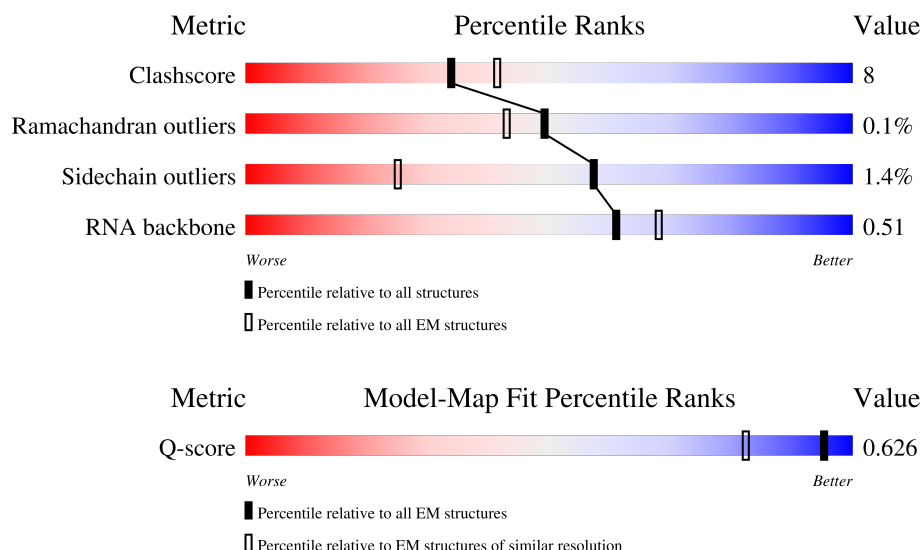
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.43 Å.

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




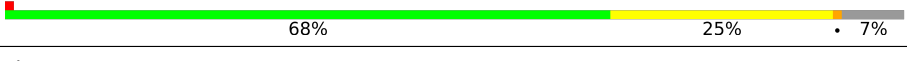
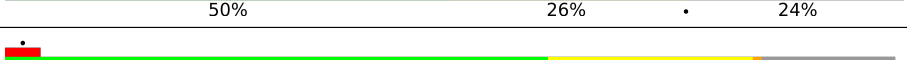
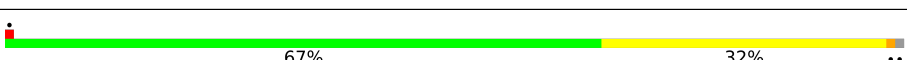
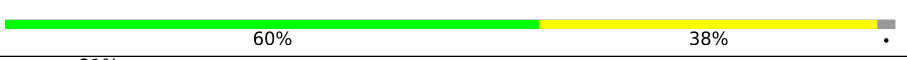

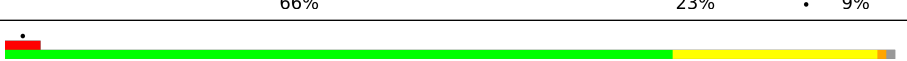
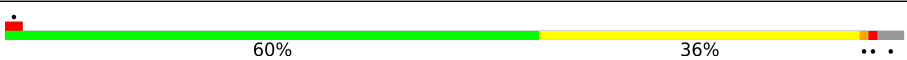
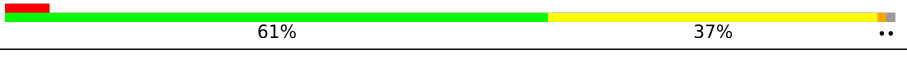

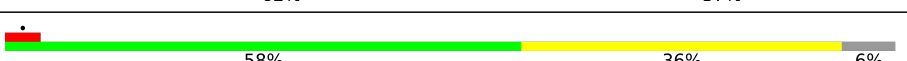


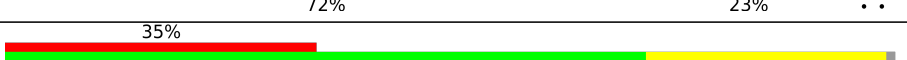
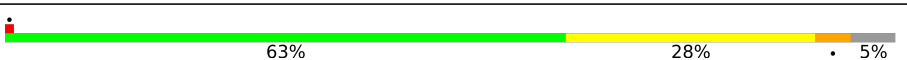




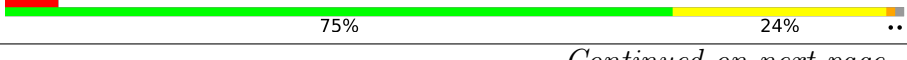



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5787 (1.94 - 2.93)

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

Mol	Chain	Length	Quality of chain
1	A	1542	
2	B	241	
3	C	233	


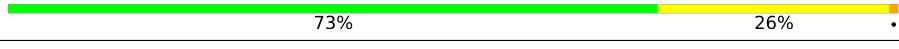
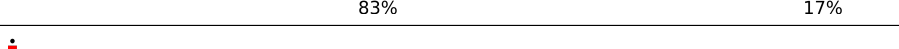
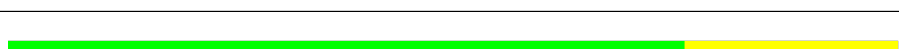



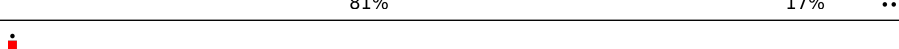



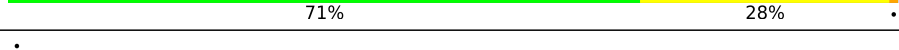
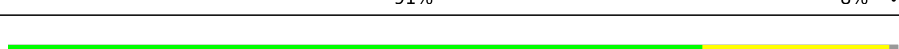
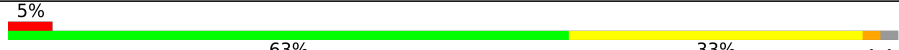


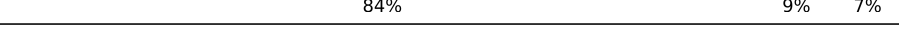







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Mol	Chain	Length	Quality of chain
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	

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Mol	Chain	Length	Quality of chain
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
46	y	59	
47	z	57	
48	0	55	
49	1	46	
50	2	65	
51	3	38	
52	4	70	
53	X	35	

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Mol	Chain	Length	Quality of chain
54	Z	77	<div><div></div><div>5%</div><div>62%</div><div>23%</div><div>14%</div></div>
55	V	76	<div><div></div><div>47%</div><div>33%</div><div>14%</div><div>• •</div></div>

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 141982 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0
			32466	14487	5964	10503	1512		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2761	Total	C	N	O	P	0	0
			59301	26460	10925	19155	2761		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

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

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	51	Total	C	N	O		0	0
			417	269	76	72			

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	11	Total	C	N	O	P	0	0
			233	105	41	76	11		

- Molecule 54 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Z	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 55 is a RNA chain called A-site tRNA-Lys.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	V	73	Total	C	N	O	P	S	0	0
			1579	712	279	514	72	2		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	83	Total	Mg	0
			83	83	
56	M	1	Total	Mg	0
			1	1	
56	a	292	Total	Mg	0
			292	292	
56	b	6	Total	Mg	0
			6	6	
56	d	1	Total	Mg	0
			1	1	
56	p	1	Total	Mg	0
			1	1	
56	z	1	Total	Mg	0
			1	1	
56	X	1	Total	Mg	0
			1	1	
56	Z	4	Total	Mg	0
			4	4	
56	V	1	Total	Mg	0
			1	1	

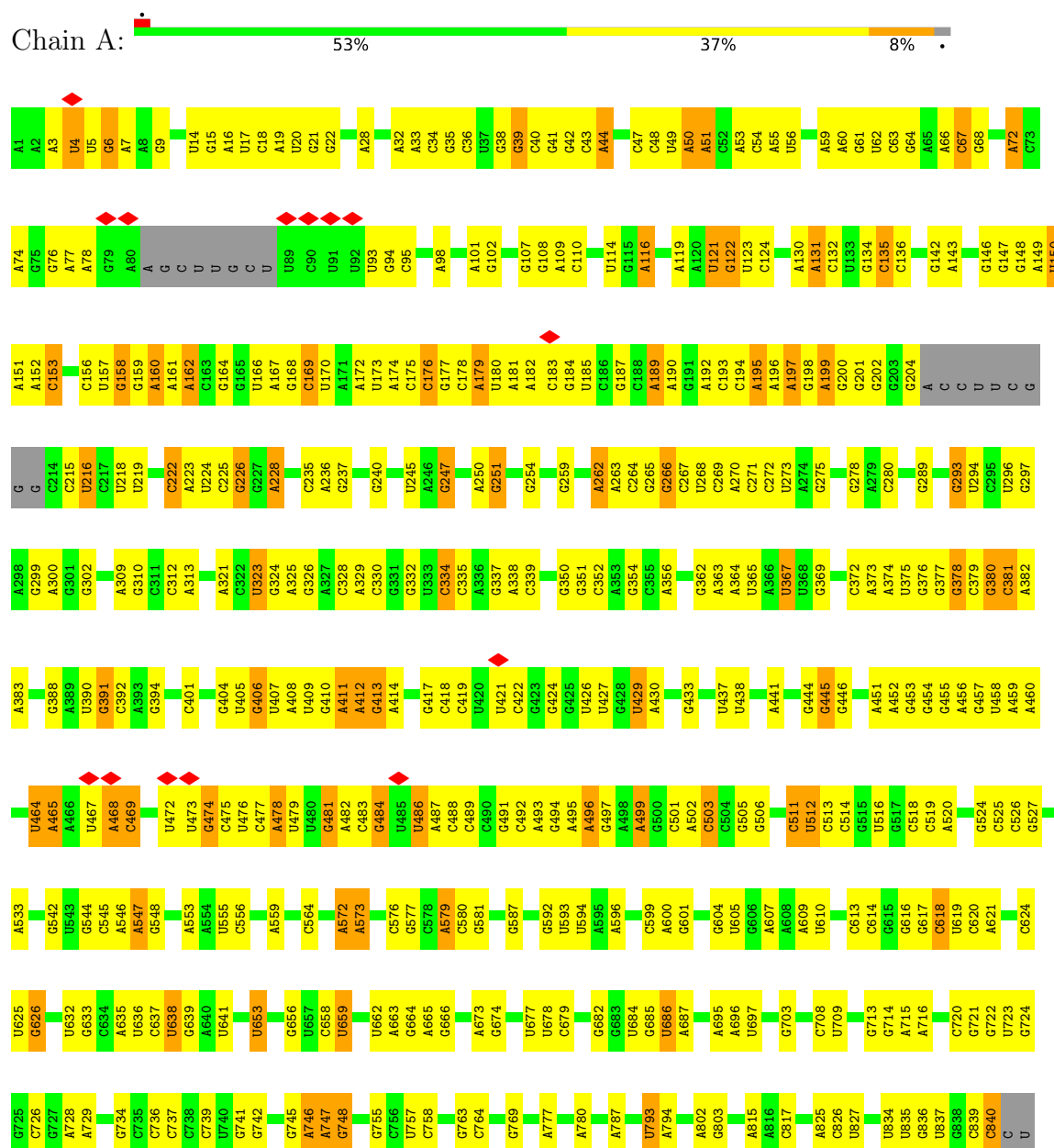
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

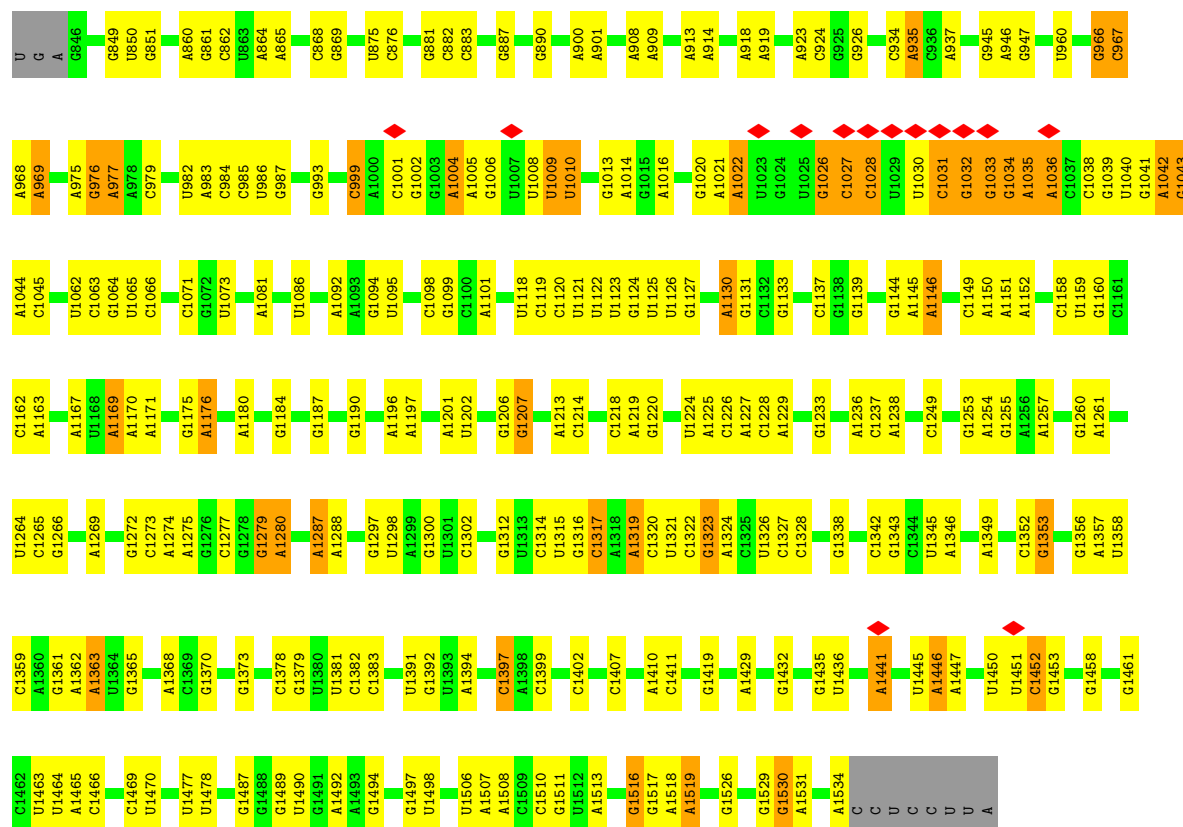
Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

3 Residue-property plots

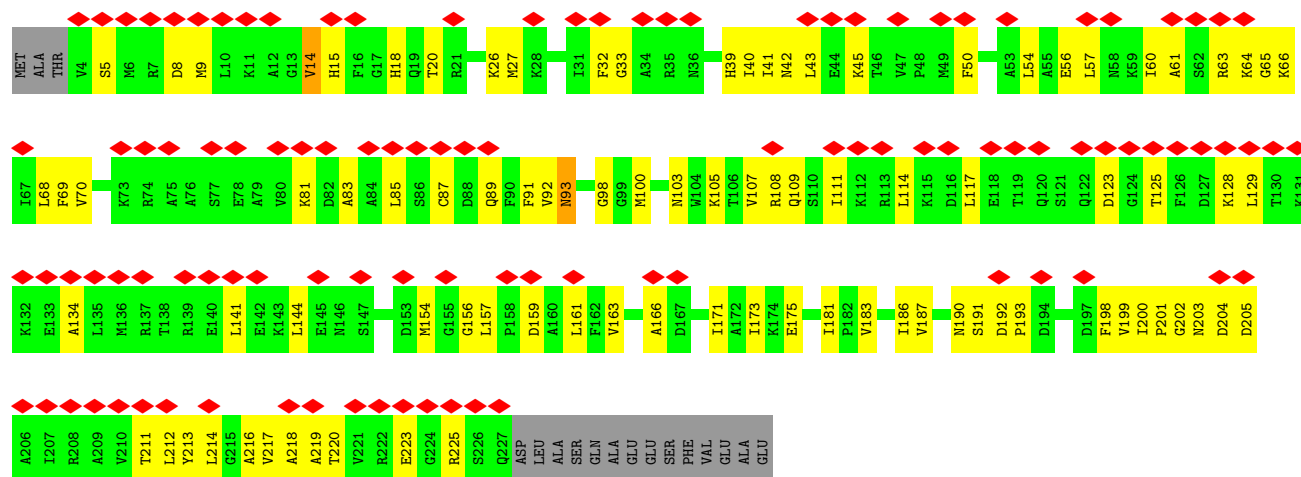
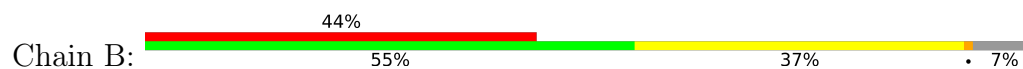
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

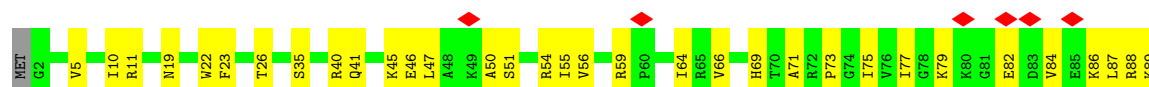


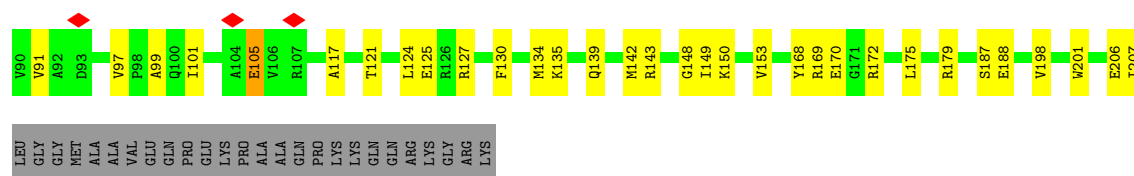


• Molecule 2: 30S ribosomal protein S2

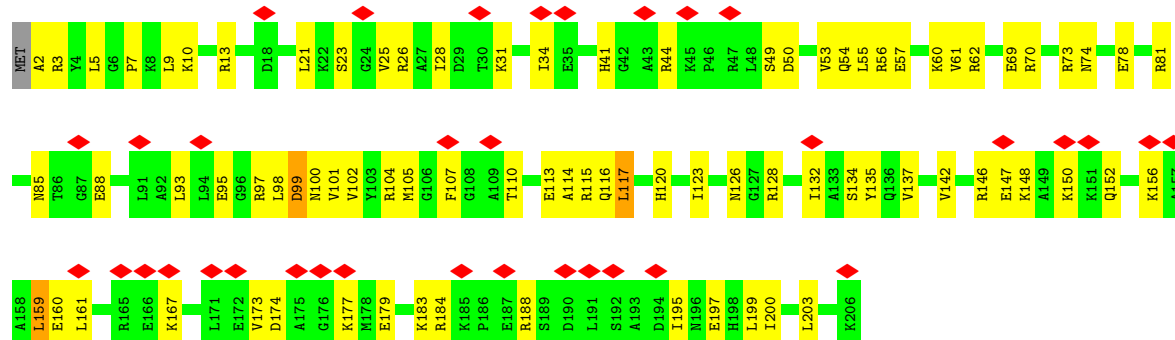


• Molecule 3: 30S ribosomal protein S3

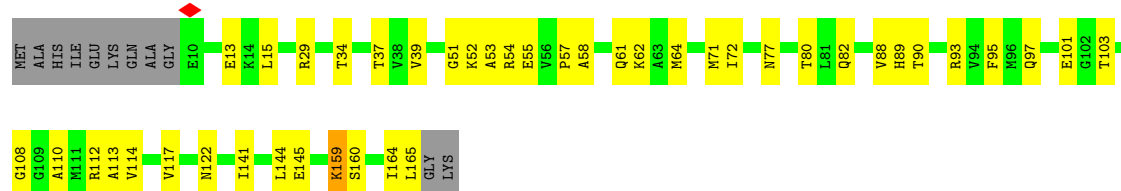




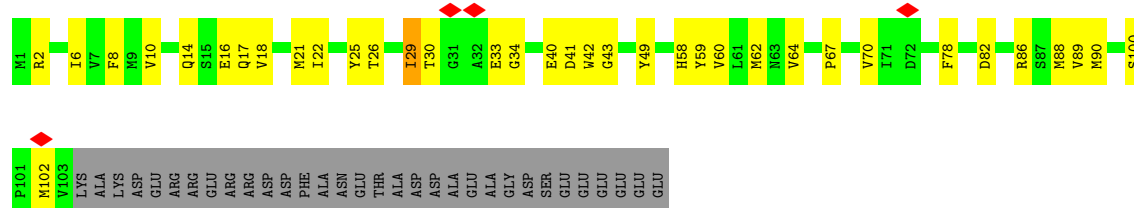
• Molecule 4: 30S ribosomal protein S4



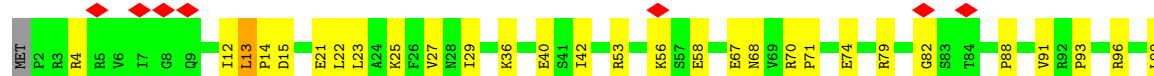
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6, fully modified isoform



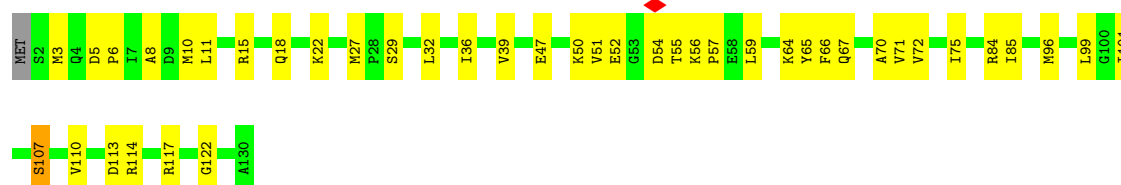
• Molecule 7: 30S ribosomal protein S7





- Molecule 8: 30S ribosomal protein S8

Chain H: 67% 32%



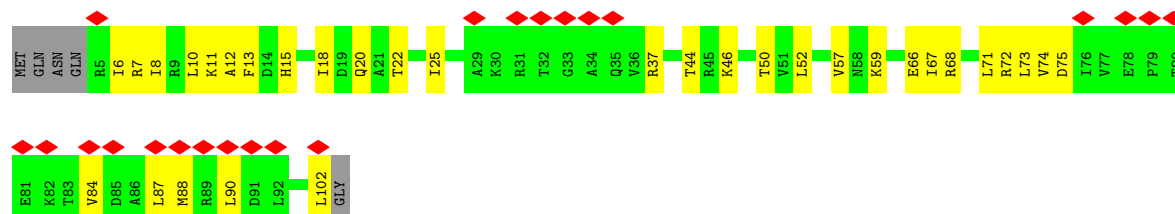
- Molecule 9: 30S ribosomal protein S9

Chain I: 60% 38%



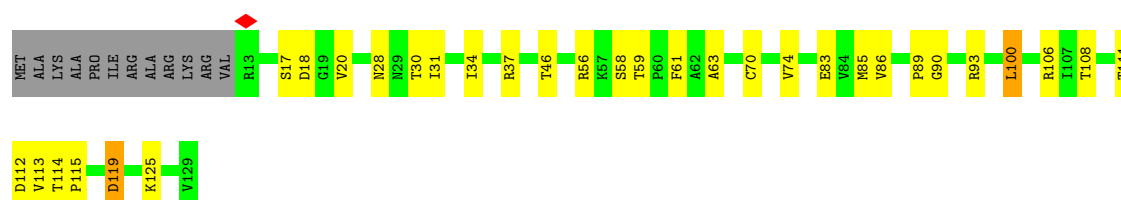
- Molecule 10: 30S ribosomal protein S10

Chain J: 21% 64% 31% 5%



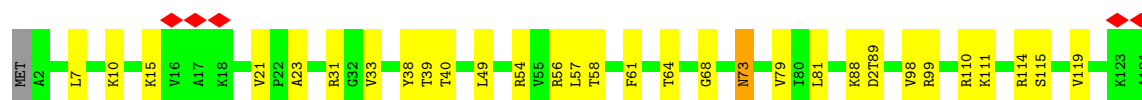
- Molecule 11: 30S ribosomal protein S11

Chain K: 66% 23% 9%

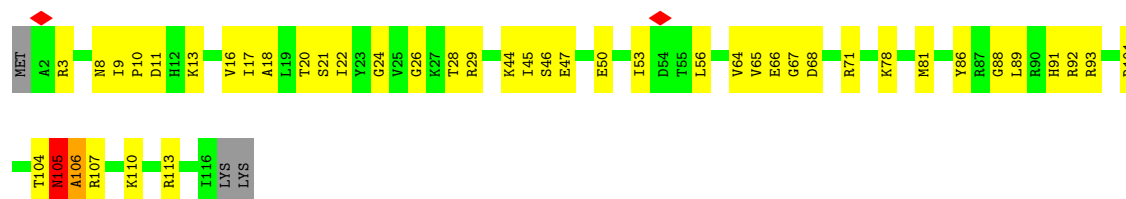


- Molecule 12: 30S ribosomal protein S12

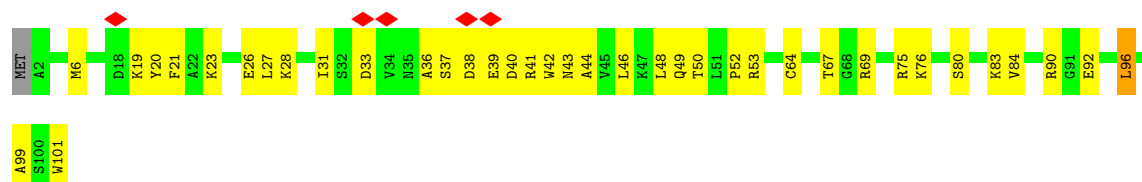
Chain L: 75% 23%



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



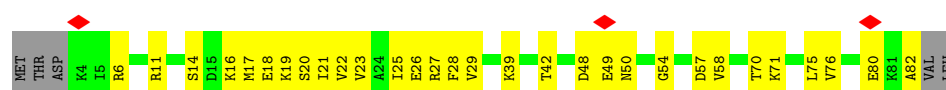
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



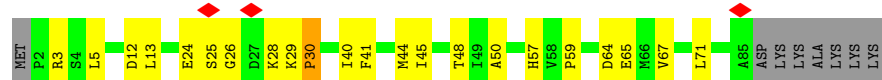
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



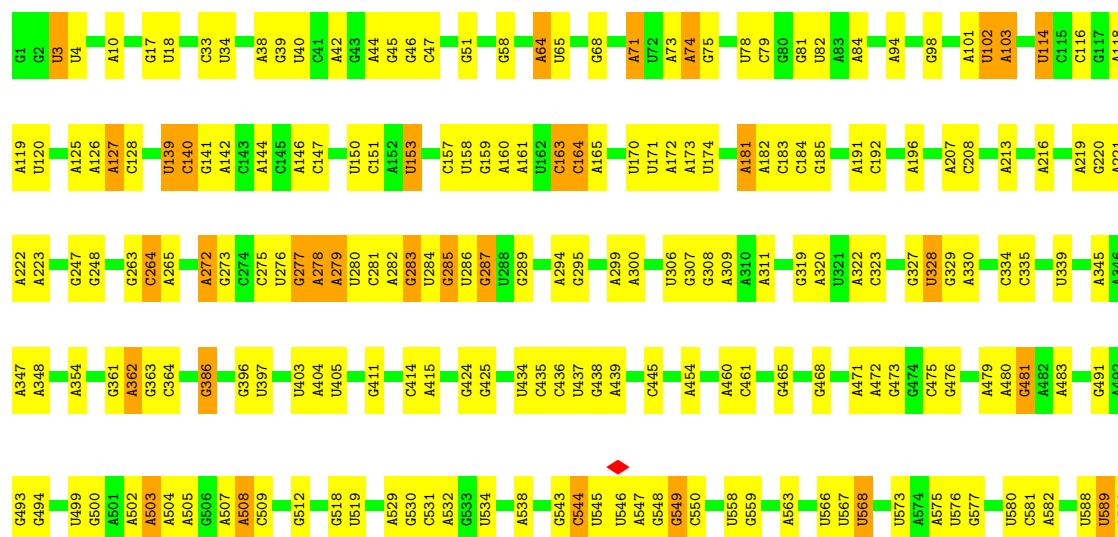
- Molecule 20: 30S ribosomal protein S20



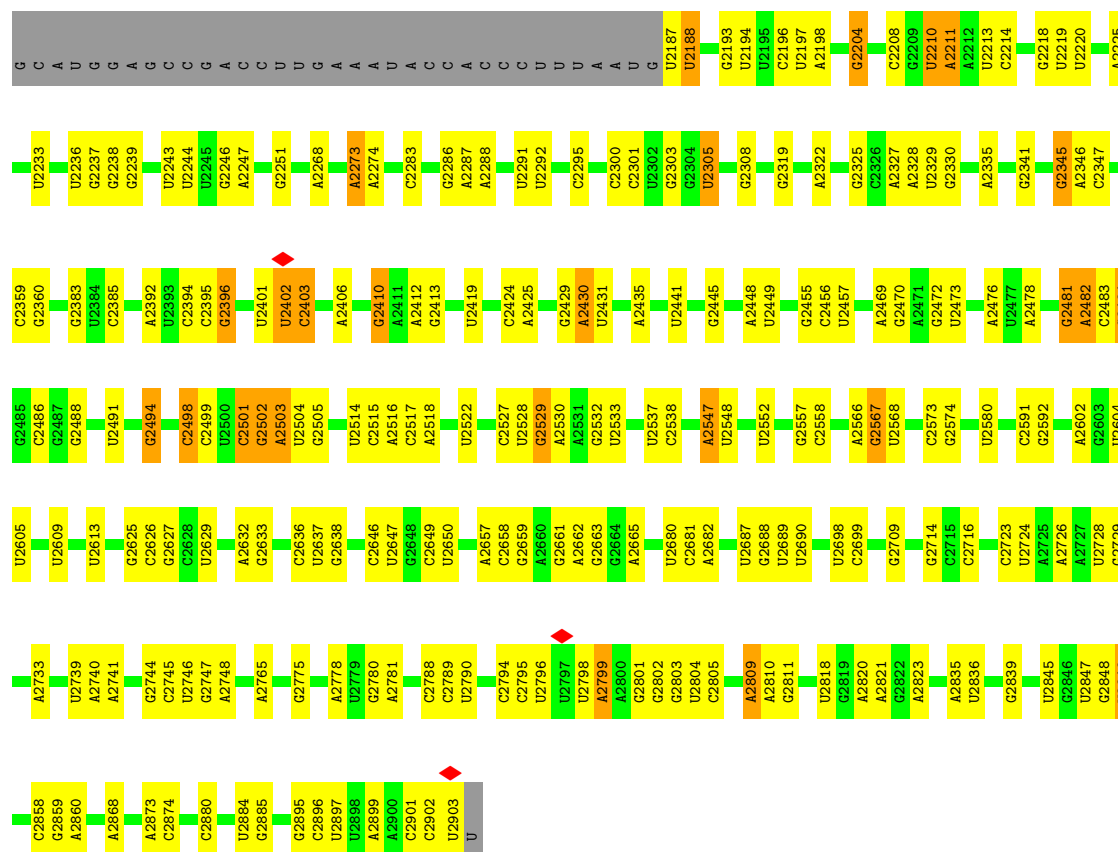
- Molecule 21: 30S ribosomal protein S21



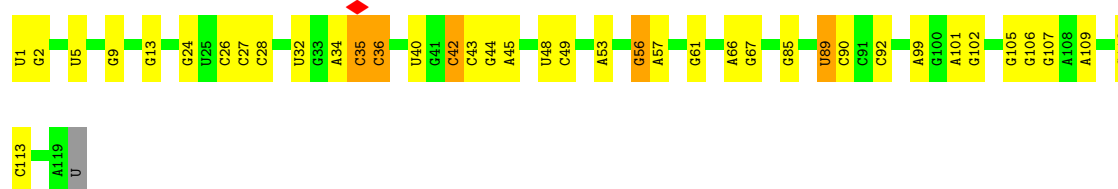
- Molecule 22: 23S rRNA



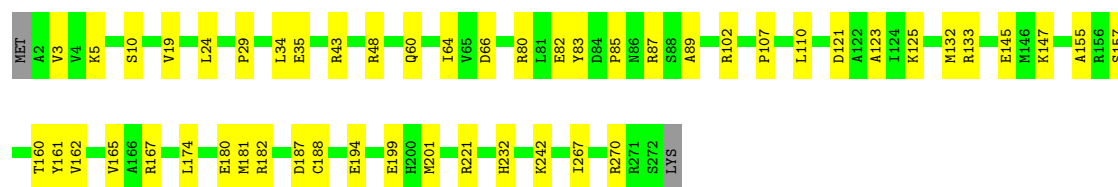
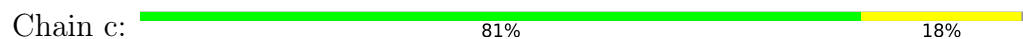




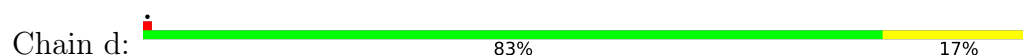
• Molecule 23: 5S rRNA



• Molecule 24: 50S ribosomal protein L2



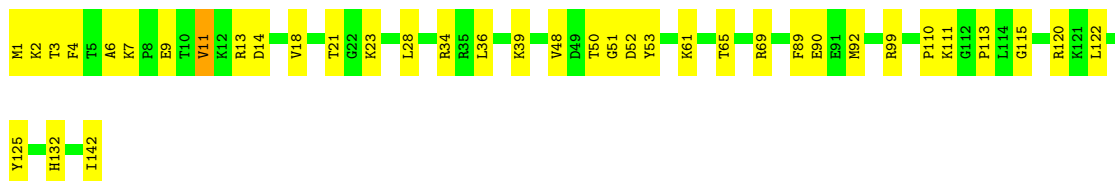
• Molecule 25: 50S ribosomal protein L3




VAL
PHE
ALA
LYS
VAL
ILE
VAL
ASN
VAL
ALA
GLU

• Molecule 30: 50S ribosomal protein L13

Chain i:  73% 26%




• Molecule 31: 50S ribosomal protein L14

Chain j:  83% 17%



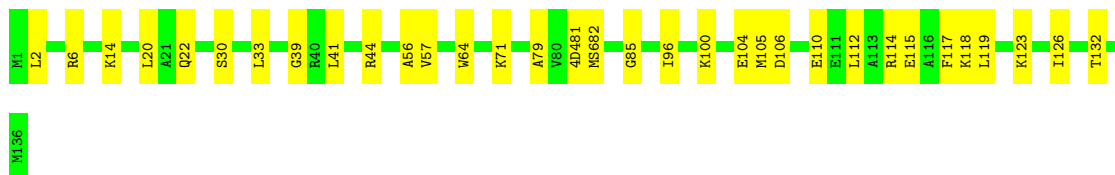
• Molecule 32: 50S ribosomal protein L15

Chain k:  83% 17%




• Molecule 33: 50S ribosomal protein L16

Chain l:  76% 24%




• Molecule 34: 50S ribosomal protein L17

Chain m:  84% 9% 7%

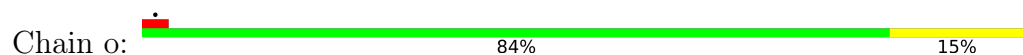


• Molecule 35: 50S ribosomal protein L18

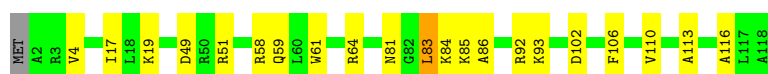
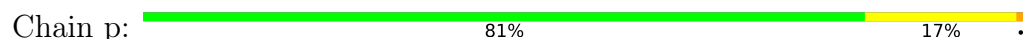
Chain n:  79% 20%



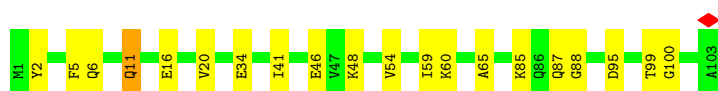
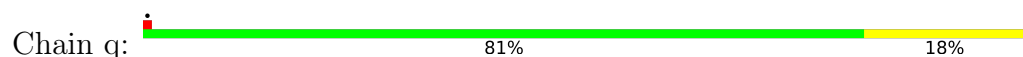
- Molecule 36: 50S ribosomal protein L19



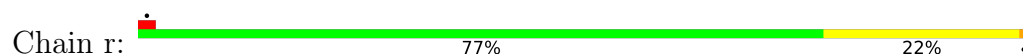
- Molecule 37: 50S ribosomal protein L20



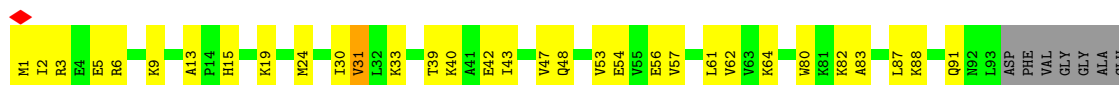
- Molecule 38: 50S ribosomal protein L21



- Molecule 39: 50S ribosomal protein L22



- Molecule 40: 50S ribosomal protein L23

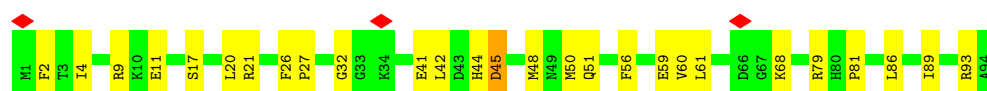


- Molecule 41: 50S ribosomal protein L24




- Molecule 42: 50S ribosomal protein L25

Chain u:  71% 28%




- Molecule 43: 50S ribosomal protein L27

Chain v:  91% 8%



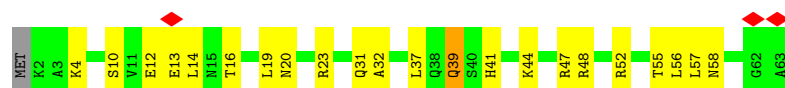
- Molecule 44: 50S ribosomal protein L28

Chain w:  78% 21%




- Molecule 45: 50S ribosomal protein L29

Chain x:  5% 63% 33%



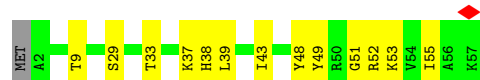
- Molecule 46: 50S ribosomal protein L30

Chain y:  83% 15%




- Molecule 47: 50S ribosomal protein L32

Chain z:  75% 23%



- Molecule 48: 50S ribosomal protein L33

Chain 0:  84% 9% 7%




- Molecule 49: 50S ribosomal protein L34

Chain 1:  91% 9%



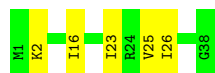
- Molecule 50: 50S ribosomal protein L35

Chain 2:  86% 11% ..



- Molecule 51: 50S ribosomal protein L36

Chain 3:  87% 13%



- Molecule 52: 50S ribosomal protein L31

Chain 4:  10% 51% 34% 14%



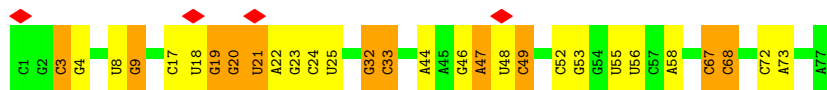
- Molecule 53: mRNA

Chain X:  31% 69%



- Molecule 54: P-site tRNA-fMet

Chain Z:  5% 62% 23% 14%



- Molecule 55: A-site tRNA-Lys

Chain V:  47% 33% 14% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	423074	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.059	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0107	Depositor
Map size (Å)	439.10498, 439.10498, 439.10498	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8285, 0.8285, 0.8285	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 6MZ, 1MA, G7M, UR3, MG, 2MU, 3TD, 4SU, MEQ, OMC, 2MG, 2MA, PSU, H2U, 1MG, IAS, MS6, D2T, OMG, 70U, 12A, 4OC, OMU, 4D4, ZN, 5MC, 5MU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/36073	0.46	0/56264
2	B	0.28	0/1784	0.51	0/2403
3	C	0.41	0/1651	0.53	0/2225
4	D	0.31	0/1665	0.50	0/2227
5	E	0.45	0/1165	0.55	0/1568
6	F	0.38	0/858	0.57	0/1160
7	G	0.35	0/1219	0.48	0/1635
8	H	0.42	0/989	0.49	0/1326
9	I	0.41	0/1034	0.57	0/1375
10	J	0.42	0/796	0.65	0/1077
11	K	0.44	0/884	0.58	0/1191
12	L	0.41	0/960	0.52	0/1286
13	M	0.39	0/900	0.56	0/1204
14	N	0.44	0/817	0.56	0/1088
15	O	0.42	0/722	0.54	0/964
16	P	0.32	0/653	0.56	0/877
17	Q	0.34	0/650	0.49	0/871
18	R	0.41	0/553	0.54	0/742
19	S	0.42	0/685	0.68	3/922 (0.3%)
20	T	0.36	0/676	0.48	0/895
21	U	0.30	0/597	0.50	0/792
22	a	0.65	0/65842	0.48	2/102711 (0.0%)
23	b	0.49	0/2850	0.41	0/4444
24	c	0.53	0/2121	0.55	0/2852
25	d	0.51	0/1576	0.53	0/2119
26	e	0.45	0/1571	0.48	0/2113
27	f	0.36	0/1434	0.49	0/1926
28	g	0.34	0/1343	0.51	0/1816
29	h	0.39	0/306	0.59	0/413
30	i	0.51	0/1152	0.51	0/1551
31	j	0.51	0/955	0.52	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	k	0.49	0/1062	0.57	0/1413
33	l	0.52	0/1073	0.60	1/1433 (0.1%)
34	m	0.53	0/958	0.55	0/1281
35	n	0.38	0/902	0.53	0/1209
36	o	0.48	0/929	0.51	0/1242
37	p	0.56	0/960	0.54	0/1278
38	q	0.49	0/829	0.53	0/1107
39	r	0.54	0/864	0.54	0/1156
40	s	0.42	0/744	0.56	0/994
41	t	0.40	0/787	0.58	0/1051
42	u	0.42	0/766	0.52	0/1025
43	v	0.49	0/642	0.51	0/848
44	w	0.48	0/635	0.56	0/848
45	x	0.39	0/502	0.53	0/667
46	y	0.47	0/453	0.54	0/605
47	z	0.51	0/450	0.53	0/599
48	0	0.45	0/424	0.52	0/565
49	1	0.51	0/380	0.56	0/498
50	2	0.54	0/513	0.51	0/676
51	3	0.51	0/303	0.56	0/397
52	4	0.31	0/488	0.54	1/649 (0.2%)
53	X	0.52	0/260	0.37	0/402
54	Z	0.44	0/1725	0.42	0/2687
55	V	0.37	0/1429	0.41	0/2217
All	All	0.55	0/152559	0.49	7/228163 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	2
50	2	0	1
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	59	PRO	CA-N-CD	-8.28	100.41	112.00
19	S	59	PRO	N-CD-CG	-7.45	92.02	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	512	G	O4'-C1'-N9	6.18	117.47	108.20
22	a	2501	C	C4'-C3'-O3'	6.13	118.60	109.40
52	4	5	ILE	N-CA-C	-5.69	108.30	113.71
19	S	30	PRO	CA-N-CD	-5.12	104.83	112.00
33	l	85	GLY	CA-C-O	-5.10	118.49	122.52

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	31	HIS	Peptide
13	M	105	ASN	Peptide
13	M	65	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32466	0	16359	483	0
2	B	1753	0	1780	75	0
3	C	1624	0	1696	42	0
4	D	1643	0	1707	74	0
5	E	1152	0	1196	30	0
6	F	839	0	833	34	0
7	G	1203	0	1254	31	0
8	H	979	0	1031	29	0
9	I	1022	0	1070	39	0
10	J	786	0	828	24	0
11	K	877	0	884	24	0
12	L	957	0	1017	24	0
13	M	891	0	952	36	0
14	N	805	0	844	33	0
15	O	714	0	734	18	0
16	P	643	0	661	24	0
17	Q	641	0	682	23	0
18	R	544	0	565	18	0
19	S	668	0	693	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	670	0	719	20	0
21	U	589	0	629	15	0
22	a	59301	0	29849	481	0
23	b	2549	0	1291	18	0
24	c	2082	0	2154	36	0
25	d	1566	0	1618	23	0
26	e	1552	0	1619	23	0
27	f	1410	0	1444	33	0
28	g	1323	0	1371	31	0
29	h	303	0	327	10	0
30	i	1129	0	1162	26	0
31	j	946	0	1023	13	0
32	k	1053	0	1129	20	0
33	l	1075	0	1144	19	0
34	m	945	0	989	8	0
35	n	892	0	923	16	0
36	o	917	0	962	13	0
37	p	947	0	1019	16	0
38	q	816	0	839	11	0
39	r	857	0	922	15	0
40	s	738	0	807	26	0
41	t	779	0	831	24	0
42	u	753	0	780	22	0
43	v	634	0	653	6	0
44	w	625	0	652	11	0
45	x	501	0	531	22	0
46	y	449	0	488	6	0
47	z	444	0	458	9	0
48	0	417	0	451	2	0
49	1	377	0	418	3	0
50	2	504	0	572	6	0
51	3	302	0	340	4	0
52	4	480	0	478	20	0
53	X	233	0	118	0	0
54	Z	1645	0	842	12	0
55	V	1579	0	820	20	0
56	A	83	0	0	0	0
56	M	1	0	0	0	0
56	V	1	0	0	0	0
56	X	1	0	0	0	0
56	Z	4	0	0	0	0
56	a	292	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	b	6	0	0	0	0
56	d	1	0	0	0	0
56	p	1	0	0	0	0
56	z	1	0	0	0	0
57	3	1	0	0	0	0
57	4	1	0	0	0	0
All	All	141982	0	95158	1922	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1922) 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:417:G:H1	1:A:426:U:H3	1.11	0.99
41:t:47:LYS:HD2	41:t:48:PRO:HD2	1.47	0.96
25:d:5:VAL:H	25:d:32:ASN:HD21	1.14	0.94
1:A:409:U:H3	1:A:433:G:H1	1.10	0.93
28:g:104:ASN:ND2	28:g:114:ASP:OD1	2.03	0.92
1:A:836:G:H1	1:A:850:U:H3	1.13	0.90
1:A:1028:C:N4	1:A:1033:G:O6	2.07	0.88
7:G:93:PRO:HA	7:G:96:ARG:HG3	1.57	0.87
22:a:1607:C:N4	22:a:1622:G:OP2	2.09	0.86
22:a:153:U:OP1	44:w:77:LYS:NZ	2.09	0.85
1:A:441:A:H61	1:A:493:A:H61	1.25	0.85
1:A:1530:G:N7	21:U:46:LYS:NZ	2.25	0.85
6:F:42:TRP:HZ3	6:F:102:MET:HE3	1.42	0.84
35:n:56:LYS:NZ	35:n:60:GLU:OE1	2.11	0.84
52:4:20:ASN:ND2	52:4:37:CYS:SG	2.51	0.83
6:F:88:MET:HE1	18:R:61:ARG:HG2	1.60	0.82
14:N:49:GLN:NE2	19:S:12:ASP:OD1	2.11	0.82
3:C:11:ARG:NH2	3:C:175:LEU:O	2.12	0.81
11:K:93:ARG:NH2	11:K:112:ASP:OD2	2.14	0.81
3:C:54:ARG:HB3	3:C:69:HIS:HB2	1.61	0.80
14:N:46:LEU:HD22	19:S:13:LEU:HD13	1.63	0.80
14:N:23:LYS:NZ	14:N:26:GLU:OE1	2.14	0.80
12:L:54:ARG:NH1	12:L:64:THR:OG1	2.15	0.80
22:a:881:G:N2	22:a:895:U:O2	2.12	0.79
5:E:39:VAL:HG13	5:E:71:MET:HE3	1.64	0.79
1:A:619:U:H4'	4:D:128:ARG:HH21	1.48	0.78
13:M:11:ASP:OD2	13:M:46:SER:OG	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:10:VAL:HA	28:g:49:THR:HG22	1.65	0.78
1:A:1027:C:H2'	1:A:1028:C:C6	2.18	0.78
33:l:30:SER:OG	33:l:106:ASP:OD1	2.02	0.78
22:a:2478:A:OP2	51:3:2:LYS:NZ	2.14	0.78
18:R:71:THR:HG23	18:R:73:ARG:H	1.48	0.78
35:n:99:TYR:OH	35:n:111:ARG:NH1	2.17	0.77
1:A:1013:G:N2	1:A:1016:A:OP2	2.17	0.77
19:S:30:PRO:HB3	19:S:48:THR:HG22	1.66	0.77
2:B:60:ILE:HA	2:B:63:ARG:HG2	1.66	0.77
14:N:39:GLU:O	14:N:43:ASN:ND2	2.17	0.77
22:a:1864:U:OP1	22:a:2410:G:O2'	2.03	0.77
30:i:125:TYR:OH	30:i:132:HIS:NE2	2.17	0.77
42:u:20:LEU:HD21	42:u:41:GLU:HG2	1.67	0.76
4:D:102:VAL:HG13	4:D:114:ALA:HB1	1.67	0.76
26:e:170:ARG:NH2	26:e:176:ASP:OD2	2.18	0.76
42:u:79:ARG:HG2	42:u:79:ARG:HH11	1.50	0.76
16:P:4:ILE:HG13	16:P:21:VAL:HG22	1.67	0.75
4:D:54:GLN:HB3	4:D:203:LEU:HD12	1.69	0.75
1:A:1229:A:OP2	13:M:113:ARG:NH1	2.20	0.75
4:D:98:LEU:HB2	4:D:135:TYR:HB3	1.67	0.75
21:U:51:SER:HA	21:U:54:LYS:HE2	1.67	0.74
22:a:870:U:OP1	33:l:6:ARG:NH2	2.20	0.74
52:4:28:VAL:HG11	52:4:32:LEU:HD11	1.68	0.74
1:A:411:A:OP1	4:D:26:ARG:NH1	2.20	0.74
44:w:72:ARG:NH1	44:w:78:TYR:OH	2.19	0.74
1:A:404:G:O6	4:D:2:ALA:N	2.20	0.74
6:F:42:TRP:CZ3	6:F:102:MET:HE3	2.23	0.74
22:a:299:A:N1	22:a:322:A:O2'	2.19	0.74
22:a:545:U:HO2'	22:a:548:G:H1	1.32	0.74
17:Q:19:LYS:HZ3	17:Q:50:ASN:H	1.35	0.73
3:C:168:TYR:OH	5:E:55:GLU:OE1	2.03	0.73
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.21	0.73
1:A:664:G:H22	1:A:741:G:H1	1.34	0.73
22:a:1365:A:OP1	44:w:3:ARG:NH2	2.20	0.73
4:D:97:ARG:HE	4:D:134:SER:HA	1.53	0.73
22:a:1047:G:HO2'	22:a:1110:G:H1	1.36	0.73
55:V:10:2MG:N2	55:V:25:C:O2	2.15	0.73
1:A:600:A:H2'	1:A:601:G:C8	2.24	0.73
2:B:15:HIS:HB3	2:B:43:LEU:HD21	1.70	0.73
1:A:180:U:H3	1:A:195:A:H62	1.34	0.73
36:o:89:ARG:NH1	36:o:113:ARG:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:C:OP1	4:D:81:ARG:NH2	2.20	0.73
39:r:31:GLN:O	39:r:35:ILE:HG13	1.89	0.73
3:C:130:PHE:O	3:C:134:MET:HG3	1.89	0.72
33:l:33:LEU:HD13	33:l:117:PHE:HB3	1.69	0.72
41:t:6:ARG:N	41:t:9:ASP:OD2	2.15	0.72
14:N:90:ARG:HB3	14:N:92:GLU:OE2	1.89	0.72
22:a:1434:A:H2'	22:a:1435:G:C8	2.24	0.72
11:K:20:VAL:HG12	11:K:83:GLU:HB2	1.72	0.72
1:A:618:C:N4	1:A:621:A:OP2	2.22	0.72
3:C:46:GLU:HG2	3:C:87:LEU:HD21	1.72	0.72
1:A:677:U:H3	1:A:713:G:H22	1.37	0.71
6:F:40:GLU:OE1	6:F:100:SER:OG	2.06	0.71
22:a:2102:G:O6	22:a:2187:U:O4	2.08	0.71
1:A:28:A:O2'	1:A:296:U:OP1	2.06	0.71
4:D:62:ARG:NH1	4:D:69:GLU:OE1	2.23	0.71
1:A:339:C:OP2	31:j:98:ARG:NH1	2.24	0.71
1:A:673:A:H2'	1:A:674:G:C8	2.26	0.71
10:J:15:HIS:HA	10:J:18:ILE:HG22	1.73	0.71
1:A:937:A:N6	1:A:1345:U:O4	2.23	0.71
2:B:186:ILE:HD13	2:B:200:ILE:HB	1.73	0.71
24:c:132:MET:HE1	24:c:174:LEU:HD21	1.72	0.71
1:A:147:G:H2'	1:A:148:G:C8	2.25	0.71
5:E:37:THR:HG21	5:E:64:MET:HE2	1.73	0.71
22:a:1800:C:OP2	24:c:182:ARG:NH1	2.24	0.71
22:a:2052:A:H4'	25:d:148:GLN:O	1.91	0.71
3:C:135:LYS:O	3:C:139:GLN:NE2	2.24	0.71
13:M:101:ARG:HE	13:M:104:THR:HG1	1.36	0.70
27:f:29:PRO:HB2	27:f:169:LEU:HD22	1.73	0.70
22:a:2204:G:OP2	24:c:147:LYS:NZ	2.24	0.70
28:g:84:THR:HG23	28:g:134:LYS:HG2	1.72	0.70
33:l:64:TRP:HB2	33:l:104:GLU:HB3	1.74	0.70
17:Q:19:LYS:NZ	17:Q:50:ASN:H	1.88	0.70
32:k:126:ARG:HG3	32:k:126:ARG:HH21	1.56	0.70
1:A:1316:G:N1	1:A:1319:A:OP2	2.24	0.70
12:L:68:GLY:O	12:L:99:ARG:NH1	2.24	0.69
22:a:545:U:O2'	22:a:548:G:N1	2.21	0.69
1:A:409:U:O2	1:A:433:G:N2	2.23	0.69
22:a:2102:G:N2	22:a:2187:U:O2	2.16	0.69
6:F:22:ILE:HD11	6:F:60:VAL:HG21	1.73	0.69
22:a:538:A:H5''	30:i:7:LYS:HE3	1.75	0.69
25:d:1:MET:HB3	25:d:205:PRO:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:42:TRP:HB2	6:F:59:TYR:HB2	1.75	0.69
22:a:639:U:H2'	22:a:640:C:C6	2.28	0.69
1:A:636:U:OP1	17:Q:6:ARG:NH1	2.26	0.69
42:u:4:ILE:HG13	42:u:50:MET:HE1	1.73	0.68
1:A:473:U:H2'	1:A:474:G:H8	1.58	0.68
8:H:3:MET:HE1	8:H:6:PRO:HG3	1.75	0.68
22:a:1434:A:H2'	22:a:1435:G:H8	1.59	0.68
20:T:79:LEU:O	20:T:83:ILE:HG13	1.93	0.68
1:A:624:C:H4'	16:P:10:GLY:HA2	1.75	0.68
3:C:35:SER:OG	3:C:59:ARG:NH2	2.26	0.68
42:u:68:LYS:HE2	42:u:68:LYS:HA	1.76	0.68
1:A:382:A:H2'	1:A:383:A:C8	2.29	0.68
22:a:1187:G:OP1	38:q:85:LYS:NZ	2.26	0.68
1:A:376:G:H4'	16:P:5:ARG:HH11	1.59	0.68
2:B:33:GLY:O	2:B:40:ILE:N	2.25	0.68
1:A:259:G:OP1	20:T:36:TYR:OH	2.11	0.68
6:F:6:ILE:HG12	6:F:89:VAL:HG22	1.75	0.68
10:J:52:LEU:HD11	10:J:59:LYS:HD2	1.75	0.68
22:a:534:U:O2'	37:p:49:ASP:OD2	2.11	0.68
1:A:404:G:OP2	4:D:115:ARG:NH2	2.19	0.67
16:P:18:GLN:OE1	16:P:35:ARG:NE	2.27	0.67
22:a:881:G:H1	22:a:895:U:H3	0.74	0.67
2:B:57:LEU:HD13	2:B:217:VAL:HG13	1.76	0.67
9:I:106:ARG:NH1	9:I:107:ASP:O	2.27	0.67
32:k:123:ARG:NH1	32:k:143:GLU:OE1	2.25	0.67
1:A:923:A:O2'	1:A:1399:C:OP2	2.12	0.67
15:O:26:GLU:H	15:O:26:GLU:CD	2.03	0.67
1:A:76:G:O6	1:A:93:U:O4	2.13	0.67
1:A:441:A:H61	1:A:493:A:N6	1.92	0.67
1:A:1062:U:H2'	1:A:1063:C:C6	2.29	0.67
24:c:107:PRO:HD2	24:c:110:LEU:HD22	1.77	0.67
14:N:20:TYR:HE2	14:N:52:PRO:HD2	1.59	0.67
1:A:108:G:N1	20:T:10:ARG:HG2	2.10	0.67
22:a:500:G:H22	22:a:503:A:H5'	1.60	0.66
1:A:76:G:N2	1:A:93:U:O2	2.20	0.66
14:N:27:LEU:HD21	14:N:44:ALA:O	1.95	0.66
4:D:57:GLU:OE2	4:D:200:ILE:HG13	1.95	0.66
1:A:472:U:H2'	1:A:473:U:H6	1.58	0.66
14:N:37:SER:OG	14:N:40:ASP:OD2	2.12	0.66
23:b:1:U:H2'	23:b:2:G:C8	2.30	0.66
27:f:56:ASP:OD2	27:f:150:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:276:U:O2'	22:a:278:A:N7	2.29	0.66
28:g:12:PRO:HD2	28:g:15:VAL:HG21	1.76	0.66
46:y:4:THR:HB	46:y:37:GLU:OE1	1.96	0.66
1:A:544:G:OP1	4:D:56:ARG:NH2	2.27	0.66
14:N:28:LYS:HA	14:N:31:ILE:HD12	1.77	0.66
22:a:1141:U:H2'	30:i:65:THR:HG21	1.76	0.66
1:A:472:U:H2'	1:A:473:U:C6	2.30	0.66
11:K:37:ARG:HG3	11:K:37:ARG:HH21	1.60	0.66
12:L:33:VAL:HG22	12:L:79:VAL:HG22	1.78	0.66
15:O:14:GLU:OE2	15:O:84:ARG:NH2	2.28	0.66
4:D:85:ASN:HB2	4:D:88:GLU:HG3	1.78	0.65
1:A:946:A:H2'	1:A:947:G:C8	2.32	0.65
1:A:1040:U:H2'	1:A:1041:G:H8	1.61	0.65
22:a:856:G:H2'	22:a:857:G:C8	2.30	0.65
22:a:2273:A:H2'	22:a:2274:A:C8	2.31	0.65
1:A:666:G:H5'	1:A:726:C:H1'	1.79	0.65
1:A:64:G:OP1	1:A:382:A:N6	2.28	0.65
1:A:1530:G:H2'	1:A:1531:A:C8	2.32	0.65
1:A:67:C:H2'	1:A:68:G:C8	2.32	0.65
3:C:117:ALA:HB1	3:C:187:SER:HB3	1.78	0.65
22:a:1548:A:H2'	22:a:1549:A:C8	2.31	0.65
10:J:10:LEU:HD12	10:J:22:THR:HG22	1.78	0.65
1:A:546:A:HO2'	1:A:548:G:HO2'	1.36	0.65
15:O:79:THR:O	15:O:83:GLU:HG2	1.97	0.65
1:A:437:U:O2'	4:D:120:HIS:ND1	2.21	0.64
16:P:14:ARG:HE	16:P:42:ILE:HD12	1.62	0.64
1:A:459:A:H2'	1:A:460:A:H8	1.60	0.64
2:B:117:LEU:HB3	2:B:141:LEU:HD12	1.80	0.64
1:A:618:C:H1'	16:P:14:ARG:HH12	1.60	0.64
4:D:57:GLU:HA	4:D:60:LYS:HG3	1.78	0.64
28:g:86:LYS:HG3	28:g:130:GLU:OE1	1.96	0.64
1:A:1073:U:O2	2:B:103:ASN:ND2	2.31	0.64
28:g:105:LEU:HD12	28:g:107:LEU:HD21	1.79	0.64
47:z:33:THR:HG22	47:z:51:GLY:HA2	1.79	0.64
2:B:213:TYR:O	2:B:217:VAL:HG23	1.98	0.64
6:F:49:TYR:OH	6:F:86:ARG:NH1	2.29	0.64
46:y:6:LYS:HD3	46:y:37:GLU:HG2	1.78	0.64
1:A:1039:G:H2'	1:A:1040:U:C6	2.33	0.64
3:C:88:ARG:HA	3:C:91:VAL:HG12	1.80	0.64
6:F:17:GLN:HB2	6:F:21:MET:HE3	1.79	0.64
16:P:6:LEU:HD22	16:P:17:TYR:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:35:VAL:HG21	20:T:54:MET:HG2	1.78	0.64
26:e:3:LEU:HD12	26:e:14:VAL:HG11	1.79	0.64
32:k:132:ARG:O	32:k:136:GLU:HG2	1.98	0.64
37:p:86:ALA:HB2	37:p:116:ALA:HB2	1.79	0.64
1:A:269:C:H2'	1:A:270:A:H8	1.63	0.64
1:A:745:G:H2'	1:A:746:A:C8	2.31	0.64
5:E:34:THR:HG22	5:E:52:LYS:HG2	1.79	0.64
24:c:232:HIS:HA	24:c:242:LYS:HE3	1.78	0.64
35:n:34:HIS:ND1	35:n:53:THR:OG1	2.23	0.64
52:4:20:ASN:HD21	52:4:39:LYS:HB2	1.62	0.64
1:A:408:A:H5'	4:D:113:GLU:HG2	1.78	0.64
1:A:437:U:HO2'	4:D:120:HIS:HD1	1.35	0.64
1:A:464:U:O2'	1:A:465:A:O5'	2.16	0.64
1:A:542:G:OP1	4:D:10:LYS:NZ	2.25	0.63
15:O:18:ASP:OD1	15:O:19:ALA:N	2.31	0.63
17:Q:58:VAL:HG12	17:Q:80:GLU:HB3	1.80	0.63
30:i:21:THR:HG23	30:i:61:LYS:HE2	1.79	0.63
4:D:99:ASP:OD1	4:D:99:ASP:N	2.31	0.63
14:N:27:LEU:HD23	14:N:31:ILE:HD11	1.80	0.63
1:A:202:G:O2'	1:A:468:A:N3	2.24	0.63
22:a:2327:A:H2'	22:a:2328:A:C8	2.33	0.63
40:s:2:ILE:HA	40:s:3:ARG:NH1	2.14	0.63
1:A:51:A:N7	1:A:114:U:O2'	2.31	0.63
22:a:127:A:H5''	22:a:128:C:C6	2.34	0.63
1:A:1086:U:H3	1:A:1099:G:H22	1.46	0.63
33:l:14:LYS:O	33:l:71:LYS:NZ	2.29	0.63
1:A:827:U:H5''	8:H:22:LYS:HE3	1.81	0.63
18:R:25:ASP:O	18:R:28:THR:OG1	2.16	0.63
9:I:41:ARG:HH11	9:I:41:ARG:HG3	1.64	0.62
22:a:1509:A:O2'	22:a:1510:G:H8	1.81	0.62
1:A:512:U:OP1	4:D:44:ARG:NH1	2.32	0.62
1:A:626:G:OP1	16:P:18:GLN:NE2	2.32	0.62
1:A:1391:U:H2'	1:A:1392:G:C8	2.34	0.62
28:g:86:LYS:HD2	28:g:132:VAL:HG22	1.81	0.62
22:a:272:A:H2'	22:a:273:G:C8	2.35	0.62
27:f:38:MET:HE3	27:f:57:LEU:HD13	1.81	0.62
13:M:10:PRO:HB2	13:M:13:LYS:HD3	1.81	0.62
13:M:66:GLU:CD	13:M:66:GLU:H	2.08	0.62
17:Q:19:LYS:HZ3	17:Q:49:GLU:HA	1.64	0.62
22:a:2659:G:OP2	28:g:158:LYS:NZ	2.32	0.62
8:H:18:GLN:NE2	8:H:70:ALA:HB1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:46:LYS:HG2	10:J:68:ARG:HG2	1.81	0.62
3:C:77:ILE:HA	3:C:84:VAL:HG13	1.81	0.62
1:A:148:G:O2'	1:A:1446:A:N3	2.28	0.62
1:A:1038:C:H2'	1:A:1039:G:C8	2.35	0.62
22:a:1115:G:O2'	22:a:1116:G:O5'	2.18	0.62
45:x:32:ALA:HB2	45:x:37:LEU:HD23	1.81	0.62
1:A:417:G:O6	1:A:426:U:O4	2.18	0.62
1:A:1261:A:N6	1:A:1274:A:O2'	2.32	0.61
14:N:27:LEU:HD22	14:N:48:LEU:HB2	1.82	0.61
30:i:11:VAL:HG21	30:i:50:THR:HG22	1.82	0.61
42:u:9:ARG:HG2	42:u:41:GLU:HG3	1.82	0.61
8:H:32:LEU:O	8:H:36:ILE:HG13	2.00	0.61
39:r:74:ILE:HD12	39:r:105:VAL:HG22	1.82	0.61
1:A:362:G:N1	1:A:365:U:OP2	2.29	0.61
1:A:459:A:H2'	1:A:460:A:C8	2.35	0.61
1:A:935:A:O2'	1:A:1383:C:O2	2.18	0.61
1:A:720:C:O2	18:R:60:LYS:NZ	2.29	0.61
22:a:363:G:H2'	22:a:364:C:H6	1.66	0.61
45:x:39:GLN:HG2	45:x:41:HIS:CE1	2.35	0.61
4:D:117:LEU:HD23	4:D:123:ILE:HD11	1.80	0.61
29:h:34:GLY:O	29:h:36:ALA:N	2.32	0.61
2:B:63:ARG:O	2:B:64:LYS:HG2	2.01	0.61
10:J:44:THR:O	10:J:46:LYS:NZ	2.34	0.61
16:P:57:ILE:O	16:P:61:VAL:HG23	2.00	0.61
22:a:2522:U:O2'	22:a:2647:U:OP1	2.15	0.61
1:A:160:A:H2'	1:A:161:A:O4'	2.00	0.61
18:R:12:ARG:NH2	18:R:16:GLU:OE2	2.34	0.61
22:a:2419:U:H4'	48:O:22:THR:HG21	1.82	0.61
1:A:1063:C:OP2	1:A:1064:G:O2'	2.17	0.61
22:a:881:G:O6	22:a:895:U:O4	2.18	0.61
24:c:165:VAL:HG11	24:c:181:MET:HE1	1.82	0.61
22:a:1179:G:H2'	22:a:1180:U:C6	2.36	0.60
1:A:299:G:H2'	1:A:300:A:C8	2.37	0.60
1:A:1034:G:O2'	1:A:1035:A:O5'	2.14	0.60
22:a:2530:A:H5'	28:g:175:LYS:HD3	1.83	0.60
27:f:158:THR:HG22	27:f:160:ALA:H	1.65	0.60
1:A:1032:G:C4	1:A:1033:G:H1'	2.36	0.60
2:B:65:GLY:O	2:B:225:ARG:NH1	2.34	0.60
54:Z:9:G:N2	54:Z:47:A:OP2	2.31	0.60
1:A:502:A:OP1	12:L:115:SER:OG	2.13	0.60
1:A:913:A:OP1	12:L:88:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1141:U:H4'	22:a:1142:A:O4'	2.01	0.60
23:b:66:A:H61	23:b:107:G:H2'	1.65	0.60
1:A:184:G:H2'	1:A:185:U:H6	1.67	0.60
4:D:41:HIS:HB3	4:D:44:ARG:HD3	1.83	0.60
22:a:2291:U:H2'	22:a:2292:U:C6	2.37	0.60
2:B:163:VAL:HG11	2:B:173:ILE:HD11	1.83	0.60
9:I:57:MET:HE2	9:I:61:LEU:HD11	1.84	0.60
22:a:2071:A:H2'	22:a:2072:C:C6	2.36	0.60
27:f:46:ASP:HB3	27:f:49:LEU:HG	1.84	0.60
1:A:1039:G:H2'	1:A:1040:U:H6	1.66	0.60
47:z:52:ARG:NH2	47:z:52:ARG:HB3	2.17	0.60
1:A:198:G:O6	1:A:219:U:O4	2.20	0.60
21:U:13:ASP:OD2	21:U:17:ARG:NH2	2.35	0.60
22:a:1528:A:OP2	22:a:1543:G:N2	2.32	0.60
2:B:68:LEU:HB3	2:B:161:LEU:HD23	1.83	0.60
17:Q:54:GLY:N	17:Q:57:ASP:OD2	2.31	0.60
17:Q:57:ASP:OD1	17:Q:82:ALA:N	2.33	0.60
9:I:83:ILE:O	9:I:87:LEU:HD13	2.01	0.59
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.84	0.59
22:a:78:U:H2'	22:a:79:C:C6	2.37	0.59
22:a:721:A:H2'	22:a:722:A:C8	2.36	0.59
1:A:39:G:H2'	1:A:40:C:H6	1.66	0.59
1:A:441:A:N6	1:A:493:A:H61	1.97	0.59
14:N:49:GLN:HE22	19:S:12:ASP:HA	1.67	0.59
22:a:2394:C:H5''	32:k:63:LYS:HE2	1.82	0.59
27:f:11:GLU:HA	27:f:14:LYS:HE2	1.82	0.59
29:h:12:LEU:HD13	29:h:19:VAL:HG21	1.84	0.59
22:a:1048:A:OP2	22:a:1110:G:N2	2.28	0.59
1:A:148:G:H1	1:A:174:A:H61	1.50	0.59
20:T:21:ASN:OD1	20:T:66:LEU:HD13	2.03	0.59
22:a:468:G:N7	49:1:39:ARG:NH2	2.44	0.59
1:A:67:C:H2'	1:A:68:G:H8	1.66	0.59
10:J:8:ILE:HD12	10:J:74:VAL:HG23	1.85	0.59
22:a:2328:A:H2'	22:a:2329:U:C6	2.37	0.59
1:A:713:G:H2'	1:A:714:G:C8	2.38	0.59
9:I:36:GLU:HA	9:I:45:ARG:HE	1.67	0.59
2:B:83:ALA:HB2	2:B:214:LEU:HD13	1.85	0.59
5:E:95:PHE:CE2	5:E:97:GLN:HG3	2.38	0.59
14:N:49:GLN:NE2	19:S:12:ASP:HA	2.17	0.59
22:a:1570:A:H2'	22:a:1571:A:C8	2.37	0.59
22:a:1590:A:H2'	22:a:1591:A:C8	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:V:2:C:H2'	55:V:3:C:H6	1.68	0.59
1:A:486:U:H2'	1:A:487:A:C8	2.38	0.59
2:B:56:GLU:HG2	2:B:198:PHE:HE2	1.67	0.59
23:b:5:U:OP1	23:b:61:G:O2'	2.17	0.59
1:A:720:C:H5''	18:R:41:PRO:HA	1.85	0.59
1:A:1009:U:H3	1:A:1020:G:H1	1.49	0.59
2:B:171:ILE:O	2:B:175:GLU:HG3	2.03	0.59
7:G:13:LEU:HD23	7:G:14:PRO:HD2	1.84	0.59
1:A:429:U:H3'	4:D:9:LEU:HD12	1.85	0.59
1:A:1035:A:H4'	1:A:1036:A:OP1	2.03	0.59
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.85	0.59
9:I:6:TYR:HB2	9:I:21:ILE:HG12	1.85	0.59
11:K:106:ARG:HH11	11:K:108:THR:HG22	1.66	0.59
27:f:13:VAL:HA	27:f:28:VAL:HG11	1.85	0.59
40:s:2:ILE:HA	40:s:3:ARG:HH11	1.68	0.59
1:A:476:U:H2'	1:A:477:C:C6	2.38	0.58
22:a:276:U:O2'	22:a:277:G:O4'	2.17	0.58
22:a:1311:G:H21	22:a:1603:A:H62	1.48	0.58
27:f:13:VAL:O	27:f:17:MET:HG2	2.02	0.58
14:N:42:TRP:O	14:N:46:LEU:HD12	2.03	0.58
22:a:2502:G:H5''	22:a:2503:2MA:H5''	1.84	0.58
1:A:202:G:H1'	1:A:468:A:H2	1.68	0.58
22:a:2547:A:H2'	22:a:2548:U:C6	2.38	0.58
38:q:6:GLN:HG2	38:q:11:GLN:HG3	1.86	0.58
42:u:2:PHE:HB2	42:u:61:LEU:HD22	1.85	0.58
1:A:742:G:H5''	15:O:58:ARG:HH21	1.68	0.58
1:A:1098:C:O2'	21:U:71:TYR:O	2.19	0.58
4:D:146:ARG:HH22	4:D:148:LYS:HD3	1.68	0.58
12:L:56:ARG:HB3	12:L:56:ARG:CZ	2.33	0.58
30:i:13:ARG:HG2	30:i:51:GLY:O	2.02	0.58
47:z:43:ILE:HG22	47:z:49:TYR:HB2	1.86	0.58
1:A:216:U:O2'	1:A:468:A:N6	2.36	0.58
1:A:573:A:N3	1:A:883:C:O2'	2.35	0.58
22:a:94:A:H8	22:a:94:A:O5'	1.87	0.58
22:a:2636:C:H2'	22:a:2637:U:C6	2.39	0.58
26:e:171:ASP:OD1	26:e:174:GLY:N	2.37	0.58
1:A:555:U:H2'	1:A:556:C:C6	2.38	0.58
1:A:1323:G:H2'	1:A:1324:A:C8	2.39	0.58
10:J:20:GLN:OE1	10:J:20:GLN:HA	2.02	0.58
1:A:323:U:OP1	20:T:25:ARG:NH2	2.34	0.58
1:A:714:G:H2'	1:A:715:A:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.85	0.58
4:D:28:ILE:HG23	4:D:34:ILE:HD11	1.86	0.58
4:D:174:ASP:HB3	4:D:179:GLU:HG2	1.84	0.58
19:S:45:ILE:H	19:S:45:ILE:HD12	1.69	0.58
24:c:199:GLU:CD	24:c:199:GLU:H	2.12	0.58
1:A:476:U:H2'	1:A:477:C:H6	1.67	0.58
22:a:1386:C:H2'	22:a:1387:A:C8	2.39	0.58
1:A:121:U:O2'	1:A:122:G:OP1	2.20	0.57
1:A:1042:A:O2'	1:A:1043:G:O5'	2.22	0.57
4:D:50:ASP:O	4:D:53:VAL:HG22	2.04	0.57
10:J:37:ARG:HG2	10:J:37:ARG:HH11	1.68	0.57
22:a:465:G:OP1	49:1:12:ARG:NH1	2.36	0.57
22:a:682:G:H5'	49:1:26:ASN:ND2	2.19	0.57
1:A:201:G:O2'	1:A:469:C:O2'	2.09	0.57
1:A:1458:G:OP1	20:T:30:THR:OG1	2.20	0.57
22:a:849:A:H2'	22:a:850:U:C6	2.38	0.57
35:n:16:ARG:HH21	35:n:16:ARG:HA	1.69	0.57
1:A:1144:G:H21	1:A:1146:A:H62	1.50	0.57
7:G:71:PRO:O	7:G:96:ARG:HD2	2.04	0.57
22:a:1199:U:H1'	37:p:4:VAL:HG22	1.84	0.57
22:a:1447:C:O2'	22:a:1544:A:N3	2.33	0.57
22:a:2097:A:H2'	22:a:2098:U:C6	2.40	0.57
51:3:16:ILE:HD13	51:3:25:VAL:HG22	1.85	0.57
1:A:262:A:H2'	1:A:263:A:C8	2.39	0.57
1:A:864:A:H5''	5:E:90:THR:HG23	1.86	0.57
19:S:45:ILE:HG12	19:S:64:ASP:OD1	2.03	0.57
1:A:187:G:N2	1:A:190:A:OP2	2.38	0.57
1:A:269:C:H2'	1:A:270:A:C8	2.38	0.57
22:a:172:A:H2'	22:a:173:A:C8	2.38	0.57
22:a:1870:C:O2'	22:a:1871:A:O4'	2.23	0.57
25:d:5:VAL:N	25:d:32:ASN:HD21	1.94	0.57
33:l:20:LEU:HD13	42:u:81:PRO:HG3	1.85	0.57
1:A:1266:G:N2	1:A:1269:A:OP2	2.30	0.57
8:H:84:ARG:C	8:H:85:ILE:HD13	2.30	0.57
16:P:3:THR:C	16:P:4:ILE:HD12	2.30	0.57
22:a:283:G:H2'	22:a:284:U:C6	2.40	0.57
40:s:39:THR:O	40:s:43:ILE:HG13	2.05	0.57
1:A:1026:G:O2'	1:A:1027:C:OP1	2.23	0.57
1:A:1073:U:O2'	2:B:105:LYS:HE2	2.05	0.57
22:a:742:A:H2'	22:a:743:A:C8	2.40	0.57
22:a:1182:G:H2'	22:a:1183:U:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:3:VAL:HG12	24:c:19:VAL:HG22	1.86	0.57
1:A:1297:G:N2	1:A:1298:U:O4	2.36	0.57
1:A:1463:U:H2'	1:A:1464:U:C6	2.39	0.57
22:a:1315:C:O2'	22:a:1392:A:N3	2.36	0.57
22:a:2210:U:H4'	22:a:2211:A:H5'	1.87	0.57
22:a:1590:A:H2'	22:a:1591:A:H8	1.70	0.57
35:n:70:ALA:O	35:n:74:VAL:HG12	2.05	0.57
42:u:79:ARG:HG2	42:u:79:ARG:NH1	2.17	0.57
1:A:39:G:H2'	1:A:40:C:C6	2.40	0.56
7:G:42:ILE:HG21	7:G:116:MET:HG3	1.86	0.56
7:G:79:ARG:CZ	7:G:82:GLY:HA2	2.35	0.56
22:a:1730:C:H1'	22:a:1731:G:C2	2.41	0.56
22:a:2728:U:HO2'	22:a:2729:G:H8	1.53	0.56
28:g:101:ASN:ND2	28:g:116:GLN:OE1	2.38	0.56
1:A:1359:C:OP2	14:N:75:ARG:NE	2.37	0.56
1:A:1530:G:H2'	1:A:1531:A:H8	1.69	0.56
27:f:14:LYS:O	27:f:18:THR:HG23	2.04	0.56
1:A:49:U:O2'	1:A:50:A:H2'	2.05	0.56
10:J:10:LEU:O	10:J:71:LEU:HA	2.06	0.56
12:L:81:LEU:HD23	12:L:98:VAL:HG11	1.87	0.56
13:M:11:ASP:HA	13:M:45:ILE:HB	1.88	0.56
22:a:1405:U:H2'	22:a:1406:U:C6	2.40	0.56
25:d:48:ILE:HG23	25:d:84:LEU:HD11	1.86	0.56
1:A:977:A:N6	1:A:1224:U:O5'	2.38	0.56
1:A:1187:G:H5'	9:I:115:LYS:HD3	1.87	0.56
4:D:146:ARG:O	4:D:150:LYS:HG3	2.05	0.56
31:j:8:LEU:HD22	31:j:84:CYS:HB3	1.88	0.56
1:A:337:G:H2'	1:A:338:A:C8	2.41	0.56
22:a:892:A:H2'	22:a:893:C:O4'	2.05	0.56
22:a:2636:C:H2'	22:a:2637:U:H6	1.70	0.56
5:E:54:ARG:HG3	5:E:54:ARG:HH11	1.70	0.56
11:K:89:PRO:HB3	21:U:32:VAL:HG11	1.88	0.56
13:M:24:GLY:O	13:M:29:ARG:NH1	2.35	0.56
14:N:80:SER:O	14:N:84:VAL:HG12	2.06	0.56
1:A:1038:C:H2'	1:A:1039:G:H8	1.68	0.56
22:a:1203:U:OP2	22:a:1204:A:O2'	2.20	0.56
22:a:1496:A:H2'	22:a:1498:C:C5	2.41	0.56
1:A:34:C:H2'	1:A:35:G:C8	2.41	0.56
14:N:46:LEU:O	14:N:50:THR:HG23	2.05	0.56
22:a:1045:C:O2	22:a:1111:A:N6	2.39	0.56
1:A:63:C:H4'	1:A:380:G:O2'	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:G:H2'	1:A:722:G:N3	2.21	0.56
4:D:107:PHE:HD1	4:D:159:LEU:HD11	1.71	0.56
12:L:57:LEU:HD12	12:L:61:PHE:HB2	1.87	0.56
21:U:63:GLU:HB3	21:U:67:ARG:HH21	1.71	0.56
22:a:1296:G:OP1	22:a:2709:G:O2'	2.22	0.56
1:A:158:G:H2'	1:A:159:G:O4'	2.06	0.55
48:0:5:ILE:HD13	48:0:28:ARG:HD3	1.87	0.55
1:A:1119:C:H2'	1:A:1120:C:H6	1.71	0.55
1:A:1317:C:H4'	14:N:48:LEU:HD21	1.87	0.55
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.88	0.55
22:a:3:U:H2'	22:a:4:U:C6	2.41	0.55
39:r:65:ASP:OD1	39:r:65:ASP:N	2.39	0.55
1:A:382:A:H2'	1:A:383:A:H8	1.72	0.55
1:A:1273:C:H2'	1:A:1274:A:O4'	2.07	0.55
22:a:191:A:H2'	22:a:192:C:C6	2.40	0.55
23:b:66:A:N6	23:b:107:G:H2'	2.21	0.55
26:e:112:LEU:HD22	26:e:117:ARG:HB2	1.88	0.55
36:o:14:LYS:HD2	36:o:77:HIS:HA	1.88	0.55
1:A:1441:A:H62	1:A:1461:G:H21	1.53	0.55
9:I:47:VAL:HG13	9:I:80:ARG:HD3	1.89	0.55
22:a:2494:G:O2'	33:l:79:ALA:HA	2.07	0.55
26:e:171:ASP:OD2	26:e:173:THR:OG1	2.20	0.55
1:A:262:A:H2'	1:A:263:A:H8	1.72	0.55
5:E:95:PHE:HE2	5:E:97:GLN:HG3	1.72	0.55
10:J:66:GLU:HG2	14:N:99:ALA:HB2	1.88	0.55
11:K:30:THR:HG21	11:K:63:ALA:HB2	1.89	0.55
15:O:57:LEU:HD21	22:a:715:A:N6	2.21	0.55
22:a:1475:G:O2'	22:a:1514:G:O6	2.24	0.55
22:a:2091:C:O3'	44:w:56:MET:HE1	2.06	0.55
24:c:167:ARG:HH21	24:c:167:ARG:HG3	1.72	0.55
1:A:1352:C:H2'	1:A:1353:G:C8	2.42	0.55
7:G:88:PRO:HG3	7:G:149:LYS:HA	1.88	0.55
22:a:140:C:H5'	22:a:141:G:C5	2.41	0.55
27:f:125:ARG:NH1	27:f:161:LYS:O	2.40	0.55
28:g:60:ASP:N	28:g:60:ASP:OD1	2.39	0.55
31:j:63:VAL:HG12	31:j:107:LEU:HD11	1.87	0.55
31:j:104:THR:HG22	31:j:106:GLU:H	1.72	0.55
32:k:57:LEU:HD22	50:2:54:ASP:HB3	1.87	0.55
37:p:106:PHE:O	37:p:110:VAL:HG23	2.06	0.55
1:A:6:G:N2	5:E:103:THR:OG1	2.38	0.55
2:B:98:GLY:HA2	2:B:171:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1048:A:N1	22:a:1112:G:O2'	2.37	0.55
17:Q:75:LEU:HD12	17:Q:76:VAL:H	1.70	0.55
22:a:182:A:H2'	22:a:183:C:H6	1.72	0.55
22:a:286:U:H2'	22:a:287:G:C8	2.42	0.55
27:f:121:SER:HB2	27:f:128:TYR:CE1	2.42	0.55
52:4:10:GLU:C	52:4:25:ARG:HG3	2.31	0.55
1:A:1516:2MG:N1	1:A:1519:MA6:OP2	2.35	0.55
11:K:59:THR:HG22	11:K:61:PHE:H	1.72	0.55
18:R:23:TYR:HB3	18:R:58:ALA:HB1	1.88	0.55
22:a:2012:G:OP1	39:r:11:ARG:NH2	2.28	0.55
7:G:22:LEU:HD12	7:G:101:MET:HE2	1.87	0.55
22:a:545:U:H2'	22:a:547:A:C5	2.42	0.55
22:a:1799:G:O2'	24:c:180:GLU:OE2	2.25	0.55
22:a:2473:U:OP1	22:a:2529:G:N2	2.39	0.55
26:e:111:GLU:OE2	26:e:115:GLN:NE2	2.32	0.55
31:j:111:LYS:NZ	31:j:111:LYS:HB3	2.22	0.55
1:A:202:G:H1'	1:A:468:A:C2	2.42	0.54
3:C:206:GLU:O	3:C:207:ILE:HG13	2.06	0.54
4:D:49:SER:O	4:D:53:VAL:HG13	2.06	0.54
40:s:53:VAL:HG13	40:s:91:GLN:HB3	1.90	0.54
1:A:1040:U:H2'	1:A:1041:G:C8	2.42	0.54
3:C:26:THR:HG23	14:N:76:LYS:HD2	1.90	0.54
8:H:47:GLU:CD	8:H:64:LYS:HB3	2.32	0.54
22:a:995:C:N4	30:i:2:LYS:HD2	2.23	0.54
22:a:2303:G:O2'	27:f:121:SER:O	2.25	0.54
1:A:1031:C:O3'	1:A:1032:G:N2	2.40	0.54
1:A:1073:U:O2'	2:B:103:ASN:OD1	2.11	0.54
13:M:17:ILE:O	13:M:20:THR:OG1	2.25	0.54
35:n:58:ILE:HD11	35:n:81:ARG:HH12	1.71	0.54
47:z:53:LYS:NZ	47:z:55:ILE:O	2.41	0.54
1:A:1180:A:OP2	9:I:99:ARG:NH2	2.41	0.54
1:A:1287:A:H2'	1:A:1288:A:C8	2.43	0.54
13:M:20:THR:HG22	13:M:26:GLY:O	2.07	0.54
14:N:27:LEU:O	14:N:31:ILE:HD12	2.07	0.54
55:V:2:C:H2'	55:V:3:C:C6	2.42	0.54
1:A:17:U:H2'	1:A:18:C:C6	2.43	0.54
1:A:483:C:H5''	1:A:484:G:OP2	2.08	0.54
4:D:28:ILE:HA	4:D:31:LYS:HB2	1.89	0.54
15:O:56:LEU:HD21	22:a:715:A:C2	2.42	0.54
40:s:54:GLU:HB2	40:s:88:LYS:HB2	1.89	0.54
1:A:1004:A:H1'	1:A:1036:A:H62	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:s:30:ILE:HD11	40:s:87:LEU:HD11	1.89	0.54
1:A:38:G:H4'	1:A:547:A:N6	2.23	0.54
4:D:102:VAL:HG23	4:D:107:PHE:CD2	2.43	0.54
22:a:44:A:H2'	22:a:45:G:O4'	2.07	0.54
22:a:163:C:H2'	22:a:164:C:C6	2.43	0.54
22:a:2845:U:H5''	36:o:52:ASN:O	2.06	0.54
1:A:695:A:H2'	1:A:696:A:C8	2.43	0.54
13:M:44:LYS:N	13:M:47:GLU:OE1	2.39	0.54
22:a:17:G:H2'	22:a:18:U:C6	2.42	0.54
22:a:157:C:H2'	22:a:158:U:O4'	2.07	0.54
22:a:549:G:H2'	22:a:550:C:C6	2.43	0.54
55:V:22:G:H2'	55:V:23:A:H8	1.72	0.54
22:a:2305:U:O2'	27:f:133:ARG:NH2	2.41	0.54
22:a:2788:C:H2'	22:a:2789:C:C6	2.43	0.54
35:n:53:THR:O	35:n:59:ALA:HB2	2.08	0.54
1:A:983:A:H5'	1:A:984:C:OP2	2.07	0.54
5:E:165:LEU:C	8:H:114:ARG:HH22	2.15	0.54
22:a:1856:U:H2'	22:a:1857:G:O4'	2.08	0.54
22:a:1937:A:O2'	22:a:1939:5MU:OP2	2.24	0.54
1:A:1277:C:H2'	1:A:1279:G:H21	1.72	0.53
27:f:71:ARG:O	27:f:81:GLN:NE2	2.40	0.53
30:i:34:ARG:HG3	30:i:39:LYS:HB2	1.91	0.53
22:a:1871:A:H2'	22:a:1872:A:C8	2.43	0.53
43:v:25:ARG:HH11	43:v:31:VAL:HG12	1.72	0.53
4:D:183:LYS:HD3	4:D:184:ARG:HB2	1.90	0.53
15:O:36:ILE:HG13	15:O:59:MET:HE3	1.90	0.53
22:a:998:C:OP1	37:p:84:LYS:NZ	2.37	0.53
25:d:19:GLY:HA3	36:o:80:VAL:HG23	1.90	0.53
41:t:98:SER:O	41:t:98:SER:OG	2.26	0.53
1:A:198:G:H1	1:A:219:U:H3	1.55	0.53
22:a:414:C:H2'	22:a:415:A:C8	2.43	0.53
22:a:2849:U:H4'	22:a:2868:A:C2	2.43	0.53
24:c:132:MET:HG3	24:c:188:CYS:O	2.08	0.53
1:A:20:U:H2'	1:A:21:G:O4'	2.07	0.53
5:E:53:ALA:HB2	5:E:62:LYS:HE2	1.90	0.53
20:T:26:SER:O	20:T:30:THR:OG1	2.26	0.53
22:a:2839:G:O2'	34:m:49:GLU:OE2	2.20	0.53
41:t:28:VAL:HG22	41:t:34:VAL:HG12	1.91	0.53
1:A:728:A:H2'	1:A:729:A:C8	2.44	0.53
3:C:23:PHE:HA	10:J:13:PHE:CE2	2.44	0.53
41:t:41:LEU:HA	41:t:61:LYS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:52:ARG:O	45:x:55:THR:HG22	2.08	0.53
1:A:109:A:C6	1:A:326:G:C6	2.96	0.53
1:A:511:C:O2'	1:A:512:U:OP2	2.19	0.53
5:E:88:VAL:HG22	5:E:93:ARG:HG3	1.91	0.53
7:G:113:ASP:HB2	7:G:119:ARG:HG3	1.91	0.53
10:J:12:ALA:HB3	10:J:18:ILE:HB	1.90	0.53
22:a:1507:C:H2'	22:a:1508:A:O4'	2.08	0.53
7:G:111:ARG:HB2	7:G:119:ARG:HG2	1.91	0.53
19:S:5:LEU:CD2	52:4:63:ARG:HH21	2.22	0.53
22:a:1183:U:H2'	22:a:1184:U:C6	2.44	0.53
35:n:35:ILE:HG23	35:n:74:VAL:HG11	1.90	0.53
3:C:150:LYS:HB2	3:C:169:ARG:HG3	1.90	0.53
4:D:21:LEU:O	4:D:110:THR:HG22	2.08	0.53
7:G:25:LYS:O	7:G:29:ILE:HG12	2.09	0.53
22:a:64:A:H2'	22:a:65:U:C6	2.44	0.53
32:k:77:ILE:CD1	32:k:108:ALA:HB1	2.39	0.53
3:C:41:GLN:O	3:C:45:LYS:HE2	2.09	0.52
22:a:347:A:H2'	22:a:348:A:C8	2.44	0.52
1:A:41:G:H2'	1:A:42:G:H8	1.73	0.52
1:A:150:U:H2'	1:A:151:A:H8	1.74	0.52
1:A:193:C:H4'	20:T:56:PRO:HG3	1.91	0.52
22:a:347:A:H2'	22:a:348:A:H8	1.74	0.52
22:a:2794:C:H2'	22:a:2795:C:C6	2.44	0.52
31:j:12:ASP:OD1	31:j:14:SER:OG	2.13	0.52
3:C:19:ASN:O	3:C:40:ARG:NH2	2.43	0.52
3:C:124:LEU:HD21	3:C:130:PHE:HB3	1.92	0.52
4:D:73:ARG:HH21	4:D:74:ASN:ND2	2.07	0.52
16:P:20:VAL:HA	16:P:35:ARG:HA	1.90	0.52
22:a:958:U:O2	23:b:89:U:H1'	2.09	0.52
33:l:41:LEU:HG	33:l:96:ILE:HG13	1.92	0.52
1:A:401:C:OP2	4:D:70:ARG:HD3	2.09	0.52
1:A:405:U:C4	4:D:5:LEU:HD11	2.44	0.52
4:D:60:LYS:NZ	4:D:195:ILE:HG23	2.25	0.52
36:o:51:ARG:HG2	36:o:53:ARG:HG2	1.92	0.52
1:A:1001:C:H2'	1:A:1002:G:H8	1.74	0.52
22:a:170:U:H2'	22:a:171:U:C6	2.44	0.52
22:a:627:A:N1	22:a:636:G:O2'	2.36	0.52
22:a:635:C:OP2	32:k:109:LYS:NZ	2.39	0.52
22:a:1521:G:OP2	22:a:1522:A:O2'	2.26	0.52
1:A:166:U:H2'	1:A:167:A:H8	1.74	0.52
1:A:999:C:N3	1:A:1042:A:N6	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:THR:HG22	2:B:39:HIS:CE1	2.45	0.52
9:I:129:LYS:HD2	9:I:130:ARG:HH22	1.74	0.52
22:a:116:C:O2'	22:a:126:A:N3	2.40	0.52
27:f:49:LEU:HD22	27:f:148:ARG:HH12	1.75	0.52
37:p:81:ASN:HD21	37:p:85:LYS:HE3	1.75	0.52
42:u:45:ASP:OD1	42:u:45:ASP:N	2.42	0.52
54:Z:48:U:H5''	54:Z:49:C:H5'	1.91	0.52
1:A:184:G:H2'	1:A:185:U:C6	2.44	0.52
1:A:664:G:P	18:R:53:ARG:HH21	2.33	0.52
2:B:211:THR:HA	2:B:214:LEU:HG	1.92	0.52
8:H:64:LYS:HG3	8:H:71:VAL:HG21	1.92	0.52
13:M:86:TYR:HA	13:M:89:LEU:HD12	1.91	0.52
22:a:1722:A:N6	22:a:1738:G:O2'	2.43	0.52
27:f:105:THR:HG22	27:f:106:ILE:HD13	1.91	0.52
30:i:13:ARG:HD2	30:i:53:TYR:CE1	2.45	0.52
37:p:58:ARG:HA	37:p:61:TRP:CE3	2.44	0.52
1:A:270:A:H2'	1:A:271:C:C6	2.45	0.52
2:B:81:LYS:HE3	2:B:85:LEU:HD11	1.92	0.52
2:B:123:ASP:OD1	2:B:125:THR:OG1	2.21	0.52
3:C:47:LEU:HB3	3:C:50:ALA:HB3	1.92	0.52
22:a:721:A:H2'	22:a:722:A:H8	1.75	0.52
22:a:2243:U:H2'	22:a:2244:U:C6	2.45	0.52
27:f:103:LEU:HA	27:f:107:ALA:HB3	1.91	0.52
36:o:2:SER:OG	36:o:3:ASN:N	2.43	0.52
37:p:61:TRP:CZ2	37:p:93:LYS:HD3	2.45	0.52
41:t:85:PHE:CE1	41:t:94:ARG:HG2	2.45	0.52
41:t:86:ARG:NH2	41:t:100:SER:OG	2.43	0.52
1:A:76:G:H2'	1:A:77:A:H8	1.74	0.52
1:A:107:G:O6	20:T:10:ARG:HD3	2.09	0.52
4:D:150:LYS:NZ	4:D:177:LYS:O	2.43	0.52
28:g:124:GLU:HG2	28:g:132:VAL:HB	1.91	0.52
36:o:63:LYS:HE2	36:o:65:SER:HB2	1.91	0.52
1:A:408:A:H2'	1:A:409:U:C6	2.45	0.52
20:T:20:HIS:O	20:T:23:SER:OG	2.25	0.52
22:a:2481:G:O2'	22:a:2482:A:H8	1.93	0.52
35:n:30:ARG:HG3	35:n:35:ILE:HD12	1.91	0.52
22:a:2801:G:H2'	22:a:2802:G:C8	2.46	0.51
24:c:145:GLU:HB3	24:c:188:CYS:HB3	1.93	0.51
26:e:97:ASN:ND2	26:e:100:MET:HE3	2.25	0.51
1:A:223:A:H2'	1:A:224:U:C6	2.46	0.51
1:A:632:U:H5''	1:A:633:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:A:H8	1:A:1005:A:O5'	1.93	0.51
3:C:73:PRO:HG3	3:C:105:GLU:HB2	1.92	0.51
11:K:85:MET:SD	11:K:111:THR:HB	2.50	0.51
13:M:66:GLU:OE1	13:M:66:GLU:N	2.41	0.51
22:a:2796:U:H3	22:a:2799:A:H61	1.58	0.51
1:A:34:C:H2'	1:A:35:G:H8	1.74	0.51
13:M:10:PRO:CB	13:M:13:LYS:HD3	2.40	0.51
22:a:861:A:H2'	22:a:862:G:O4'	2.11	0.51
35:n:27:VAL:HG21	35:n:40:ILE:HD12	1.92	0.51
1:A:107:G:N7	20:T:10:ARG:NH1	2.58	0.51
2:B:5:SER:O	2:B:9:MET:HB2	2.10	0.51
7:G:151:PHE:CZ	11:K:56:ARG:HG3	2.45	0.51
9:I:12:ARG:HG3	9:I:13:LYS:H	1.74	0.51
22:a:1357:C:H2'	22:a:1358:G:O4'	2.11	0.51
22:a:1478:G:H1	22:a:1513:U:H3	1.58	0.51
22:a:1594:U:H2'	22:a:1595:C:C6	2.45	0.51
28:g:42:GLU:OE2	28:g:44:LYS:NZ	2.40	0.51
41:t:44:LYS:HB2	41:t:61:LYS:HE2	1.92	0.51
44:w:59:ILE:HG12	44:w:67:VAL:HG21	1.91	0.51
1:A:294:U:OP1	1:A:610:U:O2'	2.23	0.51
1:A:619:U:H4'	4:D:128:ARG:NH2	2.23	0.51
1:A:1032:G:N2	1:A:1033:G:N3	2.58	0.51
13:M:101:ARG:NE	13:M:104:THR:OG1	2.22	0.51
22:a:2193:G:H2'	22:a:2194:U:C6	2.46	0.51
23:b:48:U:H2'	23:b:49:C:C6	2.46	0.51
28:g:44:LYS:O	28:g:50:LEU:HA	2.10	0.51
1:A:1001:C:H2'	1:A:1002:G:C8	2.45	0.51
6:F:16:GLU:CD	6:F:16:GLU:H	2.18	0.51
6:F:29:ILE:HG13	6:F:30:THR:N	2.24	0.51
22:a:1469:A:H2'	22:a:1470:A:C8	2.46	0.51
22:a:1703:G:H2'	22:a:1704:C:C6	2.46	0.51
22:a:2591:C:H2'	22:a:2592:G:C8	2.45	0.51
1:A:131:A:H2'	1:A:132:C:C6	2.45	0.51
1:A:268:U:H2'	1:A:269:C:C6	2.45	0.51
1:A:427:U:OP1	4:D:13:ARG:NH2	2.44	0.51
22:a:2537:U:H2'	22:a:2538:C:C6	2.45	0.51
1:A:1228:C:OP1	13:M:107:ARG:NH2	2.32	0.51
1:A:1477:U:H2'	1:A:1478:U:C6	2.46	0.51
9:I:10:GLY:HA3	9:I:78:ALA:O	2.11	0.51
22:a:139:U:H5''	22:a:140:C:H5	1.75	0.51
22:a:363:G:H2'	22:a:364:C:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.92	0.51
22:a:1496:A:N3	22:a:1577:C:O2'	2.36	0.51
24:c:60:GLN:HG2	24:c:85:PRO:HB2	1.92	0.51
47:z:52:ARG:HB3	47:z:52:ARG:HH21	1.74	0.51
52:4:42:PRO:HB2	52:4:48:GLN:HG3	1.92	0.51
1:A:14:U:O2'	1:A:16:A:N7	2.37	0.51
23:b:106:G:H2'	23:b:107:G:O4'	2.11	0.51
26:e:6:LYS:HZ3	26:e:119:ILE:HA	1.75	0.51
36:o:6:LYS:C	36:o:6:LYS:HD3	2.36	0.51
36:o:31:TRP:NE1	36:o:82:ASP:OD1	2.44	0.51
42:u:26:PHE:HE2	42:u:89:ILE:HG13	1.75	0.51
1:A:181:A:N6	1:A:195:A:N7	2.59	0.51
2:B:70:VAL:CG2	2:B:163:VAL:HG22	2.41	0.51
8:H:54:ASP:OD1	8:H:55:THR:N	2.37	0.51
19:S:5:LEU:HD23	52:4:63:ARG:HH21	1.75	0.51
1:A:502:A:H2'	1:A:503:C:O4'	2.11	0.50
3:C:22:TRP:CG	3:C:59:ARG:HD2	2.46	0.50
7:G:111:ARG:NH2	7:G:122:ASN:HB3	2.26	0.50
22:a:888:C:H2'	22:a:889:C:C6	2.46	0.50
29:h:25:TYR:HE1	29:h:29:PHE:HD2	1.59	0.50
30:i:23:LYS:HD2	30:i:28:LEU:HD13	1.93	0.50
30:i:69:ARG:HG2	30:i:90:GLU:OE1	2.11	0.50
39:r:4:ILE:HG13	39:r:106:VAL:HG22	1.93	0.50
1:A:410:G:H2'	1:A:429:U:C5	2.45	0.50
3:C:179:ARG:HG3	3:C:206:GLU:HG3	1.93	0.50
32:k:126:ARG:HG3	32:k:126:ARG:NH2	2.25	0.50
2:B:56:GLU:O	2:B:60:ILE:HG13	2.11	0.50
2:B:60:ILE:HD12	2:B:61:ALA:N	2.27	0.50
9:I:25:ASN:HA	9:I:59:GLU:O	2.12	0.50
17:Q:11:ARG:HH12	17:Q:26:GLU:H	1.57	0.50
22:a:876:C:H2'	22:a:877:A:O4'	2.11	0.50
22:a:2430:A:N3	22:a:2430:A:H2'	2.26	0.50
1:A:662:U:H2'	1:A:663:A:C8	2.46	0.50
1:A:1441:A:C2	36:o:114:LEU:HD12	2.46	0.50
30:i:14:ASP:O	30:i:52:ASP:HB3	2.11	0.50
41:t:10:GLU:OE1	41:t:22:ARG:NH1	2.44	0.50
1:A:123:U:OP1	1:A:312:C:H5'	2.11	0.50
1:A:222:C:H2'	1:A:223:A:H8	1.76	0.50
1:A:1144:G:N2	1:A:1146:A:H62	2.10	0.50
20:T:66:LEU:HG	20:T:67:ILE:HG23	1.94	0.50
22:a:3:U:H2'	22:a:4:U:H6	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:548:G:H2'	22:a:549:G:O4'	2.11	0.50
22:a:600:G:H1'	26:e:100:MET:HE2	1.92	0.50
22:a:1156:A:C8	37:p:51:ARG:HG2	2.47	0.50
22:a:1332:G:N7	22:a:1609:A:O2'	2.40	0.50
22:a:1483:G:H2'	22:a:1484:U:C6	2.47	0.50
40:s:13:ALA:HB3	40:s:33:LYS:HD2	1.93	0.50
1:A:272:C:H2'	1:A:273:U:H6	1.76	0.50
1:A:635:A:H2'	1:A:636:U:C6	2.46	0.50
2:B:32:PHE:HB2	2:B:42:ASN:HB2	1.94	0.50
6:F:86:ARG:NH1	18:R:64:TYR:O	2.36	0.50
22:a:2801:G:H2'	22:a:2802:G:H8	1.77	0.50
38:q:34:GLU:OE1	38:q:60:LYS:HG3	2.11	0.50
1:A:1034:G:O2'	1:A:1035:A:C8	2.65	0.50
1:A:1035:A:C8	1:A:1036:A:H2	2.29	0.50
1:A:1063:C:H3'	1:A:1064:G:H2'	1.93	0.50
1:A:1124:G:H1'	1:A:1125:U:H5	1.75	0.50
1:A:1127:G:H1	1:A:1145:A:H61	1.58	0.50
22:a:1212:G:O2'	22:a:1236:G:N2	2.38	0.50
22:a:1223:G:N2	22:a:1226:A:OP2	2.40	0.50
24:c:24:LEU:HD13	24:c:83:TYR:HB2	1.93	0.50
28:g:86:LYS:CD	28:g:132:VAL:HG22	2.41	0.50
44:w:66:THR:O	44:w:70:GLU:OE1	2.30	0.50
1:A:156:C:H2'	1:A:157:U:O4'	2.12	0.50
1:A:520:A:OP1	12:L:49:LEU:HB2	2.11	0.50
1:A:747:A:H2'	1:A:748:G:O4'	2.12	0.50
5:E:58:ALA:HA	5:E:61:GLN:HG2	1.94	0.50
18:R:33:ILE:HD12	18:R:37:GLY:HA2	1.93	0.50
22:a:995:C:O2	30:i:3:THR:OG1	2.26	0.50
22:a:2395:C:H2'	22:a:2396:G:O4'	2.11	0.50
22:a:2501:C:H4'	22:a:2502:G:OP2	2.11	0.50
22:a:2661:G:H2'	22:a:2662:A:C8	2.47	0.50
24:c:133:ARG:HH11	24:c:187:ASP:CG	2.20	0.50
27:f:60:ILE:HG13	27:f:141:ILE:HD11	1.93	0.50
45:x:31:GLN:OE1	45:x:31:GLN:HA	2.11	0.50
1:A:1328:C:OP1	13:M:28:THR:HG21	2.12	0.50
1:A:1465:A:H2'	1:A:1466:C:C6	2.47	0.50
3:C:187:SER:OG	3:C:188:GLU:N	2.45	0.50
17:Q:17:MET:HG3	17:Q:20:SER:OG	2.12	0.50
22:a:146:A:H2'	22:a:147:C:C6	2.47	0.50
22:a:306:U:H2'	22:a:307:G:O4'	2.12	0.50
22:a:544:C:H2'	22:a:545:U:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:839:U:H2'	22:a:840:C:C6	2.47	0.50
22:a:1212:G:H1'	22:a:1237:A:N6	2.27	0.50
22:a:1397:U:OP2	22:a:1398:C:N4	2.40	0.50
47:z:48:TYR:CE1	47:z:53:LYS:HD2	2.46	0.50
1:A:312:C:H2'	1:A:313:A:C8	2.46	0.49
1:A:769:G:H4'	1:A:1513:A:H4'	1.94	0.49
9:I:36:GLU:HA	9:I:45:ARG:NE	2.27	0.49
19:S:26:GLY:O	19:S:28:LYS:HG2	2.11	0.49
22:a:103:A:H8	22:a:103:A:OP1	1.95	0.49
26:e:46:GLN:O	26:e:88:ARG:NH1	2.45	0.49
45:x:10:SER:N	45:x:13:GLU:OE2	2.44	0.49
1:A:116:A:H61	1:A:313:A:H1'	1.77	0.49
1:A:173:U:H5''	1:A:197:A:O4'	2.12	0.49
4:D:78:GLU:OE2	4:D:93:LEU:HD22	2.11	0.49
13:M:18:ALA:O	13:M:21:SER:OG	2.30	0.49
22:a:279:A:N6	22:a:361:G:H1'	2.27	0.49
22:a:593:U:H2'	22:a:594:U:C6	2.47	0.49
45:x:44:LYS:NZ	45:x:47:ARG:HH11	2.10	0.49
1:A:76:G:H2'	1:A:77:A:C8	2.46	0.49
1:A:482:A:H2'	1:A:483:C:O4'	2.12	0.49
1:A:1169:A:H2'	1:A:1170:A:C8	2.47	0.49
15:O:75:VAL:O	15:O:79:THR:OG1	2.26	0.49
22:a:645:C:O2'	22:a:646:U:H5''	2.11	0.49
22:a:1419:A:O2'	22:a:1421:G:N7	2.36	0.49
32:k:77:ILE:HD13	32:k:108:ALA:HB1	1.94	0.49
1:A:407:U:H2'	1:A:408:A:C8	2.47	0.49
2:B:219:ALA:O	2:B:223:GLU:HG2	2.13	0.49
10:J:7:ARG:NH1	10:J:75:ASP:OD2	2.45	0.49
11:K:90:GLY:O	11:K:93:ARG:HG3	2.12	0.49
22:a:479:A:N3	22:a:481:G:H5''	2.28	0.49
22:a:2038:G:H2'	22:a:2039:U:O4'	2.12	0.49
33:l:39:GLY:HA3	33:l:126:ILE:HD11	1.94	0.49
1:A:43:C:H2'	1:A:44:A:O4'	2.11	0.49
1:A:151:A:C5	1:A:152:A:C8	3.01	0.49
1:A:1004:A:H1'	1:A:1036:A:N6	2.27	0.49
7:G:27:VAL:HG11	7:G:40:GLU:HG3	1.93	0.49
22:a:1210:G:OP1	22:a:1211:C:O2'	2.11	0.49
27:f:58:ALA:HB2	27:f:65:PRO:HD3	1.94	0.49
40:s:24:MET:O	40:s:24:MET:HE3	2.13	0.49
3:C:142:MET:HG3	3:C:170:GLU:CD	2.38	0.49
9:I:43:THR:HA	9:I:46:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2532:G:O2'	22:a:2657:A:N1	2.39	0.49
28:g:55:ARG:HB2	28:g:58:TYR:HD2	1.78	0.49
1:A:376:G:H4'	16:P:5:ARG:NH1	2.28	0.49
1:A:780:A:H5''	11:K:125:LYS:HD3	1.95	0.49
2:B:163:VAL:HG21	2:B:173:ILE:CD1	2.43	0.49
5:E:159:LYS:HB2	5:E:164:ILE:HD11	1.95	0.49
22:a:558:U:OP1	30:i:113:PRO:HD2	2.11	0.49
22:a:2218:G:C6	22:a:2219:U:C4	3.01	0.49
39:r:12:SER:O	39:r:101:SER:OG	2.27	0.49
54:Z:47:A:H2'	54:Z:48:U:H5'	1.95	0.49
55:V:75:C:H2'	55:V:76:A:C8	2.47	0.49
6:F:49:TYR:HH	6:F:86:ARG:HH12	1.60	0.49
7:G:140:ASP:O	7:G:144:MET:HG3	2.11	0.49
9:I:42:GLU:OE2	9:I:45:ARG:NH1	2.40	0.49
1:A:900:A:H2'	1:A:901:A:C8	2.47	0.49
2:B:173:ILE:HD13	2:B:173:ILE:N	2.26	0.49
10:J:18:ILE:O	10:J:22:THR:HG23	2.12	0.49
22:a:518:G:H2'	22:a:519:U:C6	2.48	0.49
32:k:29:LYS:O	32:k:29:LYS:HG2	2.13	0.49
40:s:43:ILE:O	40:s:47:VAL:HG12	2.11	0.49
1:A:501:C:H2'	1:A:502:A:C8	2.47	0.49
22:a:81:G:H2'	22:a:82:U:O4'	2.13	0.49
22:a:611:C:H2'	22:a:612:G:O4'	2.13	0.49
22:a:756:A:H2'	22:a:757:G:O4'	2.13	0.49
29:h:5:LEU:O	29:h:6:LEU:HD23	2.12	0.49
32:k:10:GLU:OE1	32:k:10:GLU:HA	2.12	0.49
1:A:181:A:O2'	1:A:194:C:N4	2.46	0.48
1:A:270:A:H2'	1:A:271:C:H6	1.78	0.48
1:A:491:G:H2'	1:A:492:C:C6	2.48	0.48
1:A:839:C:H2'	1:A:840:C:C6	2.48	0.48
9:I:119:ARG:HD3	9:I:123:ARG:HG3	1.95	0.48
13:M:67:GLY:HA3	27:f:113:ASP:HB2	1.95	0.48
22:a:743:A:O2'	22:a:1659:G:OP1	2.29	0.48
22:a:2557:G:H2'	22:a:2558:C:C6	2.48	0.48
42:u:32:GLY:O	42:u:93:ARG:NH1	2.43	0.48
1:A:108:G:H1	20:T:10:ARG:HG2	1.79	0.48
1:A:235:C:H2'	1:A:236:A:C8	2.48	0.48
1:A:600:A:H2'	1:A:601:G:H8	1.76	0.48
1:A:716:A:N3	11:K:119:IAS:HB2	2.27	0.48
5:E:77:ASN:HB2	5:E:82:GLN:OE1	2.12	0.48
9:I:113:ARG:HD3	14:N:101:TRP:OXT	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:73:ASN:C	12:L:73:ASN:HD22	2.20	0.48
22:a:784:G:H5'	22:a:785:G:OP1	2.11	0.48
22:a:1149:G:H2'	22:a:1150:C:C6	2.48	0.48
22:a:1170:C:H2'	22:a:1171:G:C8	2.48	0.48
22:a:1199:U:H2'	22:a:1200:C:C6	2.48	0.48
22:a:1510:G:H2'	22:a:1511:G:C8	2.48	0.48
22:a:2074:U:H2'	22:a:2075:U:C6	2.48	0.48
22:a:2901:C:H2'	22:a:2902:C:H6	1.77	0.48
42:u:26:PHE:CZ	42:u:42:LEU:HD12	2.48	0.48
1:A:1464:U:H2'	1:A:1465:A:H8	1.77	0.48
5:E:72:ILE:HD12	5:E:145:GLU:HB3	1.95	0.48
8:H:51:VAL:HG22	8:H:59:LEU:HD13	1.94	0.48
9:I:118:LEU:HA	9:I:125:PRO:HD3	1.95	0.48
25:d:55:LYS:HD3	25:d:60:VAL:HG12	1.95	0.48
45:x:10:SER:O	45:x:14:LEU:HG	2.14	0.48
1:A:437:U:H2'	1:A:438:U:O4'	2.13	0.48
1:A:678:U:H2'	1:A:679:C:C6	2.48	0.48
1:A:755:G:OP2	15:O:65:LYS:HD3	2.13	0.48
1:A:1236:A:H2'	1:A:1237:C:C6	2.48	0.48
6:F:67:PRO:O	6:F:70:VAL:HG12	2.14	0.48
6:F:88:MET:HG2	6:F:90:MET:SD	2.54	0.48
9:I:84:THR:HG22	9:I:88:MET:HE1	1.96	0.48
11:K:17:SER:OG	11:K:18:ASP:OD1	2.32	0.48
52:4:59:ARG:HH11	52:4:63:ARG:HD2	1.79	0.48
1:A:350:G:H2'	1:A:351:G:C8	2.49	0.48
1:A:475:C:H2'	1:A:476:U:C6	2.48	0.48
1:A:982:U:H5''	14:N:6:MET:HE3	1.96	0.48
1:A:1272:G:H2'	1:A:1273:C:C6	2.49	0.48
10:J:37:ARG:HG2	10:J:37:ARG:NH1	2.28	0.48
17:Q:19:LYS:HZ3	17:Q:50:ASN:N	2.08	0.48
28:g:17:VAL:HG12	28:g:26:ILE:HG12	1.94	0.48
45:x:44:LYS:HZ3	45:x:47:ARG:HH11	1.60	0.48
1:A:195:A:H2'	1:A:196:A:C8	2.48	0.48
1:A:616:G:O2'	16:P:47:GLU:OE2	2.24	0.48
2:B:105:LYS:H	2:B:105:LYS:CD	2.27	0.48
3:C:153:VAL:HG22	3:C:198:VAL:HG22	1.95	0.48
10:J:11:LYS:HG2	10:J:71:LEU:HD13	1.96	0.48
22:a:2402:U:O2'	22:a:2403:C:O5'	2.30	0.48
23:b:40:U:O2'	23:b:43:C:OP2	2.29	0.48
1:A:1035:A:N9	1:A:1036:A:H2	2.11	0.48
5:E:57:PRO:O	5:E:61:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:50:GLU:O	13:M:53:ILE:HG22	2.13	0.48
13:M:106:ALA:O	13:M:110:LYS:HB2	2.12	0.48
18:R:49:ALA:O	18:R:53:ARG:HG3	2.12	0.48
39:r:21:ALA:HB1	39:r:74:ILE:HG12	1.95	0.48
1:A:152:A:H3'	1:A:153:C:H6	1.77	0.48
2:B:32:PHE:N	2:B:40:ILE:O	2.41	0.48
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.96	0.48
14:N:27:LEU:CD2	14:N:48:LEU:HB2	2.44	0.48
22:a:102:U:O4	45:x:4:LYS:HG3	2.13	0.48
22:a:438:G:H2'	22:a:439:A:C8	2.49	0.48
23:b:112:G:H2'	23:b:113:C:C6	2.48	0.48
24:c:162:VAL:HG11	24:c:174:LEU:HD13	1.96	0.48
29:h:41:LYS:HA	29:h:41:LYS:HE2	1.96	0.48
1:A:167:A:H2'	1:A:168:G:H8	1.78	0.48
1:A:373:A:N1	1:A:391:G:O2'	2.39	0.48
1:A:404:G:N7	4:D:2:ALA:HB3	2.29	0.48
1:A:685:G:O2'	1:A:686:U:H5'	2.14	0.48
2:B:93:ASN:OD1	2:B:93:ASN:N	2.42	0.48
8:H:101:ILE:C	8:H:101:ILE:HD12	2.38	0.48
22:a:322:A:OP2	26:e:163:ASN:HB2	2.14	0.48
22:a:765:C:H2'	22:a:766:U:C6	2.49	0.48
22:a:927:A:H2'	22:a:928:A:C8	2.48	0.48
22:a:2632:A:H2'	22:a:2633:G:C8	2.49	0.48
22:a:2740:A:H2'	22:a:2741:A:C8	2.49	0.48
1:A:187:G:O2'	1:A:189:A:N6	2.44	0.48
1:A:237:G:H5''	17:Q:27:ARG:NH2	2.28	0.48
2:B:8:ASP:OD1	2:B:9:MET:N	2.46	0.48
2:B:114:LEU:HD12	2:B:144:LEU:HB3	1.94	0.48
2:B:187:VAL:O	2:B:201:PRO:HA	2.14	0.48
3:C:54:ARG:HD3	3:C:69:HIS:ND1	2.29	0.48
4:D:7:PRO:HB2	4:D:10:LYS:HG3	1.96	0.48
4:D:98:LEU:O	4:D:102:VAL:HG12	2.14	0.48
11:K:113:VAL:HA	18:R:73:ARG:HH11	1.79	0.48
17:Q:28:PHE:CE1	17:Q:39:LYS:HG3	2.49	0.48
22:a:810:U:C4	32:k:29:LYS:O	2.67	0.48
22:a:2412:A:H2'	22:a:2413:G:O4'	2.14	0.48
27:f:5:HIS:HB2	27:f:97:TRP:CG	2.48	0.48
1:A:275:G:H5'	17:Q:16:LYS:HD3	1.96	0.47
1:A:496:A:H5'	1:A:497:G:OP2	2.14	0.47
1:A:637:C:H2'	1:A:638:U:C6	2.49	0.47
1:A:1225:A:H2'	1:A:1226:C:C5	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:VAL:HG23	4:D:107:PHE:HD2	1.79	0.47
5:E:101:GLU:OE1	5:E:122:ASN:ND2	2.47	0.47
22:a:1108:U:H2'	22:a:1109:C:C6	2.48	0.47
55:V:58:1MA:O2'	55:V:60:U:OP2	2.28	0.47
2:B:105:LYS:H	2:B:105:LYS:HD3	1.78	0.47
3:C:40:ARG:HG2	3:C:55:ILE:HG21	1.96	0.47
6:F:14:GLN:OE1	6:F:14:GLN:N	2.46	0.47
6:F:29:ILE:O	6:F:34:GLY:N	2.40	0.47
27:f:136:ILE:HD13	27:f:143:TYR:HD1	1.80	0.47
28:g:55:ARG:HB2	28:g:58:TYR:CD2	2.48	0.47
1:A:254:G:O2'	17:Q:18:GLU:O	2.32	0.47
17:Q:58:VAL:CG1	17:Q:80:GLU:HB3	2.44	0.47
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.96	0.47
1:A:223:A:H2'	1:A:224:U:H6	1.80	0.47
1:A:451:A:N6	1:A:481:G:H5'	2.29	0.47
4:D:126:ASN:OD1	4:D:142:VAL:N	2.37	0.47
5:E:113:ALA:O	5:E:117:VAL:HG22	2.15	0.47
10:J:87:LEU:HD23	10:J:87:LEU:HA	1.67	0.47
11:K:70:CYS:O	11:K:74:VAL:HG22	2.14	0.47
16:P:2:VAL:HG11	16:P:60:TRP:CE3	2.49	0.47
22:a:284:U:H2'	22:a:285:G:C8	2.49	0.47
22:a:1311:G:N2	22:a:1603:A:H62	2.11	0.47
22:a:1509:A:O2'	22:a:1510:G:O5'	2.33	0.47
22:a:2329:U:H2'	22:a:2330:G:C8	2.48	0.47
22:a:2625:G:H2'	22:a:2626:C:O4'	2.15	0.47
35:n:58:ILE:HG22	35:n:62:LEU:HD11	1.97	0.47
42:u:4:ILE:HG21	42:u:42:LEU:HD22	1.97	0.47
4:D:70:ARG:O	4:D:74:ASN:OD1	2.33	0.47
5:E:54:ARG:HG3	5:E:54:ARG:NH1	2.28	0.47
16:P:44:SER:O	16:P:47:GLU:HB2	2.13	0.47
22:a:634:C:H2'	22:a:635:C:C6	2.49	0.47
22:a:1814:G:OP2	22:a:1815:A:O2'	2.29	0.47
22:a:2401:U:O2'	22:a:2402:U:H2'	2.14	0.47
22:a:276:U:H1'	22:a:278:A:H62	1.79	0.47
22:a:893:C:H2'	22:a:894:U:O4'	2.14	0.47
22:a:1047:G:N2	22:a:1110:G:O2'	2.45	0.47
25:d:108:ASP:OD1	25:d:173:GLN:HA	2.14	0.47
28:g:42:GLU:O	28:g:52:PHE:HA	2.14	0.47
42:u:9:ARG:NH2	42:u:11:GLU:O	2.48	0.47
1:A:72:A:H61	1:A:98:A:H2	1.63	0.47
1:A:519:C:H2'	1:A:520:A:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:A:H5''	12:L:21:VAL:HG21	1.97	0.47
1:A:968:A:C6	1:A:1062:U:O2'	2.67	0.47
1:A:1064:G:H1'	1:A:1190:G:N2	2.29	0.47
3:C:5:VAL:HG21	3:C:10:ILE:HD12	1.96	0.47
6:F:33:GLU:HG3	6:F:33:GLU:O	2.14	0.47
7:G:67:GLU:HG2	7:G:70:ARG:HH12	1.79	0.47
13:M:9:ILE:HD12	13:M:18:ALA:HB1	1.96	0.47
14:N:38:ASP:OD1	14:N:41:ARG:NH1	2.47	0.47
22:a:588:U:H2'	22:a:589:U:C6	2.49	0.47
22:a:638:G:H2'	22:a:639:U:C6	2.49	0.47
22:a:871:U:H2'	22:a:872:U:C6	2.50	0.47
22:a:2086:U:H2'	22:a:2087:G:C8	2.50	0.47
22:a:2305:U:H5''	27:f:131:GLY:HA3	1.96	0.47
22:a:2455:G:H2'	22:a:2456:C:C6	2.50	0.47
25:d:121:THR:HB	25:d:127:PHE:CD2	2.49	0.47
27:f:49:LEU:HD22	27:f:148:ARG:NH1	2.30	0.47
30:i:111:LYS:HD2	30:i:111:LYS:N	2.29	0.47
35:n:27:VAL:CG2	35:n:40:ILE:HD12	2.44	0.47
38:q:41:ILE:HD12	38:q:54:VAL:HG11	1.97	0.47
40:s:5:GLU:N	40:s:5:GLU:OE2	2.47	0.47
41:t:94:ARG:CB	41:t:103:ILE:HD12	2.45	0.47
46:y:6:LYS:HB2	46:y:58:GLU:HB2	1.95	0.47
51:3:26:ILE:HG13	51:3:26:ILE:O	2.14	0.47
55:V:10:2MG:H2'	55:V:11:C:C6	2.49	0.47
55:V:13:C:H2'	55:V:14:A:H5''	1.96	0.47
5:E:15:LEU:HD12	5:E:37:THR:HG22	1.97	0.47
10:J:67:ILE:HG13	14:N:96:LEU:HD12	1.97	0.47
22:a:68:G:N2	22:a:74:A:OP2	2.45	0.47
22:a:319:G:H2'	22:a:320:A:O4'	2.15	0.47
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.96	0.47
1:A:77:A:H2'	1:A:78:A:H8	1.80	0.47
1:A:131:A:H2'	1:A:132:C:H6	1.80	0.47
1:A:175:C:O2'	1:A:1447:A:N1	2.39	0.47
1:A:524:G:H2'	1:A:525:C:C6	2.50	0.47
14:N:33:ASP:CG	14:N:36:ALA:HB2	2.40	0.47
17:Q:11:ARG:NH2	17:Q:26:GLU:HB3	2.30	0.47
22:a:813:U:H2'	22:a:814:C:C6	2.50	0.47
22:a:1842:G:H2'	22:a:1843:C:C6	2.50	0.47
55:V:10:2MG:O2'	55:V:11:C:OP1	2.30	0.47
1:A:1397:C:OP2	5:E:29:ARG:NH2	2.48	0.47
4:D:85:ASN:HB2	4:D:88:GLU:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:66:PHE:CD2	8:H:67:GLN:HG2	2.49	0.47
22:a:703:U:H2'	22:a:704:G:O4'	2.15	0.47
22:a:851:C:O2'	46:y:43:ALA:O	2.32	0.47
22:a:1723:G:H2'	22:a:1724:G:O4'	2.15	0.47
22:a:2065:C:H2'	22:a:2066:C:C6	2.50	0.47
22:a:2483:C:N3	33:l:123:LYS:NZ	2.57	0.47
1:A:109:A:H5'	1:A:110:C:C5	2.49	0.46
1:A:218:U:H2'	1:A:219:U:O4'	2.15	0.46
1:A:268:U:H2'	1:A:269:C:H6	1.80	0.46
1:A:968:A:C8	1:A:1062:U:H4'	2.49	0.46
9:I:33:ARG:HH11	9:I:37:GLN:HG2	1.79	0.46
22:a:1591:A:H2'	22:a:1592:C:C6	2.50	0.46
25:d:12:THR:OG1	25:d:13:ARG:N	2.48	0.46
50:2:24:HIS:ND1	50:2:25:LYS:O	2.39	0.46
54:Z:24:C:H2'	54:Z:25:U:C6	2.50	0.46
1:A:148:G:H1	1:A:174:A:N6	2.12	0.46
1:A:1218:C:H2'	1:A:1219:A:C8	2.50	0.46
2:B:100:MET:HA	2:B:107:VAL:HG21	1.97	0.46
5:E:144:LEU:HD23	5:E:144:LEU:HA	1.80	0.46
6:F:41:ASP:OD1	6:F:58:HIS:NE2	2.48	0.46
22:a:1027:A:C2	22:a:2488:G:H5'	2.50	0.46
22:a:1046:A:H3'	22:a:1047:G:H5'	1.98	0.46
22:a:2658:C:H2'	22:a:2659:G:O4'	2.15	0.46
33:l:118:LYS:HE3	33:l:118:LYS:HB2	1.64	0.46
54:Z:67:C:O2'	54:Z:68:C:OP1	2.32	0.46
1:A:312:C:H2'	1:A:313:A:H8	1.80	0.46
1:A:473:U:C2	1:A:474:G:C8	3.03	0.46
3:C:66:VAL:HB	3:C:101:ILE:HD13	1.96	0.46
9:I:88:MET:HE1	9:I:104:VAL:HG22	1.98	0.46
16:P:52:LEU:HD23	16:P:78:VAL:HG11	1.97	0.46
21:U:39:GLU:HA	21:U:39:GLU:OE2	2.14	0.46
22:a:2064:C:H2'	22:a:2065:C:C6	2.51	0.46
24:c:161:TYR:HB3	24:c:194:GLU:HG2	1.96	0.46
30:i:110:PRO:O	30:i:115:GLY:HA3	2.15	0.46
33:l:112:LEU:O	33:l:115:GLU:HG3	2.15	0.46
41:t:22:ARG:NH1	41:t:22:ARG:HB3	2.30	0.46
44:w:17:ASN:OD1	44:w:27:ARG:HD2	2.15	0.46
52:4:12:ILE:C	52:4:12:ILE:HD12	2.41	0.46
1:A:444:G:C6	1:A:491:G:C6	3.03	0.46
1:A:1026:G:HO2'	1:A:1027:C:P	2.37	0.46
3:C:139:GLN:O	3:C:143:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:188:ARG:HE	4:D:197:GLU:CD	2.24	0.46
22:a:1794:A:H2'	22:a:1795:C:C6	2.50	0.46
22:a:2345:G:H4'	22:a:2346:A:O5'	2.15	0.46
52:4:26:SER:OG	52:4:28:VAL:HG12	2.15	0.46
1:A:1122:U:H2'	1:A:1123:U:C6	2.50	0.46
1:A:1131:G:H5'	9:I:5:GLN:HE22	1.80	0.46
1:A:1206:G:H2'	1:A:1207:2MG:O4'	2.16	0.46
3:C:56:VAL:O	3:C:66:VAL:HA	2.15	0.46
7:G:68:ASN:O	7:G:138:ARG:NH2	2.48	0.46
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.98	0.46
18:R:71:THR:HG22	18:R:74:HIS:CD2	2.50	0.46
22:a:219:A:H2'	22:a:220:G:O4'	2.16	0.46
22:a:595:C:H2'	22:a:596:U:H6	1.81	0.46
22:a:693:A:O2'	22:a:1353:A:N3	2.45	0.46
22:a:1510:G:H2'	22:a:1511:G:H8	1.81	0.46
22:a:1932:A:H2'	22:a:1933:G:O4'	2.15	0.46
22:a:2687:U:H2'	22:a:2688:G:O4'	2.15	0.46
27:f:69:LYS:HA	27:f:84:PRO:HA	1.97	0.46
29:h:30:LEU:HB3	29:h:36:ALA:HB3	1.98	0.46
1:A:35:G:H2'	1:A:36:C:C6	2.51	0.46
1:A:1009:U:H2'	1:A:1010:U:H6	1.80	0.46
3:C:79:LYS:O	3:C:82:GLU:HG3	2.16	0.46
7:G:113:ASP:OD2	7:G:122:ASN:ND2	2.49	0.46
11:K:28:ASN:O	11:K:58:SER:OG	2.32	0.46
22:a:1340:U:OP1	40:s:19:LYS:NZ	2.47	0.46
22:a:1710:G:H4'	22:a:2858:C:O2	2.15	0.46
26:e:119:ILE:HD11	26:e:185:LYS:HD2	1.97	0.46
8:H:10:MET:HG3	8:H:27:MET:SD	2.55	0.46
9:I:12:ARG:O	9:I:13:LYS:C	2.59	0.46
11:K:34:ILE:HD12	11:K:74:VAL:HG21	1.98	0.46
12:L:23:ALA:HA	12:L:61:PHE:CD2	2.51	0.46
17:Q:19:LYS:O	17:Q:48:ASP:N	2.43	0.46
22:a:160:A:N3	22:a:2208:C:O2'	2.48	0.46
22:a:644:A:H2'	22:a:645:C:O4'	2.15	0.46
22:a:858:G:OP1	43:v:78:LYS:HE3	2.15	0.46
22:a:959:A:H2'	22:a:960:A:C8	2.50	0.46
22:a:1902:C:H4'	24:c:242:LYS:O	2.15	0.46
22:a:2847:U:H2'	22:a:2848:G:O4'	2.16	0.46
24:c:87:ARG:HG3	24:c:89:ALA:H	1.79	0.46
41:t:100:SER:OG	41:t:100:SER:O	2.31	0.46
1:A:150:U:H2'	1:A:151:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:C:C2'	1:A:179:A:H5'	2.46	0.46
1:A:264:C:H2'	1:A:265:G:O4'	2.16	0.46
2:B:41:ILE:HD13	2:B:202:GLY:HA2	1.96	0.46
8:H:96:MET:HE3	8:H:99:LEU:HB3	1.96	0.46
13:M:71:ARG:NH2	27:f:113:ASP:OD1	2.44	0.46
17:Q:20:SER:HB3	17:Q:71:LYS:NZ	2.31	0.46
22:a:139:U:H3'	22:a:140:C:H6	1.81	0.46
22:a:285:G:H2'	22:a:285:G:N3	2.31	0.46
22:a:2193:G:H2'	22:a:2194:U:H6	1.80	0.46
22:a:2484:G:OP1	33:l:44:ARG:HD2	2.16	0.46
39:r:33:LEU:HA	39:r:33:LEU:HD23	1.78	0.46
42:u:20:LEU:HD23	42:u:27:PRO:HD3	1.98	0.46
1:A:836:G:O6	1:A:850:U:O4	2.34	0.46
1:A:881:G:H2'	1:A:882:C:O4'	2.16	0.46
1:A:1264:U:H2'	1:A:1265:C:C6	2.51	0.46
6:F:88:MET:CE	18:R:61:ARG:HG2	2.37	0.46
21:U:52:ALA:HA	21:U:55:ARG:HG2	1.98	0.46
22:a:849:A:H2'	22:a:850:U:H6	1.81	0.46
22:a:1341:G:C2	22:a:1398:C:H4'	2.51	0.46
22:a:1418:G:N1	22:a:1579:A:OP2	2.40	0.46
22:a:1802:A:H2'	22:a:1803:A:C8	2.50	0.46
22:a:2196:C:H2'	22:a:2197:U:C6	2.51	0.46
26:e:145:ASP:HA	26:e:166:LYS:O	2.15	0.46
29:h:34:GLY:C	29:h:36:ALA:H	2.24	0.46
1:A:408:A:H2'	1:A:409:U:H6	1.80	0.46
1:A:453:G:H2'	1:A:454:G:O4'	2.15	0.46
1:A:547:A:OP2	4:D:2:ALA:HA	2.16	0.46
1:A:1162:C:H2'	1:A:1163:A:H8	1.80	0.46
8:H:113:ASP:OD1	8:H:113:ASP:N	2.48	0.46
22:a:600:G:H2'	22:a:601:C:C6	2.50	0.46
25:d:128:ARG:HA	25:d:128:ARG:NE	2.30	0.46
33:l:110:GLU:O	33:l:114:ARG:HG3	2.15	0.46
36:o:51:ARG:CZ	36:o:53:ARG:HG3	2.46	0.46
1:A:406:G:H21	4:D:116:GLN:HE22	1.64	0.45
2:B:191:SER:OG	2:B:192:ASP:N	2.47	0.45
2:B:217:VAL:HA	2:B:220:THR:HG22	1.97	0.45
13:M:93:ARG:HA	13:M:93:ARG:HD3	1.70	0.45
19:S:41:PHE:HB2	19:S:44:MET:SD	2.57	0.45
22:a:139:U:H3'	22:a:140:C:C6	2.51	0.45
22:a:1204:A:H4'	22:a:1205:A:O5'	2.16	0.45
22:a:1319:C:O2'	22:a:1320:C:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2745:C:H2'	22:a:2746:U:C6	2.51	0.45
44:w:6:GLN:HG2	44:w:76:GLU:OE2	2.16	0.45
1:A:41:G:H2'	1:A:42:G:C8	2.51	0.45
1:A:272:C:H2'	1:A:273:U:C6	2.51	0.45
1:A:418:C:H2'	1:A:419:C:C6	2.52	0.45
1:A:736:C:H2'	1:A:737:C:C6	2.51	0.45
1:A:1158:C:C4	1:A:1160:G:C8	3.05	0.45
2:B:69:PHE:O	2:B:91:PHE:HA	2.15	0.45
4:D:54:GLN:HG2	4:D:199:LEU:HB3	1.98	0.45
12:L:114:ARG:HB3	12:L:119:VAL:HB	1.98	0.45
22:a:1242:U:H2'	22:a:1243:C:C6	2.52	0.45
22:a:1405:U:H2'	22:a:1406:U:H6	1.80	0.45
24:c:35:GLU:CD	24:c:64:ILE:HD11	2.41	0.45
46:y:23:THR:HG23	46:y:47:MET:HG2	1.98	0.45
1:A:3:A:H5''	1:A:4:U:O4'	2.17	0.45
1:A:875:U:O2'	8:H:15:ARG:NH1	2.49	0.45
1:A:1220:G:OP2	14:N:53:ARG:NH1	2.23	0.45
4:D:97:ARG:HA	4:D:135:TYR:O	2.16	0.45
9:I:55:VAL:HG23	9:I:57:MET:HB3	1.98	0.45
12:L:110:ARG:O	12:L:111:LYS:HD3	2.16	0.45
22:a:639:U:H2'	22:a:640:C:H6	1.80	0.45
22:a:657:U:H2'	22:a:658:U:C6	2.51	0.45
22:a:1548:A:H2'	22:a:1549:A:H8	1.79	0.45
22:a:1607:C:H4'	22:a:1608:A:O5'	2.16	0.45
22:a:1720:U:H2'	22:a:1721:G:O4'	2.17	0.45
22:a:2723:C:H2'	22:a:2724:U:O4'	2.17	0.45
31:j:7:MET:HE2	31:j:7:MET:HB2	1.69	0.45
37:p:61:TRP:CH2	37:p:93:LYS:HB2	2.51	0.45
37:p:81:ASN:ND2	37:p:85:LYS:HE3	2.31	0.45
55:V:22:G:H2'	55:V:23:A:C8	2.50	0.45
1:A:151:A:C2	1:A:152:A:H1'	2.52	0.45
1:A:483:C:O5'	1:A:483:C:H6	2.00	0.45
2:B:107:VAL:O	2:B:111:ILE:HG12	2.16	0.45
8:H:50:LYS:NZ	8:H:52:GLU:OE1	2.49	0.45
13:M:81:MET:HE3	13:M:81:MET:HB2	1.67	0.45
22:a:173:A:H2'	22:a:174:U:C6	2.51	0.45
22:a:1853:A:N3	22:a:2233:U:O2'	2.48	0.45
27:f:34:ILE:HD12	27:f:96:MET:HG2	1.98	0.45
28:g:155:GLU:OE2	28:g:158:LYS:N	2.47	0.45
34:m:79:LEU:HD23	34:m:83:LEU:HD12	1.98	0.45
39:r:82:MET:HB2	39:r:98:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:V:44:G:H2'	55:V:45:G:O4'	2.17	0.45
1:A:658:C:H1'	15:O:22:THR:HG21	1.97	0.45
2:B:154:MET:HG2	2:B:156:GLY:O	2.15	0.45
2:B:199:VAL:HG12	2:B:201:PRO:HD3	1.98	0.45
10:J:90:LEU:HD12	10:J:90:LEU:HA	1.69	0.45
22:a:71:A:N1	22:a:114:U:H1'	2.31	0.45
22:a:483:A:C8	41:t:45:HIS:HD2	2.35	0.45
22:a:549:G:H2'	22:a:550:C:H6	1.80	0.45
22:a:1020:A:C2	22:a:1141:U:C2	3.05	0.45
22:a:2804:U:H2'	22:a:2805:C:C6	2.51	0.45
24:c:66:ASP:OD2	24:c:102:ARG:NH1	2.50	0.45
36:o:37:LYS:H	36:o:37:LYS:HE2	1.81	0.45
55:V:37:12A:N1	55:V:37:12A:N	2.64	0.45
1:A:323:U:H2'	1:A:324:G:O4'	2.17	0.45
1:A:491:G:H2'	1:A:492:C:H6	1.80	0.45
1:A:545:C:H5'	4:D:69:GLU:HG2	1.97	0.45
1:A:1373:G:H5''	7:G:36:LYS:HE2	1.99	0.45
12:L:38:TYR:CE2	12:L:40:THR:HG23	2.51	0.45
34:m:24:MET:HE1	34:m:40:LYS:HD3	1.99	0.45
1:A:161:A:H2'	1:A:162:A:C8	2.51	0.45
1:A:169:C:H2'	1:A:170:U:H6	1.81	0.45
1:A:678:U:H2'	1:A:679:C:H6	1.82	0.45
1:A:1092:A:H5''	7:G:4:ARG:HH12	1.81	0.45
2:B:128:LYS:HE2	2:B:128:LYS:HB2	1.86	0.45
9:I:42:GLU:OE2	9:I:45:ARG:HD2	2.15	0.45
22:a:2796:U:H3	22:a:2799:A:N6	2.14	0.45
26:e:168:ASP:OD1	26:e:169:VAL:N	2.50	0.45
30:i:9:GLU:CD	30:i:9:GLU:H	2.24	0.45
33:l:105:MET:HE2	33:l:117:PHE:CE1	2.52	0.45
40:s:62:VAL:O	40:s:64:LYS:NZ	2.41	0.45
1:A:123:U:H2'	1:A:124:C:C6	2.52	0.45
1:A:1249:C:O2'	9:I:70:GLY:O	2.30	0.45
2:B:212:LEU:HD12	2:B:212:LEU:HA	1.85	0.45
13:M:88:GLY:O	13:M:92:ARG:HG3	2.16	0.45
23:b:53:A:H8	23:b:53:A:O5'	1.99	0.45
28:g:90:VAL:HG12	28:g:91:GLY:H	1.82	0.45
41:t:99:ASN:O	41:t:101:GLU:N	2.50	0.45
45:x:39:GLN:HG2	45:x:41:HIS:HE1	1.79	0.45
1:A:77:A:H2'	1:A:78:A:C8	2.51	0.45
1:A:334:C:H2'	1:A:335:C:H6	1.82	0.45
1:A:1297:G:N2	7:G:114:LYS:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:111:THR:HG23	21:U:3:VAL:HB	1.99	0.45
22:a:150:U:H2'	22:a:151:C:C6	2.52	0.45
22:a:283:G:H2'	22:a:284:U:O4'	2.16	0.45
22:a:566:U:H2'	22:a:567:U:O4'	2.17	0.45
26:e:47:LYS:HA	26:e:51:GLU:OE2	2.17	0.45
26:e:124:PHE:HE1	26:e:141:MET:SD	2.40	0.45
28:g:84:THR:HA	28:g:133:LEU:O	2.16	0.45
1:A:486:U:H2'	1:A:487:A:H8	1.79	0.45
1:A:487:A:H2'	1:A:488:C:O4'	2.16	0.45
1:A:1410:A:H2'	1:A:1411:C:C6	2.53	0.45
2:B:50:PHE:CD1	2:B:200:ILE:HD13	2.51	0.45
4:D:167:LYS:HA	4:D:167:LYS:HD3	1.72	0.45
19:S:29:LYS:HB3	19:S:30:PRO:HD3	1.99	0.45
22:a:434:U:O2	22:a:436:C:N4	2.49	0.45
22:a:595:C:H2'	22:a:596:U:C6	2.52	0.45
22:a:1796:U:H2'	22:a:1797:G:C8	2.52	0.45
23:b:48:U:H2'	23:b:49:C:H6	1.81	0.45
39:r:13:SER:HB3	39:r:16:LYS:HD2	1.99	0.45
43:v:30:SER:HA	43:v:65:GLY:O	2.17	0.45
55:V:8:U:O2'	55:V:21:A:N1	2.38	0.45
1:A:362:G:N2	1:A:365:U:OP2	2.47	0.44
1:A:1040:U:O2'	1:A:1041:G:H5'	2.16	0.44
1:A:1342:C:H2'	1:A:1343:G:C8	2.53	0.44
2:B:68:LEU:HD23	2:B:161:LEU:HD21	1.99	0.44
2:B:87:CYS:O	2:B:89:GLN:HG2	2.17	0.44
21:U:63:GLU:HB3	21:U:67:ARG:NH2	2.31	0.44
22:a:471:A:H2'	22:a:472:A:O4'	2.17	0.44
22:a:581:C:H2'	22:a:582:A:C8	2.52	0.44
22:a:1483:G:H2'	22:a:1484:U:H6	1.82	0.44
22:a:1495:A:H2'	22:a:1496:A:C8	2.52	0.44
22:a:1499:C:H2'	22:a:1500:G:H8	1.80	0.44
22:a:1715:G:O2'	22:a:1743:G:O6	2.23	0.44
26:e:130:LYS:HE3	26:e:130:LYS:HB3	1.72	0.44
30:i:92:MET:HE3	30:i:99:ARG:HB3	1.99	0.44
31:j:114:LYS:HE2	31:j:114:LYS:HB2	1.78	0.44
33:l:57:VAL:HG11	33:l:105:MET:SD	2.57	0.44
1:A:362:G:O2'	1:A:364:A:N7	2.48	0.44
1:A:501:C:H2'	1:A:502:A:H8	1.81	0.44
1:A:625:U:H2'	1:A:626:G:C8	2.52	0.44
1:A:1005:A:H2'	1:A:1006:G:O4'	2.17	0.44
1:A:1162:C:H2'	1:A:1163:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:MET:HE1	2:B:187:VAL:CG1	2.47	0.44
8:H:22:LYS:O	8:H:65:TYR:OH	2.33	0.44
15:O:32:LEU:HD21	15:O:62:GLN:HE22	1.81	0.44
21:U:34:ARG:NE	21:U:34:ARG:HA	2.32	0.44
22:a:2295:C:OP1	35:n:10:ARG:NH2	2.50	0.44
24:c:80:ARG:NE	24:c:82:GLU:OE1	2.45	0.44
25:d:11:MET:HE2	25:d:11:MET:HB3	1.82	0.44
1:A:452:A:H2'	1:A:453:G:O4'	2.17	0.44
1:A:483:C:OP2	1:A:484:G:O2'	2.31	0.44
1:A:985:C:H2'	1:A:986:U:C6	2.52	0.44
4:D:156:LYS:O	4:D:160:GLU:HG2	2.18	0.44
20:T:56:PRO:O	20:T:60:ARG:HG3	2.17	0.44
22:a:1677:A:H2'	22:a:1678:A:C8	2.52	0.44
22:a:2020:A:H5'	47:z:9:THR:CG2	2.47	0.44
22:a:2065:C:H2'	22:a:2066:C:H6	1.81	0.44
22:a:2809:A:H2'	22:a:2810:A:C8	2.53	0.44
37:p:83:LEU:HD23	37:p:113:ALA:HB2	1.99	0.44
39:r:20:VAL:HG11	39:r:44:ALA:HA	2.00	0.44
40:s:56:GLU:OE2	40:s:88:LYS:HA	2.17	0.44
41:t:95:PHE:CD2	41:t:100:SER:HA	2.53	0.44
1:A:381:C:H2'	1:A:382:A:O4'	2.18	0.44
2:B:166:ALA:HB3	2:B:191:SER:HG	1.83	0.44
4:D:102:VAL:CG1	4:D:114:ALA:HB1	2.41	0.44
14:N:28:LYS:HA	14:N:31:ILE:CD1	2.45	0.44
14:N:67:THR:CG2	14:N:83:LYS:HE3	2.48	0.44
22:a:997:G:OP1	37:p:92:ARG:HD2	2.18	0.44
37:p:17:ILE:HA	37:p:17:ILE:HD13	1.78	0.44
45:x:16:THR:O	45:x:20:ASN:ND2	2.45	0.44
1:A:271:C:H2'	1:A:272:C:H6	1.82	0.44
22:a:2097:A:H2'	22:a:2098:U:H6	1.82	0.44
24:c:35:GLU:OE2	24:c:64:ILE:HD11	2.18	0.44
28:g:91:GLY:HA2	28:g:160:LYS:HE2	1.99	0.44
47:z:29:SER:O	47:z:37:LYS:HA	2.18	0.44
52:4:12:ILE:HD13	52:4:32:LEU:HD13	2.00	0.44
1:A:109:A:H2'	1:A:326:G:N2	2.33	0.44
1:A:1123:U:O2'	1:A:1124:G:H5'	2.17	0.44
1:A:1233:G:H5'	9:I:119:ARG:NH2	2.32	0.44
1:A:1510:C:H2'	1:A:1511:G:C8	2.53	0.44
9:I:57:MET:HA	9:I:60:LYS:NZ	2.32	0.44
10:J:7:ARG:HG3	10:J:73:LEU:HD11	2.00	0.44
13:M:64:VAL:HG13	13:M:68:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:78:LYS:HB3	13:M:78:LYS:HE2	1.69	0.44
19:S:24:GLU:OE2	19:S:25:SER:OG	2.30	0.44
22:a:362:A:H2'	22:a:362:A:N3	2.32	0.44
22:a:882:G:H2'	22:a:883:G:H8	1.83	0.44
22:a:1796:U:H2'	22:a:1797:G:H8	1.83	0.44
40:s:5:GLU:OE2	45:x:19:LEU:HD21	2.18	0.44
40:s:64:LYS:N	40:s:64:LYS:HD2	2.32	0.44
1:A:592:G:H2'	1:A:593:U:H6	1.83	0.44
1:A:918:A:H2'	1:A:919:A:C8	2.53	0.44
1:A:967:5MC:OP2	1:A:968:A:O2'	2.20	0.44
1:A:1361:G:H2'	1:A:1362:A:O4'	2.17	0.44
1:A:1363:A:O2'	1:A:1365:G:N7	2.40	0.44
6:F:18:VAL:HG11	6:F:58:HIS:NE2	2.32	0.44
7:G:58:GLU:H	7:G:58:GLU:HG2	1.64	0.44
22:a:81:G:C2	22:a:82:U:H1'	2.53	0.44
22:a:424:G:H2'	22:a:425:G:O4'	2.18	0.44
22:a:476:G:H4'	22:a:502:A:N1	2.32	0.44
22:a:948:C:H1'	22:a:984:A:C8	2.53	0.44
22:a:2632:A:H2'	22:a:2633:G:H8	1.83	0.44
22:a:2902:C:H3'	22:a:2903:U:C6	2.53	0.44
38:q:5:PHE:HB3	38:q:59:ILE:HD12	2.00	0.44
40:s:1:MET:HE2	40:s:1:MET:HA	1.99	0.44
54:Z:52:C:H2'	54:Z:53:G:O4'	2.17	0.44
1:A:373:A:O2'	1:A:481:G:C2	2.71	0.44
1:A:908:A:H2'	1:A:909:A:C8	2.53	0.44
7:G:99:LEU:HB3	7:G:103:TRP:CZ2	2.53	0.44
9:I:51:PRO:O	9:I:55:VAL:HG22	2.18	0.44
22:a:170:U:H2'	22:a:171:U:H6	1.83	0.44
22:a:247:G:H4'	22:a:386:G:C5	2.53	0.44
22:a:362:A:C4	22:a:363:G:C8	3.05	0.44
22:a:1746:A:H2'	22:a:1747:U:C6	2.53	0.44
22:a:2895:G:H2'	22:a:2896:C:C6	2.53	0.44
26:e:138:LEU:HD23	26:e:138:LEU:HA	1.63	0.44
27:f:80:ARG:HB2	27:f:83:TYR:CE1	2.53	0.44
34:m:106:ASP:OD1	34:m:106:ASP:N	2.50	0.44
47:z:38:HIS:ND1	47:z:39:LEU:O	2.50	0.44
1:A:513:C:H2'	1:A:514:C:C6	2.53	0.44
1:A:868:C:H2'	1:A:869:G:O4'	2.18	0.44
1:A:1464:U:H2'	1:A:1465:A:C8	2.52	0.44
2:B:108:ARG:HG2	2:B:108:ARG:HH11	1.83	0.44
12:L:73:ASN:C	12:L:73:ASN:ND2	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:361:G:H8	22:a:361:G:OP2	2.01	0.44
22:a:436:C:H2'	22:a:437:U:H6	1.83	0.44
22:a:594:U:H2'	22:a:595:C:C6	2.52	0.44
22:a:2798:U:H4'	22:a:2799:A:H5'	2.00	0.44
23:b:36:C:N4	23:b:49:C:O2	2.51	0.44
26:e:1:MET:HB2	26:e:16:GLU:OE1	2.18	0.44
31:j:71:ARG:HH21	31:j:104:THR:HG23	1.83	0.44
1:A:451:A:H61	1:A:481:G:H5'	1.83	0.43
1:A:599:C:H4'	8:H:122:GLY:C	2.43	0.43
1:A:604:G:H2'	1:A:605:U:O4'	2.18	0.43
1:A:1356:G:H2'	1:A:1357:A:C8	2.52	0.43
2:B:166:ALA:HB3	2:B:191:SER:OG	2.18	0.43
22:a:580:U:H2'	22:a:581:C:C6	2.53	0.43
22:a:620:G:H4'	22:a:621:A:O5'	2.18	0.43
22:a:1579:A:H2'	22:a:1580:A:C8	2.53	0.43
22:a:1728:C:O2'	22:a:1729:U:H5''	2.17	0.43
25:d:157:LYS:HE3	25:d:157:LYS:HB2	1.76	0.43
41:t:73:PHE:CZ	41:t:78:GLY:HA2	2.52	0.43
41:t:84:GLY:HA3	41:t:95:PHE:CE1	2.53	0.43
22:a:636:G:N1	32:k:76:GLU:OE2	2.36	0.43
23:b:24:G:N7	23:b:56:G:H2'	2.33	0.43
31:j:4:GLU:OE2	31:j:23:LYS:HA	2.17	0.43
40:s:9:LYS:HE2	40:s:9:LYS:HA	2.00	0.43
1:A:33:A:H2'	1:A:34:C:C6	2.53	0.43
1:A:198:G:H2'	1:A:199:A:H8	1.83	0.43
1:A:222:C:H2'	1:A:223:A:C8	2.53	0.43
1:A:1201:A:H4'	1:A:1202:U:O5'	2.17	0.43
2:B:203:ASN:O	2:B:213:TYR:OH	2.25	0.43
3:C:86:LYS:HG3	3:C:87:LEU:N	2.32	0.43
3:C:125:GLU:O	3:C:127:ARG:HD3	2.19	0.43
4:D:146:ARG:HH12	4:D:148:LYS:HG2	1.82	0.43
7:G:138:ARG:NE	7:G:139:GLU:OE1	2.42	0.43
16:P:75:ILE:O	16:P:79:ASN:HB2	2.18	0.43
21:U:49:LYS:HE2	21:U:49:LYS:HB2	1.87	0.43
22:a:278:A:N6	22:a:362:A:N7	2.66	0.43
22:a:558:U:H2'	22:a:559:G:H8	1.83	0.43
22:a:2031:A:C6	22:a:2498:OMC:H1'	2.53	0.43
22:a:2514:U:H2'	22:a:2515:C:C6	2.52	0.43
31:j:53:LYS:HD3	31:j:53:LYS:HA	1.55	0.43
35:n:109:ALA:HA	35:n:112:GLU:OE1	2.18	0.43
1:A:175:C:O2	1:A:1447:A:H2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:C:H2'	1:A:226:G:O4'	2.19	0.43
1:A:407:U:H2'	1:A:408:A:H8	1.82	0.43
1:A:445:G:C2	1:A:446:G:C8	3.07	0.43
1:A:739:C:OP1	6:F:2:ARG:NH2	2.47	0.43
1:A:999:C:C4	1:A:1042:A:N6	2.87	0.43
2:B:105:LYS:O	2:B:109:GLN:HG3	2.18	0.43
4:D:105:MET:HB2	4:D:173:VAL:HG12	1.99	0.43
18:R:42:SER:HB2	18:R:52:GLN:HG2	2.00	0.43
22:a:1584:U:H5'	22:a:1585:C:C5	2.54	0.43
24:c:157:SER:O	24:c:160:THR:OG1	2.29	0.43
27:f:73:SER:OG	27:f:80:ARG:HA	2.18	0.43
30:i:36:LEU:HD11	30:i:122:LEU:HB2	1.99	0.43
30:i:69:ARG:O	30:i:89:PHE:HB3	2.17	0.43
54:Z:9:G:N3	54:Z:46:G:H2'	2.32	0.43
1:A:1021:A:C6	1:A:1022:A:N7	2.86	0.43
1:A:1326:U:H2'	1:A:1327:C:C6	2.54	0.43
1:A:1391:U:H2'	1:A:1392:G:H8	1.81	0.43
1:A:1450:U:H2'	1:A:1452:C:C5	2.54	0.43
7:G:71:PRO:HG3	7:G:103:TRP:CH2	2.54	0.43
22:a:45:G:H5''	22:a:46:G:O5'	2.19	0.43
22:a:729:G:OP1	24:c:10:SER:OG	2.32	0.43
22:a:1361:G:H2'	22:a:1362:C:C6	2.53	0.43
22:a:1485:U:H2'	22:a:1486:U:H6	1.84	0.43
22:a:2698:U:H2'	22:a:2699:C:C6	2.53	0.43
22:a:2859:G:H2'	22:a:2860:A:C8	2.53	0.43
35:n:56:LYS:HE2	35:n:56:LYS:HB2	1.83	0.43
1:A:152:A:C8	1:A:153:C:C5	3.07	0.43
1:A:455:G:C6	1:A:456:A:C5	3.07	0.43
1:A:1121:U:H2'	1:A:1122:U:C6	2.53	0.43
1:A:1297:G:H21	7:G:114:LYS:HB3	1.84	0.43
2:B:27:MET:HE1	2:B:187:VAL:HG12	2.00	0.43
2:B:50:PHE:HD1	2:B:200:ILE:HD13	1.83	0.43
6:F:16:GLU:OE2	6:F:17:GLN:NE2	2.51	0.43
8:H:5:ASP:OD2	8:H:8:ALA:HB2	2.19	0.43
11:K:31:ILE:HG12	11:K:46:THR:HG22	2.01	0.43
11:K:59:THR:HG22	11:K:61:PHE:N	2.32	0.43
16:P:6:LEU:HB3	16:P:17:TYR:CD1	2.54	0.43
22:a:1348:C:C5	22:a:1349:C:C5	3.07	0.43
22:a:1407:G:H2'	22:a:1408:G:H8	1.84	0.43
22:a:1522:A:H8	22:a:1522:A:OP1	2.01	0.43
22:a:2025:C:H2'	22:a:2026:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:27:LYS:HE2	28:g:32:GLU:OE1	2.18	0.43
42:u:59:GLU:HG2	42:u:60:VAL:H	1.83	0.43
45:x:19:LEU:HD23	45:x:19:LEU:HA	1.74	0.43
54:Z:20:G:H3'	54:Z:21:H2U:O2	2.19	0.43
1:A:592:G:H2'	1:A:593:U:C6	2.53	0.43
1:A:860:A:H2'	1:A:861:G:O4'	2.18	0.43
1:A:1014:A:C2	1:A:1219:A:H1'	2.54	0.43
5:E:110:ALA:O	5:E:114:VAL:HG23	2.18	0.43
8:H:113:ASP:O	8:H:117:ARG:HG2	2.18	0.43
9:I:33:ARG:NH1	9:I:38:TYR:HA	2.33	0.43
20:T:61:GLN:OE1	20:T:61:GLN:HA	2.17	0.43
22:a:64:A:H2'	22:a:65:U:H6	1.83	0.43
22:a:2047:C:H2'	22:a:2048:G:H8	1.84	0.43
22:a:2527:C:H2'	22:a:2528:U:O4'	2.18	0.43
32:k:85:VAL:HG13	32:k:94:THR:HG22	2.00	0.43
34:m:86:ARG:HH21	34:m:117:ASP:CG	2.22	0.43
52:4:16:CYS:SG	52:4:17:SER:N	2.92	0.43
1:A:968:A:H4'	1:A:969:A:OP2	2.19	0.43
7:G:12:ILE:HG13	7:G:13:LEU:N	2.34	0.43
15:O:53:ARG:O	15:O:57:LEU:HD23	2.19	0.43
22:a:207:A:H2'	22:a:208:C:O4'	2.18	0.43
22:a:632:A:H2'	22:a:633:A:C8	2.54	0.43
22:a:1020:A:N1	22:a:1141:U:O2'	2.46	0.43
22:a:1283:G:H1'	22:a:1329:U:O2	2.18	0.43
22:a:1378:A:O2'	22:a:1380:G:N7	2.52	0.43
22:a:1492:G:C6	22:a:1496:A:N6	2.87	0.43
22:a:1744:A:H3'	22:a:1745:A:H8	1.84	0.43
22:a:1880:U:H2'	22:a:1881:C:C6	2.54	0.43
22:a:2469:A:H2'	22:a:2470:G:O4'	2.19	0.43
24:c:121:ASP:OD1	24:c:121:ASP:N	2.51	0.43
24:c:167:ARG:HG3	24:c:167:ARG:NH2	2.34	0.43
25:d:35:THR:HA	25:d:71:ALA:HB1	2.01	0.43
32:k:62:PRO:HG2	50:2:25:LYS:HB3	2.01	0.43
35:n:94:ARG:HD2	35:n:97:PHE:O	2.18	0.43
39:r:18:ARG:HG3	39:r:76:VAL:HB	2.00	0.43
50:2:23:LYS:HA	50:2:48:ALA:O	2.19	0.43
54:Z:19:G:C6	54:Z:58:A:C6	3.07	0.43
1:A:251:G:C6	1:A:266:G:C6	3.07	0.43
1:A:593:U:H2'	1:A:594:U:C6	2.54	0.43
1:A:696:A:H2'	1:A:697:U:H6	1.83	0.43
1:A:1032:G:C2	1:A:1033:G:H1'	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:108:GLY:O	5:E:112:ARG:N	2.41	0.43
6:F:8:PHE:HE2	6:F:62:MET:HE2	1.84	0.43
10:J:6:ILE:HG13	10:J:102:LEU:HG	2.00	0.43
17:Q:14:SER:HB3	17:Q:22:VAL:CG1	2.49	0.43
22:a:158:U:H2'	22:a:159:G:O4'	2.18	0.43
22:a:163:C:H2'	22:a:164:C:H6	1.84	0.43
22:a:817:C:O2'	22:a:839:U:H5''	2.18	0.43
22:a:1428:C:C5	22:a:1569:A:H5''	2.54	0.43
25:d:181:ASP:OD2	25:d:184:ARG:NE	2.39	0.43
28:g:155:GLU:OE1	28:g:157:TYR:N	2.43	0.43
30:i:125:TYR:HH	30:i:132:HIS:CD2	2.33	0.43
34:m:56:LYS:HE2	34:m:87:PHE:O	2.19	0.43
38:q:46:GLU:HG3	38:q:48:LYS:HZ2	1.82	0.43
1:A:158:G:N2	1:A:164:G:H1'	2.33	0.43
1:A:377:G:H2'	1:A:378:G:H8	1.84	0.43
3:C:22:TRP:CD1	3:C:59:ARG:HD2	2.53	0.43
11:K:106:ARG:NH1	11:K:108:THR:HG22	2.33	0.43
22:a:760:G:H2'	22:a:761:A:O4'	2.19	0.43
22:a:1881:C:H2'	22:a:1882:U:O4'	2.19	0.43
27:f:98:GLU:OE2	52:4:25:ARG:NH2	2.52	0.43
43:v:50:ASN:HB2	43:v:82:ILE:HB	2.01	0.43
1:A:53:A:H2'	1:A:54:C:O4'	2.19	0.42
1:A:477:C:H2'	1:A:478:A:C8	2.54	0.42
1:A:945:G:C2	1:A:946:A:C8	3.07	0.42
2:B:129:LEU:HD23	2:B:134:ALA:HA	2.01	0.42
13:M:81:MET:HE2	13:M:91:HIS:HB3	2.00	0.42
13:M:92:ARG:O	22:a:888:C:H5'	2.19	0.42
13:M:92:ARG:NH1	22:a:887:U:H5''	2.33	0.42
16:P:73:ALA:O	16:P:76:LYS:HG2	2.18	0.42
19:S:40:ILE:HG22	19:S:67:VAL:HA	2.01	0.42
22:a:272:A:H2'	22:a:273:G:H8	1.79	0.42
22:a:493:G:H2'	22:a:494:G:O4'	2.19	0.42
22:a:833:A:H2'	22:a:834:G:C8	2.54	0.42
22:a:1599:U:H2'	22:a:1600:C:C6	2.53	0.42
22:a:2219:U:H2'	22:a:2220:U:O4'	2.19	0.42
45:x:12:GLU:OE1	45:x:12:GLU:N	2.42	0.42
45:x:14:LEU:HD23	45:x:14:LEU:HA	1.80	0.42
1:A:976:G:OP2	1:A:1358:U:O2'	2.37	0.42
1:A:1526:G:OP1	21:U:45:ARG:NH2	2.46	0.42
2:B:117:LEU:HD23	2:B:117:LEU:HA	1.86	0.42
3:C:88:ARG:HG3	3:C:89:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:GLY:HA2	6:F:58:HIS:CE1	2.54	0.42
10:J:10:LEU:HD11	10:J:25:ILE:HD12	2.01	0.42
12:L:10:LYS:HE2	12:L:10:LYS:HB3	1.72	0.42
15:O:9:ALA:HA	15:O:12:VAL:HG12	2.01	0.42
22:a:1582:C:H2'	22:a:1583:A:O4'	2.19	0.42
24:c:267:ILE:HG21	24:c:270:ARG:HD2	2.01	0.42
28:g:126:PRO:HD2	28:g:130:GLU:OE2	2.19	0.42
30:i:6:ALA:O	30:i:48:VAL:HG21	2.18	0.42
40:s:40:LYS:HA	40:s:43:ILE:HD12	2.01	0.42
45:x:12:GLU:HG2	45:x:13:GLU:N	2.34	0.42
45:x:58:ASN:C	45:x:58:ASN:HD22	2.20	0.42
1:A:367:U:H5'	1:A:394:G:H21	1.84	0.42
1:A:1326:U:H2'	1:A:1327:C:H6	1.84	0.42
2:B:157:LEU:HD23	2:B:181:ILE:HD11	2.02	0.42
2:B:204:ASP:OD1	2:B:205:ASP:N	2.53	0.42
4:D:102:VAL:CG2	4:D:107:PHE:HB2	2.49	0.42
6:F:43:GLY:O	6:F:58:HIS:HA	2.19	0.42
9:I:115:LYS:HB2	9:I:118:LEU:HD12	2.00	0.42
12:L:31:ARG:O	12:L:58:THR:HG23	2.19	0.42
19:S:30:PRO:HB3	19:S:48:THR:CG2	2.45	0.42
22:a:590:A:H2'	22:a:591:U:C6	2.54	0.42
22:a:685:A:H5''	22:a:788:A:H62	1.85	0.42
22:a:848:C:H2'	22:a:849:A:C8	2.55	0.42
22:a:1292:G:H2'	22:a:1293:C:C6	2.53	0.42
22:a:1436:G:H2'	22:a:1437:C:O4'	2.19	0.42
23:b:42:C:C6	27:f:66:LEU:HB2	2.54	0.42
25:d:36:GLN:NE2	25:d:67:HIS:HE1	2.18	0.42
52:4:41:HIS:CE1	52:4:43:PHE:H	2.36	0.42
1:A:684:U:H2'	1:A:685:G:O4'	2.19	0.42
1:A:1151:A:HO2'	1:A:1152:A:H8	1.66	0.42
5:E:160:SER:O	5:E:164:ILE:HG12	2.20	0.42
6:F:10:VAL:HG23	6:F:58:HIS:O	2.19	0.42
8:H:18:GLN:NE2	8:H:72:VAL:H	2.18	0.42
22:a:1842:G:H2'	22:a:1843:C:H6	1.85	0.42
22:a:2030:6MZ:C2	22:a:2499:C:H5''	2.50	0.42
22:a:2359:C:H2'	22:a:2360:G:C8	2.55	0.42
42:u:48:MET:HE3	42:u:51:GLN:NE2	2.35	0.42
51:3:23:ILE:HD13	51:3:23:ILE:HA	1.88	0.42
54:Z:72:C:H2'	54:Z:73:A:C8	2.54	0.42
1:A:653:U:C5	8:H:56:LYS:HG2	2.54	0.42
1:A:1130:A:H2'	1:A:1131:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:SER:HG	2:B:192:ASP:H	1.68	0.42
3:C:121:THR:HG21	3:C:187:SER:OG	2.19	0.42
4:D:104:ARG:HA	4:D:104:ARG:HE	1.83	0.42
8:H:39:VAL:HG21	8:H:110:VAL:HG12	2.01	0.42
22:a:322:A:H1'	22:a:339:U:O2	2.20	0.42
22:a:1736:U:H2'	22:a:1737:G:O4'	2.20	0.42
22:a:2392:A:OP2	50:2:31:HIS:NE2	2.35	0.42
22:a:2472:G:H2'	22:a:2529:G:N2	2.34	0.42
22:a:2657:A:O3'	28:g:160:LYS:NZ	2.46	0.42
22:a:2902:C:H2'	22:a:2903:U:O4'	2.19	0.42
24:c:155:ALA:HB2	24:c:162:VAL:HG23	2.01	0.42
25:d:46:ARG:NH1	25:d:85:ALA:O	2.51	0.42
30:i:4:PHE:O	37:p:64:ARG:NH2	2.46	0.42
41:t:94:ARG:HB3	41:t:103:ILE:HD12	2.01	0.42
52:4:30:HIS:ND1	52:4:31:ASP:O	2.45	0.42
54:Z:3:C:H2'	54:Z:4:G:H8	1.84	0.42
1:A:101:A:C6	1:A:102:G:N7	2.88	0.42
1:A:123:U:H2'	1:A:124:C:H6	1.82	0.42
1:A:374:A:C6	1:A:375:U:C4	3.07	0.42
1:A:411:A:H4'	1:A:412:A:O5'	2.18	0.42
1:A:473:U:H2'	1:A:474:G:C8	2.46	0.42
1:A:715:A:H2'	1:A:716:A:C8	2.55	0.42
13:M:3:ARG:HG2	52:4:35:ASP:OD2	2.18	0.42
14:N:64:CYS:HB3	14:N:69:ARG:H	1.84	0.42
19:S:45:ILE:HD12	19:S:45:ILE:N	2.32	0.42
20:T:27:MET:SD	20:T:57:ILE:HG21	2.59	0.42
22:a:141:G:H3'	22:a:141:G:N3	2.34	0.42
22:a:181:A:H1'	22:a:435:C:H5'	2.01	0.42
22:a:263:G:H2'	22:a:264:C:O4'	2.19	0.42
22:a:1401:G:H2'	22:a:1402:U:O4'	2.18	0.42
22:a:2072:C:H2'	22:a:2073:C:H6	1.83	0.42
29:h:1:MET:N	29:h:21:VAL:O	2.45	0.42
40:s:31:VAL:HA	40:s:83:ALA:O	2.19	0.42
40:s:56:GLU:HB3	40:s:57:VAL:HG23	2.01	0.42
45:x:13:GLU:O	45:x:16:THR:HG22	2.19	0.42
1:A:175:C:H2'	1:A:176:C:C6	2.54	0.42
1:A:446:G:C2	1:A:489:C:C2	3.07	0.42
1:A:834:U:H2'	1:A:835:U:C6	2.55	0.42
1:A:1225:A:H2'	1:A:1226:C:C6	2.54	0.42
2:B:66:LYS:O	2:B:159:ASP:N	2.46	0.42
6:F:59:TYR:CE2	18:R:67:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:21:VAL:O	16:P:33:ILE:N	2.52	0.42
22:a:2591:C:H2'	22:a:2592:G:H8	1.85	0.42
30:i:18:VAL:HG21	30:i:142:ILE:HD12	2.01	0.42
38:q:41:ILE:HB	38:q:48:LYS:HE2	2.02	0.42
1:A:1009:U:H2'	1:A:1010:U:C6	2.54	0.42
1:A:1175:G:H2'	1:A:1176:A:H8	1.84	0.42
2:B:26:LYS:HD3	2:B:193:PRO:HD2	2.01	0.42
17:Q:25:ILE:HB	17:Q:42:THR:CG2	2.50	0.42
22:a:78:U:H2'	22:a:79:C:H6	1.83	0.42
22:a:1028:A:N3	22:a:2486:C:O2'	2.49	0.42
22:a:1519:G:H2'	22:a:1520:U:O4'	2.20	0.42
22:a:1827:U:OP2	24:c:221:ARG:HD2	2.19	0.42
32:k:2:ARG:HD3	32:k:2:ARG:HA	1.91	0.42
40:s:3:ARG:HD3	40:s:3:ARG:N	2.34	0.42
1:A:134:G:H1'	1:A:325:A:C5	2.54	0.42
1:A:499:A:C2	1:A:547:A:C5	3.08	0.42
6:F:22:ILE:O	6:F:26:THR:HG23	2.20	0.42
19:S:65:GLU:OE2	19:S:65:GLU:HA	2.20	0.42
21:U:58:LYS:HE3	21:U:62:ARG:NH2	2.35	0.42
22:a:171:U:H2'	22:a:172:A:H8	1.85	0.42
22:a:182:A:H2'	22:a:183:C:C6	2.52	0.42
22:a:184:C:H2'	22:a:185:G:C8	2.55	0.42
22:a:1730:C:O2	22:a:1730:C:H2'	2.19	0.42
36:o:63:LYS:HB2	36:o:63:LYS:HE3	1.82	0.42
42:u:68:LYS:HA	42:u:68:LYS:CE	2.47	0.42
1:A:169:C:O2'	1:A:170:U:H5'	2.19	0.42
1:A:235:C:H2'	1:A:236:A:H8	1.85	0.42
1:A:309:A:O2'	1:A:607:A:N1	2.44	0.42
1:A:864:A:H2'	1:A:865:A:C8	2.55	0.42
1:A:1120:C:C2	1:A:1121:U:C5	3.07	0.42
2:B:70:VAL:HG12	2:B:92:VAL:CG2	2.50	0.42
4:D:101:VAL:HG21	4:D:137:VAL:HG21	2.02	0.42
5:E:13:GLU:HG2	5:E:39:VAL:HG23	2.01	0.42
15:O:67:LEU:HD12	15:O:67:LEU:HA	1.81	0.42
19:S:71:LEU:HA	19:S:71:LEU:HD23	1.87	0.42
22:a:73:A:OP1	45:x:48:ARG:NH1	2.52	0.42
22:a:645:C:H2'	22:a:647:G:C8	2.55	0.42
22:a:1526:C:H2'	22:a:1527:G:O4'	2.20	0.42
22:a:1930:G:O2'	22:a:1968:G:O6	2.34	0.42
22:a:2014:A:H2'	22:a:2015:A:C8	2.54	0.42
22:a:2896:C:H2'	22:a:2897:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:50:LEU:HD21	27:f:67:ILE:HD12	2.02	0.42
28:g:30:ASN:HB3	28:g:79:VAL:HA	2.01	0.42
38:q:16:GLU:CD	38:q:100:GLY:HA2	2.44	0.42
42:u:44:HIS:CD2	42:u:86:LEU:HB2	2.55	0.42
55:V:4:U:O2'	55:V:5:G:O5'	2.30	0.42
1:A:134:G:H2'	1:A:135:C:O4'	2.20	0.41
1:A:178:C:O2'	1:A:179:A:H5'	2.20	0.41
1:A:228:A:H8	1:A:228:A:OP2	2.03	0.41
1:A:363:A:OP2	12:L:58:THR:HG21	2.19	0.41
1:A:547:A:H4'	1:A:548:G:O5'	2.19	0.41
1:A:580:C:H2'	1:A:581:G:O4'	2.20	0.41
1:A:1507:A:H2'	1:A:1508:A:C8	2.55	0.41
4:D:147:GLU:HA	4:D:150:LYS:HD2	2.01	0.41
7:G:56:LYS:H	7:G:56:LYS:HG2	1.68	0.41
9:I:55:VAL:HG12	9:I:97:GLU:OE1	2.20	0.41
11:K:100:LEU:HD12	11:K:100:LEU:HA	1.75	0.41
22:a:38:A:H2'	22:a:39:G:O4'	2.20	0.41
22:a:184:C:H2'	22:a:185:G:H8	1.85	0.41
22:a:277:G:H1'	22:a:278:A:C6	2.55	0.41
22:a:323:C:H6	22:a:1205:A:C2	2.38	0.41
22:a:894:U:H2'	22:a:895:U:O4'	2.20	0.41
22:a:1203:U:C4	22:a:1204:A:C5	3.07	0.41
24:c:145:GLU:CB	24:c:188:CYS:HB3	2.50	0.41
26:e:177:PRO:O	26:e:181:ILE:HG13	2.19	0.41
34:m:71:ARG:HA	34:m:71:ARG:HD2	1.78	0.41
37:p:102:ASP:OD2	38:q:2:TYR:OH	2.32	0.41
38:q:65:ALA:HB3	38:q:95:ASP:HB2	2.02	0.41
55:V:4:U:HO2'	55:V:5:G:P	2.42	0.41
1:A:169:C:H2'	1:A:170:U:C6	2.55	0.41
1:A:293:G:OP1	1:A:609:A:N6	2.37	0.41
1:A:329:A:C6	1:A:332:G:C2	3.08	0.41
1:A:579:A:H2'	1:A:580:C:C6	2.55	0.41
2:B:14:VAL:O	2:B:203:ASN:N	2.49	0.41
2:B:166:ALA:HB2	2:B:187:VAL:HG22	2.02	0.41
17:Q:21:ILE:HG23	17:Q:48:ASP:HB2	2.03	0.41
22:a:172:A:H2'	22:a:173:A:H8	1.83	0.41
22:a:917:A:H5''	22:a:2268:A:H61	1.85	0.41
22:a:1820:U:C2	24:c:201:MET:HB3	2.56	0.41
28:g:94:TYR:HA	28:g:106:SER:O	2.20	0.41
29:h:1:MET:O	29:h:20:ASN:HA	2.20	0.41
52:4:9:TYR:CE2	52:4:25:ARG:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:V:23:A:H2'	55:V:24:G:C8	2.54	0.41
1:A:405:U:OP1	1:A:406:G:O2'	2.31	0.41
1:A:1435:G:H2'	1:A:1436:U:C6	2.54	0.41
5:E:80:THR:OG1	5:E:122:ASN:O	2.36	0.41
7:G:15:ASP:OD2	7:G:23:LEU:HB3	2.20	0.41
12:L:23:ALA:HA	12:L:61:PHE:HD2	1.85	0.41
17:Q:11:ARG:O	17:Q:23:VAL:HG13	2.20	0.41
22:a:171:U:H2'	22:a:172:A:C8	2.54	0.41
22:a:278:A:C6	22:a:362:A:N7	2.89	0.41
22:a:327:G:H2'	22:a:328:U:O4'	2.20	0.41
22:a:499:U:H5''	41:t:43:LYS:HE2	2.01	0.41
22:a:576:U:H2'	22:a:577:G:C8	2.55	0.41
22:a:577:G:O2'	22:a:1254:A:OP1	2.36	0.41
22:a:1499:C:C2	22:a:1500:G:C8	3.09	0.41
22:a:2627:G:O2'	22:a:2781:A:N1	2.45	0.41
22:a:2649:C:H2'	22:a:2650:U:H6	1.84	0.41
27:f:140:GLU:HG3	52:4:28:VAL:HB	2.03	0.41
39:r:109:ASP:OD1	39:r:110:ARG:N	2.53	0.41
41:t:74:ASN:C	41:t:76:ALA:H	2.27	0.41
41:t:96:PHE:CE1	41:t:103:ILE:HG12	2.56	0.41
43:v:25:ARG:HD3	43:v:25:ARG:HA	1.85	0.41
45:x:57:LEU:HD23	45:x:57:LEU:HA	1.87	0.41
50:2:55:LEU:HD12	50:2:55:LEU:HA	1.90	0.41
52:4:20:ASN:HD21	52:4:39:LYS:CB	2.30	0.41
1:A:61:G:H2'	1:A:62:U:O4'	2.20	0.41
1:A:297:G:N2	1:A:299:G:H3'	2.35	0.41
1:A:356:A:H5'	1:A:367:U:H5	1.85	0.41
1:A:641:U:H4'	8:H:107:SER:O	2.21	0.41
1:A:757:U:H2'	1:A:758:C:O4'	2.20	0.41
1:A:861:G:H2'	1:A:862:C:O4'	2.20	0.41
1:A:1264:U:H2'	1:A:1265:C:H6	1.85	0.41
1:A:1489:G:C6	1:A:1490:U:C4	3.08	0.41
2:B:45:LYS:HA	2:B:45:LYS:HD3	1.82	0.41
3:C:175:LEU:HD21	3:C:201:TRP:CD1	2.55	0.41
4:D:152:GLN:O	4:D:156:LYS:HG2	2.20	0.41
11:K:114:THR:HA	11:K:115:PRO:HD3	1.93	0.41
13:M:56:LEU:HA	13:M:56:LEU:HD23	1.75	0.41
13:M:81:MET:HG2	22:a:888:C:C4	2.56	0.41
14:N:19:LYS:HD2	14:N:19:LYS:C	2.45	0.41
16:P:22:ALA:HA	16:P:33:ILE:HD12	2.01	0.41
22:a:880:G:H2'	22:a:881:G:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1199:U:H2'	22:a:1200:C:H6	1.85	0.41
22:a:1446:C:H2'	22:a:1447:C:C6	2.55	0.41
22:a:1877:A:H2'	22:a:1878:G:O4'	2.21	0.41
22:a:2680:U:O2'	22:a:2681:C:H5'	2.19	0.41
24:c:123:ALA:HB3	24:c:125:LYS:HE3	2.01	0.41
34:m:86:ARG:NH2	34:m:117:ASP:OD1	2.32	0.41
1:A:180:U:O2'	1:A:181:A:H5'	2.20	0.41
1:A:247:G:O6	1:A:278:G:C6	2.73	0.41
1:A:613:C:H2'	1:A:614:C:C6	2.55	0.41
1:A:1469:C:H2'	1:A:1470:U:O4'	2.20	0.41
8:H:114:ARG:HA	8:H:114:ARG:HD2	1.89	0.41
9:I:7:TYR:HE1	9:I:18:ARG:HB3	1.85	0.41
22:a:286:U:H2'	22:a:287:G:H8	1.85	0.41
22:a:2214:C:H6	22:a:2214:C:O5'	2.03	0.41
22:a:2780:G:OP2	30:i:120:ARG:HD3	2.20	0.41
23:b:101:A:H2'	23:b:102:G:O4'	2.21	0.41
32:k:19:LEU:HD23	32:k:27:LEU:HD13	2.01	0.41
42:u:26:PHE:CE1	42:u:42:LEU:HB2	2.56	0.41
55:V:4:U:O2'	55:V:5:G:H8	2.03	0.41
1:A:76:G:H1	1:A:93:U:H3	0.64	0.41
1:A:157:U:O2'	1:A:158:G:H5'	2.20	0.41
1:A:658:C:O2'	1:A:659:U:H5'	2.21	0.41
1:A:923:A:H2'	1:A:924:C:O4'	2.20	0.41
1:A:1314:C:H2'	1:A:1315:U:C6	2.55	0.41
2:B:161:LEU:HB2	2:B:183:VAL:HG22	2.02	0.41
13:M:22:ILE:HG23	13:M:66:GLU:OE2	2.20	0.41
20:T:79:LEU:HD13	20:T:79:LEU:HA	1.83	0.41
22:a:739:A:H1'	22:a:740:C:H5	1.85	0.41
22:a:1843:C:H2'	22:a:1844:C:C6	2.56	0.41
22:a:2236:U:H2'	22:a:2237:G:O4'	2.20	0.41
22:a:2803:G:H2'	22:a:2804:U:H6	1.85	0.41
40:s:48:GLN:HG2	40:s:53:VAL:O	2.20	0.41
1:A:19:A:O2'	1:A:572:A:N1	2.51	0.41
1:A:620:C:C2	4:D:132:ILE:HG21	2.56	0.41
2:B:54:LEU:HD11	2:B:216:ALA:HB1	2.02	0.41
2:B:186:ILE:HD13	2:B:186:ILE:HA	1.76	0.41
4:D:23:SER:HB2	4:D:25:VAL:HG22	2.03	0.41
6:F:59:TYR:HE2	18:R:67:LEU:HD11	1.86	0.41
13:M:81:MET:HG2	22:a:888:C:N3	2.36	0.41
22:a:864:G:O2'	22:a:865:C:H5'	2.20	0.41
22:a:914:G:H3'	22:a:915:C:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1563:U:H2'	22:a:1564:C:C6	2.56	0.41
22:a:2082:A:H2'	22:a:2083:G:O4'	2.21	0.41
22:a:2300:C:H2'	22:a:2301:C:C6	2.55	0.41
22:a:2533:U:OP1	22:a:2665:A:O2'	2.35	0.41
31:j:111:LYS:HB3	31:j:111:LYS:HZ1	1.86	0.41
41:t:49:VAL:HG13	41:t:52:LEU:O	2.20	0.41
1:A:32:A:H2'	1:A:33:A:C8	2.56	0.41
1:A:263:A:OP2	20:T:74:ARG:NH2	2.54	0.41
1:A:708:C:H2'	1:A:709:U:C6	2.56	0.41
2:B:57:LEU:HA	2:B:60:ILE:HD11	2.03	0.41
22:a:903:C:C2	22:a:904:G:C8	3.09	0.41
22:a:1009:A:OP2	30:i:39:LYS:NZ	2.54	0.41
22:a:2246:G:H2'	22:a:2247:A:C8	2.55	0.41
22:a:2286:G:H2'	22:a:2286:G:N3	2.36	0.41
22:a:2300:C:H2'	22:a:2301:C:H6	1.86	0.41
32:k:132:ARG:NH2	32:k:142:ILE:HG21	2.36	0.41
46:y:30:ARG:HB2	46:y:31:ARG:NH1	2.36	0.41
1:A:142:G:H3'	1:A:143:A:H8	1.85	0.41
1:A:151:A:C4	1:A:152:A:C8	3.09	0.41
1:A:168:G:C2	1:A:169:C:C5	3.09	0.41
1:A:215:C:H2'	1:A:216:U:C6	2.56	0.41
1:A:375:U:H2'	1:A:376:G:C8	2.56	0.41
1:A:405:U:H5	4:D:3:ARG:HB2	1.86	0.41
1:A:412:A:O2'	1:A:413:G:H4'	2.20	0.41
1:A:513:C:H2'	1:A:514:C:H6	1.85	0.41
1:A:546:A:OP1	4:D:69:GLU:N	2.54	0.41
1:A:825:A:H2'	1:A:826:C:O4'	2.20	0.41
1:A:1272:G:C6	1:A:1273:C:C4	3.09	0.41
1:A:1319:A:OP1	19:S:3:ARG:HD2	2.21	0.41
1:A:1322:C:H6	1:A:1322:C:OP1	2.03	0.41
1:A:1349:A:OP1	9:I:123:ARG:N	2.48	0.41
1:A:1489:G:H2'	1:A:1490:U:O4'	2.20	0.41
2:B:18:HIS:CG	2:B:190:ASN:HD22	2.38	0.41
2:B:87:CYS:SG	2:B:218:ALA:HA	2.61	0.41
3:C:51:SER:OG	3:C:71:ALA:HB3	2.21	0.41
4:D:57:GLU:OE2	4:D:199:LEU:HB2	2.20	0.41
4:D:95:GLU:O	4:D:100:ASN:ND2	2.54	0.41
5:E:89:HIS:O	5:E:90:THR:C	2.63	0.41
6:F:42:TRP:HZ2	6:F:100:SER:OG	2.04	0.41
9:I:36:GLU:N	9:I:36:GLU:CD	2.79	0.41
12:L:7:LEU:HD23	12:L:7:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:15:LYS:HE2	12:L:15:LYS:HB2	1.79	0.41
21:U:41:PRO:O	21:U:45:ARG:HG3	2.21	0.41
22:a:460:A:H2'	22:a:461:C:O4'	2.21	0.41
22:a:475:C:O2	22:a:479:A:N6	2.52	0.41
22:a:480:A:O2'	41:t:43:LYS:O	2.36	0.41
22:a:612:G:C2	22:a:614:A:H5''	2.56	0.41
22:a:874:G:C6	22:a:904:G:C6	3.09	0.41
22:a:1019:U:OP1	22:a:1035:U:O2'	2.26	0.41
22:a:1028:A:N6	22:a:1125:G:H2'	2.36	0.41
22:a:1231:U:H2'	22:a:1232:G:H8	1.84	0.41
22:a:1265:A:H8	22:a:1265:A:OP1	2.04	0.41
22:a:1339:G:P	40:s:15:HIS:HE2	2.44	0.41
22:a:2567:G:H2'	22:a:2568:U:C6	2.56	0.41
22:a:2638:G:O2'	22:a:2775:G:N2	2.39	0.41
22:a:2810:A:H2'	22:a:2811:G:O4'	2.20	0.41
23:b:1:U:H2'	23:b:2:G:H8	1.78	0.41
25:d:37:VAL:HG22	25:d:48:ILE:HG22	2.02	0.41
25:d:124:ARG:HA	25:d:165:MET:HE3	2.03	0.41
25:d:128:ARG:HA	25:d:128:ARG:HE	1.86	0.41
26:e:128:ALA:O	26:e:130:LYS:N	2.53	0.41
29:h:25:TYR:CE1	29:h:29:PHE:HD2	2.38	0.41
33:l:22:GLN:O	33:l:100:LYS:NZ	2.52	0.41
33:l:56:ALA:HB2	33:l:119:LEU:HD12	2.02	0.41
44:w:6:GLN:O	44:w:74:ARG:NH2	2.53	0.41
45:x:19:LEU:HB3	45:x:23:ARG:HH21	1.85	0.41
55:V:1:G:O2'	55:V:2:C:H5'	2.21	0.41
55:V:70:G:H2'	55:V:71:G:C8	2.56	0.41
1:A:624:C:H2'	1:A:625:U:C6	2.56	0.41
1:A:1149:C:H2'	1:A:1150:A:C8	2.55	0.41
12:L:54:ARG:HH11	12:L:64:THR:HG1	1.65	0.41
18:R:24:LYS:O	18:R:26:ILE:N	2.54	0.41
22:a:507:A:H5''	22:a:508:A:H3'	2.02	0.41
22:a:1430:G:H2'	22:a:1431:A:O4'	2.21	0.41
22:a:2747:G:OP1	28:g:138:LYS:NZ	2.54	0.41
24:c:43:ARG:HA	24:c:48:ARG:O	2.21	0.41
41:t:54:GLN:N	41:t:55:PRO:HD2	2.36	0.41
42:u:17:SER:HB3	42:u:21:ARG:NH2	2.36	0.41
43:v:25:ARG:NH1	43:v:31:VAL:HG12	2.36	0.41
45:x:13:GLU:HA	45:x:16:THR:HG22	2.03	0.41
55:V:10:2MG:O2'	55:V:11:C:P	2.79	0.41
1:A:271:C:C2	1:A:272:C:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:G:O2'	1:A:556:C:H5''	2.21	0.40
1:A:763:G:H2'	1:A:764:C:C6	2.55	0.40
1:A:793:U:H6	1:A:793:U:H2'	1.72	0.40
1:A:986:U:H2'	1:A:987:G:O4'	2.21	0.40
1:A:1121:U:H2'	1:A:1122:U:H6	1.85	0.40
1:A:1126:U:O2	1:A:1280:A:H2'	2.21	0.40
3:C:149:ILE:HA	3:C:201:TRP:O	2.22	0.40
4:D:101:VAL:HG12	4:D:105:MET:HE3	2.03	0.40
5:E:34:THR:HA	5:E:51:GLY:O	2.20	0.40
6:F:25:TYR:CE2	6:F:78:PHE:HE1	2.39	0.40
7:G:53:ARG:HH12	7:G:122:ASN:HA	1.87	0.40
11:K:34:ILE:HG13	11:K:70:CYS:SG	2.61	0.40
12:L:38:TYR:HE2	12:L:40:THR:HG23	1.86	0.40
15:O:14:GLU:HG2	15:O:15:PHE:CD2	2.56	0.40
22:a:1044:C:O2'	22:a:1111:A:N1	2.53	0.40
22:a:1339:G:N2	22:a:1603:A:H1'	2.36	0.40
25:d:40:LEU:CD1	25:d:46:ARG:HG3	2.51	0.40
25:d:152:PRO:HG3	25:d:156:PHE:CZ	2.56	0.40
52:4:58:ASP:O	52:4:62:LYS:HG2	2.20	0.40
1:A:62:U:H2'	1:A:63:C:C6	2.57	0.40
1:A:198:G:O6	1:A:219:U:C4	2.73	0.40
4:D:60:LYS:HD2	4:D:61:VAL:N	2.35	0.40
6:F:29:ILE:HD13	6:F:64:VAL:HG13	2.03	0.40
7:G:67:GLU:HG2	7:G:70:ARG:NH1	2.36	0.40
10:J:22:THR:HG21	10:J:72:ARG:HG3	2.02	0.40
14:N:21:PHE:C	14:N:21:PHE:CD1	2.99	0.40
16:P:51:ARG:O	16:P:52:LEU:HD13	2.21	0.40
22:a:160:A:H2'	22:a:161:A:C8	2.55	0.40
22:a:308:G:H2'	22:a:309:A:C8	2.56	0.40
22:a:645:C:H2'	22:a:647:G:N7	2.36	0.40
22:a:1342:A:O2'	22:a:1344:U:OP1	2.38	0.40
22:a:1354:A:H2'	22:a:1355:G:O4'	2.22	0.40
22:a:1818:U:H5''	24:c:157:SER:OG	2.21	0.40
22:a:1874:C:H2'	22:a:1875:G:O4'	2.21	0.40
25:d:48:ILE:HG21	25:d:90:PHE:HB2	2.04	0.40
26:e:40:ARG:HD3	26:e:92:HIS:CG	2.56	0.40
32:k:91:ASP:OD1	32:k:92:LEU:N	2.54	0.40
54:Z:32:G:H2'	54:Z:33:OMC:C6	2.56	0.40
1:A:16:A:N1	1:A:919:A:H2	2.18	0.40
1:A:375:U:OP1	16:P:70:ARG:HD3	2.20	0.40
1:A:405:U:C5	4:D:3:ARG:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:A:O2'	1:A:979:C:OP2	2.37	0.40
1:A:1118:U:H2'	1:A:1119:C:H6	1.86	0.40
1:A:1170:A:H2'	1:A:1171:A:O4'	2.21	0.40
10:J:84:VAL:O	10:J:88:MET:SD	2.79	0.40
16:P:45:GLU:O	16:P:46:LYS:HB3	2.21	0.40
22:a:403:U:H5'	22:a:404:A:OP1	2.20	0.40
22:a:1427:A:H4'	22:a:1428:C:O5'	2.22	0.40
22:a:1495:A:C6	22:a:1496:A:C6	3.10	0.40
22:a:2072:C:H2'	22:a:2073:C:C6	2.56	0.40
22:a:2187:U:H2'	22:a:2188:U:H6	1.87	0.40
22:a:2516:A:O2'	22:a:2517:C:H5'	2.21	0.40
22:a:2646:C:H2'	22:a:2647:U:O4'	2.22	0.40
26:e:105:LEU:HD23	26:e:105:LEU:HA	1.82	0.40
28:g:91:GLY:HA2	28:g:160:LYS:HG2	2.02	0.40
31:j:34:GLY:N	31:j:37:ASP:OD2	2.46	0.40
33:l:2:LEU:HD23	33:l:2:LEU:HA	1.85	0.40
39:r:6:LYS:HA	39:r:103:ILE:O	2.21	0.40
40:s:61:LEU:HD11	40:s:82:LYS:HE2	2.03	0.40
42:u:51:GLN:HA	42:u:56:PHE:CG	2.56	0.40
1:A:377:G:H2'	1:A:378:G:C8	2.56	0.40
1:A:379:C:H2'	1:A:380:G:O4'	2.21	0.40
1:A:802:A:H2'	1:A:803:G:O4'	2.22	0.40
1:A:875:U:O2'	8:H:15:ARG:HD2	2.21	0.40
1:A:1254:A:H2'	1:A:1255:G:C8	2.56	0.40
1:A:1272:G:C5	1:A:1273:C:C4	3.10	0.40
3:C:64:ILE:O	3:C:99:ALA:HA	2.22	0.40
3:C:148:GLY:HA3	3:C:172:ARG:O	2.21	0.40
6:F:18:VAL:HG21	6:F:58:HIS:CD2	2.56	0.40
20:T:48:GLN:OE1	20:T:52:ASN:OD1	2.39	0.40
22:a:183:C:H42	22:a:213:A:H61	1.70	0.40
22:a:221:A:N1	22:a:265:A:O2'	2.53	0.40
22:a:397:U:H5''	44:w:32:ASN:HB2	2.03	0.40
22:a:754:U:H2'	22:a:755:U:C6	2.57	0.40
22:a:1445:G:C5	22:a:1446:C:C5	3.10	0.40
32:k:110:VAL:HB	32:k:127:VAL:HG23	2.03	0.40
40:s:15:HIS:CE1	40:s:80:TRP:HH2	2.40	0.40
1:A:496:A:C2	1:A:497:G:C5	3.09	0.40
1:A:1321:U:H4'	13:M:86:TYR:CZ	2.57	0.40
9:I:18:ARG:NH1	9:I:66:THR:OG1	2.50	0.40
9:I:71:GLY:O	9:I:75:GLN:HG3	2.22	0.40
22:a:687:C:H2'	22:a:688:U:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1406:U:H2'	22:a:1407:G:C8	2.57	0.40
22:a:1485:U:H2'	22:a:1486:U:C6	2.55	0.40
22:a:2016:U:H2'	22:a:2017:U:C6	2.57	0.40
23:b:27:C:C4	23:b:28:C:C4	3.10	0.40
23:b:34:A:HO2'	23:b:35:C:H5	1.69	0.40
38:q:87:GLN:HG2	38:q:88:GLY:N	2.37	0.40
39:r:25:ARG:NH2	39:r:74:ILE:O	2.49	0.40
40:s:6:ARG:NE	40:s:42:GLU:OE2	2.55	0.40
44:w:69:ALA:HA	44:w:72:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	203 (91%)	19 (9%)	0	100	100
3	C	204/233 (88%)	191 (94%)	13 (6%)	0	100	100
4	D	203/206 (98%)	186 (92%)	17 (8%)	0	100	100
5	E	154/167 (92%)	146 (95%)	8 (5%)	0	100	100
6	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
7	G	151/179 (84%)	139 (92%)	12 (8%)	0	100	100
8	H	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
9	I	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
10	J	96/103 (93%)	87 (91%)	8 (8%)	1 (1%)	12	13
11	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
12	L	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
13	M	113/118 (96%)	102 (90%)	9 (8%)	2 (2%)	6	5
14	N	98/101 (97%)	92 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
17	Q	77/84 (92%)	69 (90%)	8 (10%)	0	100	100
18	R	64/75 (85%)	58 (91%)	6 (9%)	0	100	100
19	S	82/92 (89%)	76 (93%)	6 (7%)	0	100	100
20	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	U	68/71 (96%)	68 (100%)	0	0	100	100
24	c	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
25	d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
26	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
27	f	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
28	g	174/177 (98%)	153 (88%)	21 (12%)	0	100	100
29	h	39/149 (26%)	32 (82%)	7 (18%)	0	100	100
30	i	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
31	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
32	k	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
33	l	132/136 (97%)	123 (93%)	9 (7%)	0	100	100
34	m	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
35	n	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
36	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
37	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
38	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
39	r	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
40	s	91/100 (91%)	80 (88%)	11 (12%)	0	100	100
41	t	100/104 (96%)	89 (89%)	11 (11%)	0	100	100
42	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
43	v	82/85 (96%)	78 (95%)	4 (5%)	0	100	100
44	w	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
45	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
47	z	54/57 (95%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	6
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/70 (80%)	54 (96%)	2 (4%)	0	100	100
All	All	5487/5913 (93%)	5161 (94%)	322 (6%)	4 (0%)	49	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL
13	M	105	ASN
13	M	106	ALA
50	2	32	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	184 (99%)	2 (1%)	65	75
3	C	170/190 (90%)	167 (98%)	3 (2%)	51	64
4	D	172/173 (99%)	167 (97%)	5 (3%)	37	49
5	E	119/126 (94%)	117 (98%)	2 (2%)	53	66
6	F	90/116 (78%)	88 (98%)	2 (2%)	45	59
7	G	126/147 (86%)	124 (98%)	2 (2%)	55	68
8	H	104/105 (99%)	103 (99%)	1 (1%)	68	77
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	85 (99%)	1 (1%)	63	74
11	K	89/98 (91%)	87 (98%)	2 (2%)	45	59
12	L	102/103 (99%)	100 (98%)	2 (2%)	48	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	93/96 (97%)	90 (97%)	3 (3%)	34	46
14	N	83/84 (99%)	82 (99%)	1 (1%)	63	74
15	O	76/77 (99%)	75 (99%)	1 (1%)	61	72
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	71 (97%)	2 (3%)	39	52
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	61 (94%)	4 (6%)	16	22
21	U	60/61 (98%)	60 (100%)	0	100	100
24	c	216/218 (99%)	215 (100%)	1 (0%)	81	87
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	163 (99%)	2 (1%)	63	74
27	f	148/150 (99%)	147 (99%)	1 (1%)	76	83
28	g	137/138 (99%)	132 (96%)	5 (4%)	31	42
29	h	32/114 (28%)	32 (100%)	0	100	100
30	i	116/116 (100%)	114 (98%)	2 (2%)	53	66
31	j	104/104 (100%)	101 (97%)	3 (3%)	37	49
32	k	103/103 (100%)	102 (99%)	1 (1%)	68	77
33	l	107/107 (100%)	106 (99%)	1 (1%)	70	80
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	85 (99%)	1 (1%)	63	74
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	86 (97%)	3 (3%)	32	45
38	q	84/84 (100%)	81 (96%)	3 (4%)	31	42
39	r	93/93 (100%)	92 (99%)	1 (1%)	65	75
40	s	80/84 (95%)	79 (99%)	1 (1%)	61	72
41	t	83/85 (98%)	83 (100%)	0	100	100
42	u	78/78 (100%)	77 (99%)	1 (1%)	61	72
43	v	62/63 (98%)	62 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	52 (96%)	2 (4%)	30	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100
48	0	46/49 (94%)	44 (96%)	2 (4%)	26	36
49	1	38/38 (100%)	37 (97%)	1 (3%)	40	53
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	55/62 (89%)	55 (100%)	0	100	100
All	All	4576/4825 (95%)	4512 (99%)	64 (1%)	57	70

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	14	VAL
2	B	93	ASN
3	C	75	ILE
3	C	97	VAL
3	C	105	GLU
4	D	55	LEU
4	D	99	ASP
4	D	117	LEU
4	D	159	LEU
4	D	161	LEU
5	E	141	ILE
5	E	159	LYS
6	F	29	ILE
6	F	82	ASP
7	G	13	LEU
7	G	21	GLU
8	H	107	SER
10	J	50	THR
11	K	86	VAL
11	K	100	LEU
12	L	39	THR
12	L	73	ASN
13	M	8	ASN
13	M	16	VAL
13	M	105	ASN
14	N	96	LEU
15	O	17	ARG
17	Q	29	VAL

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Mol	Chain	Res	Type
17	Q	70	THR
20	T	30	THR
20	T	49	LYS
20	T	67	ILE
20	T	79	LEU
24	c	5	LYS
26	e	13	THR
26	e	199	MET
27	f	32	GLU
28	g	4	VAL
28	g	84	THR
28	g	106	SER
28	g	113	VAL
28	g	153	ARG
30	i	1	MET
30	i	11	VAL
31	j	17	ARG
31	j	58	LEU
31	j	91	SER
32	k	103	ILE
33	l	132	THR
35	n	12	THR
37	p	19	LYS
37	p	59	GLN
37	p	83	LEU
38	q	11	GLN
38	q	20	VAL
38	q	99	THR
39	r	4	ILE
40	s	31	VAL
42	u	45	ASP
45	x	39	GLN
45	x	56	LEU
48	0	12	VAL
48	0	48	ILE
49	1	24	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	18	HIS
2	B	120	GLN

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Mol	Chain	Res	Type
2	B	168	HIS
2	B	190	ASN
3	C	3	GLN
4	D	71	GLN
4	D	164	GLN
5	E	148	ASN
6	F	17	GLN
6	F	52	ASN
7	G	130	ASN
7	G	148	ASN
7	G	153	HIS
8	H	18	GLN
9	I	5	GLN
14	N	49	GLN
16	P	63	GLN
19	S	14	HIS
21	U	9	ASN
21	U	56	HIS
24	c	25	HIS
24	c	143	ASN
25	d	32	ASN
25	d	173	GLN
26	e	115	GLN
26	e	156	ASN
27	f	5	HIS
28	g	30	ASN
28	g	104	ASN
28	g	128	GLN
30	i	80	HIS
31	j	5	GLN
34	m	107	ASN
35	n	29	HIS
36	o	75	GLN
37	p	81	ASN
44	w	36	HIS
45	x	36	GLN
45	x	39	GLN
48	0	45	GLN
52	4	20	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1542 (97%)	262 (17%)	7 (0%)
22	a	2757/2904 (94%)	361 (13%)	0
23	b	118/120 (98%)	19 (16%)	0
53	X	10/35 (28%)	0	0
54	Z	76/77 (98%)	13 (17%)	1 (1%)
55	V	70/76 (92%)	12 (17%)	2 (2%)
All	All	4539/4754 (95%)	667 (14%)	10 (0%)

All (667) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	7	A
1	A	9	G
1	A	15	G
1	A	22	G
1	A	39	G
1	A	44	A
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	55	A
1	A	56	U
1	A	59	A
1	A	60	A
1	A	66	A
1	A	67	C
1	A	72	A
1	A	74	A
1	A	94	G
1	A	95	C
1	A	116	A
1	A	119	A
1	A	121	U
1	A	122	G
1	A	130	A
1	A	131	A
1	A	135	C
1	A	136	C
1	A	146	G

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Mol	Chain	Res	Type
1	A	149	A
1	A	150	U
1	A	153	C
1	A	158	G
1	A	160	A
1	A	162	A
1	A	169	C
1	A	172	A
1	A	176	C
1	A	177	G
1	A	179	A
1	A	182	A
1	A	183	C
1	A	189	A
1	A	192	A
1	A	195	A
1	A	197	A
1	A	199	A
1	A	200	G
1	A	204	G
1	A	216	U
1	A	222	C
1	A	226	G
1	A	228	A
1	A	240	G
1	A	245	U
1	A	247	G
1	A	250	A
1	A	251	G
1	A	262	A
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	293	G
1	A	310	G
1	A	321	A
1	A	323	U
1	A	328	C
1	A	330	C
1	A	334	C
1	A	352	C

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Mol	Chain	Res	Type
1	A	354	G
1	A	367	U
1	A	369	G
1	A	372	C
1	A	378	G
1	A	380	G
1	A	381	C
1	A	388	G
1	A	390	U
1	A	391	G
1	A	392	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	445	G
1	A	457	G
1	A	458	U
1	A	464	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	474	G
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	494	G
1	A	495	A
1	A	496	A
1	A	499	A
1	A	503	C
1	A	505	G
1	A	506	G

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Mol	Chain	Res	Type
1	A	511	C
1	A	512	U
1	A	518	C
1	A	526	C
1	A	533	A
1	A	547	A
1	A	559	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	587	G
1	A	596	A
1	A	617	G
1	A	618	C
1	A	626	G
1	A	638	U
1	A	639	G
1	A	653	U
1	A	656	G
1	A	659	U
1	A	665	A
1	A	682	G
1	A	686	U
1	A	687	A
1	A	703	G
1	A	721	G
1	A	723	U
1	A	724	G
1	A	734	G
1	A	746	A
1	A	747	A
1	A	748	G
1	A	777	A
1	A	787	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	837	U

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Mol	Chain	Res	Type
1	A	840	C
1	A	849	G
1	A	851	G
1	A	876	C
1	A	887	G
1	A	890	G
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	993	G
1	A	999	C
1	A	1004	A
1	A	1008	U
1	A	1009	U
1	A	1010	U
1	A	1022	A
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1035	A
1	A	1036	A
1	A	1042	A
1	A	1043	G
1	A	1044	A
1	A	1045	C
1	A	1065	U
1	A	1066	C
1	A	1071	C
1	A	1081	A
1	A	1094	G

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Mol	Chain	Res	Type
1	A	1095	U
1	A	1101	A
1	A	1130	A
1	A	1133	G
1	A	1137	C
1	A	1139	G
1	A	1146	A
1	A	1159	U
1	A	1167	A
1	A	1169	A
1	A	1176	A
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1253	G
1	A	1257	A
1	A	1260	G
1	A	1275	A
1	A	1279	G
1	A	1280	A
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1312	G
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1323	G
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1368	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1382	C

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Mol	Chain	Res	Type
1	A	1394	A
1	A	1397	C
1	A	1419	G
1	A	1429	A
1	A	1432	G
1	A	1441	A
1	A	1445	U
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1487	G
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1534	A
22	a	3	U
22	a	10	A
22	a	33	C
22	a	34	U
22	a	40	U
22	a	42	A
22	a	47	C
22	a	51	G
22	a	58	G
22	a	64	A
22	a	71	A
22	a	74	A
22	a	75	G
22	a	84	A
22	a	98	G
22	a	101	A
22	a	102	U
22	a	103	A
22	a	114	U
22	a	118	A
22	a	119	A
22	a	120	U

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Mol	Chain	Res	Type
22	a	125	A
22	a	127	A
22	a	139	U
22	a	140	C
22	a	142	A
22	a	144	A
22	a	153	U
22	a	163	C
22	a	164	C
22	a	165	A
22	a	181	A
22	a	196	A
22	a	216	A
22	a	222	A
22	a	223	A
22	a	248	G
22	a	264	C
22	a	272	A
22	a	275	C
22	a	277	G
22	a	278	A
22	a	279	A
22	a	280	U
22	a	281	C
22	a	282	A
22	a	283	G
22	a	285	G
22	a	287	G
22	a	289	G
22	a	294	A
22	a	295	G
22	a	300	A
22	a	311	A
22	a	328	U
22	a	329	G
22	a	330	A
22	a	334	C
22	a	335	C
22	a	345	A
22	a	354	A
22	a	362	A
22	a	386	G

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Mol	Chain	Res	Type
22	a	396	G
22	a	405	U
22	a	411	G
22	a	445	C
22	a	454	A
22	a	473	G
22	a	481	G
22	a	491	G
22	a	503	A
22	a	504	A
22	a	505	A
22	a	508	A
22	a	509	C
22	a	529	A
22	a	530	G
22	a	531	C
22	a	532	A
22	a	543	G
22	a	544	C
22	a	546	U
22	a	549	G
22	a	563	A
22	a	568	U
22	a	573	U
22	a	575	A
22	a	589	U
22	a	602	A
22	a	603	A
22	a	614	A
22	a	615	U
22	a	620	G
22	a	627	A
22	a	637	A
22	a	645	C
22	a	647	G
22	a	654	A
22	a	659	G
22	a	668	A
22	a	685	A
22	a	686	U
22	a	717	C
22	a	723	C

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Mol	Chain	Res	Type
22	a	730	A
22	a	738	G
22	a	747	5MU
22	a	764	A
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	789	A
22	a	791	C
22	a	805	G
22	a	811	U
22	a	812	C
22	a	827	U
22	a	828	U
22	a	845	A
22	a	846	U
22	a	847	U
22	a	859	G
22	a	866	A
22	a	884	U
22	a	888	C
22	a	890	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	898	C
22	a	900	A
22	a	903	C
22	a	910	A
22	a	914	G
22	a	915	C
22	a	916	G
22	a	931	U
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	989	G
22	a	996	A
22	a	1012	U

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Mol	Chain	Res	Type
22	a	1013	C
22	a	1022	G
22	a	1025	G
22	a	1033	U
22	a	1040	A
22	a	1041	G
22	a	1045	C
22	a	1047	G
22	a	1108	U
22	a	1111	A
22	a	1112	G
22	a	1115	G
22	a	1116	G
22	a	1122	G
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1144	A
22	a	1171	G
22	a	1172	C
22	a	1205	A
22	a	1250	G
22	a	1253	A
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1275	A
22	a	1284	A
22	a	1286	A
22	a	1300	G
22	a	1301	A
22	a	1306	C
22	a	1312	U
22	a	1321	A
22	a	1329	U
22	a	1344	U
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1386	C

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Mol	Chain	Res	Type
22	a	1416	G
22	a	1417	C
22	a	1427	A
22	a	1428	C
22	a	1437	C
22	a	1452	G
22	a	1453	A
22	a	1482	G
22	a	1485	U
22	a	1493	C
22	a	1508	A
22	a	1509	A
22	a	1510	G
22	a	1515	A
22	a	1523	U
22	a	1524	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1538	G
22	a	1560	G
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1586	A
22	a	1588	G
22	a	1608	A
22	a	1610	A
22	a	1626	A
22	a	1634	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1669	A
22	a	1674	G
22	a	1714	U
22	a	1715	G
22	a	1724	G

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Mol	Chain	Res	Type
22	a	1729	U
22	a	1730	C
22	a	1732	C
22	a	1738	G
22	a	1764	C
22	a	1773	A
22	a	1782	U
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1847	A
22	a	1848	A
22	a	1858	A
22	a	1867	G
22	a	1871	A
22	a	1872	A
22	a	1876	A
22	a	1906	G
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1965	C
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2020	A
22	a	2023	C
22	a	2030	6MZ
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G

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Mol	Chain	Res	Type
22	a	2062	A
22	a	2069	G7M
22	a	2188	U
22	a	2198	A
22	a	2204	G
22	a	2210	U
22	a	2211	A
22	a	2213	U
22	a	2225	A
22	a	2238	G
22	a	2239	G
22	a	2273	A
22	a	2283	C
22	a	2287	A
22	a	2288	A
22	a	2305	U
22	a	2308	G
22	a	2319	G
22	a	2322	A
22	a	2325	G
22	a	2335	A
22	a	2341	G
22	a	2345	G
22	a	2347	C
22	a	2383	G
22	a	2385	C
22	a	2396	G
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2410	G
22	a	2424	C
22	a	2425	A
22	a	2429	G
22	a	2430	A
22	a	2431	U
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2476	A
22	a	2481	G
22	a	2482	A

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Mol	Chain	Res	Type
22	a	2484	G
22	a	2491	U
22	a	2494	G
22	a	2502	G
22	a	2505	G
22	a	2518	A
22	a	2529	G
22	a	2547	A
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2574	G
22	a	2602	A
22	a	2609	U
22	a	2613	U
22	a	2629	U
22	a	2663	G
22	a	2682	A
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2716	C
22	a	2726	A
22	a	2733	A
22	a	2739	U
22	a	2744	G
22	a	2748	A
22	a	2765	A
22	a	2778	A
22	a	2790	U
22	a	2799	A
22	a	2809	A
22	a	2818	U
22	a	2820	A
22	a	2821	A
22	a	2823	A
22	a	2835	A
22	a	2836	U
22	a	2849	U
22	a	2873	A
22	a	2874	C
22	a	2880	C

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Mol	Chain	Res	Type
22	a	2884	U
22	a	2885	G
22	a	2899	A
23	b	9	G
23	b	13	G
23	b	26	C
23	b	32	U
23	b	35	C
23	b	36	C
23	b	42	C
23	b	44	G
23	b	45	A
23	b	56	G
23	b	57	A
23	b	67	G
23	b	85	G
23	b	89	U
23	b	90	C
23	b	92	C
23	b	99	A
23	b	105	G
23	b	109	A
54	Z	3	C
54	Z	9	G
54	Z	17	C
54	Z	18	U
54	Z	19	G
54	Z	20	G
54	Z	22	A
54	Z	23	G
54	Z	32	G
54	Z	44	A
54	Z	47	A
54	Z	49	C
54	Z	68	C
55	V	2	C
55	V	5	G
55	V	8	U
55	V	11	C
55	V	14	A
55	V	19	G
55	V	46	G7M

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Mol	Chain	Res	Type
55	V	47	H2U
55	V	48	5MC
55	V	49	5MC
55	V	50	A
55	V	74	C

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	121	U
1	A	199	A
1	A	334	C
1	A	723	U
1	A	1026	G
1	A	1034	G
1	A	1035	A
54	Z	67	C
55	V	10	2MG
55	V	48	5MC

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	2MG	V	10	55	23,26,27	2.69	7 (30%)	33,38,41	2.25	10 (30%)
55	2MG	V	6	55	23,26,27	2.67	7 (30%)	33,38,41	2.09	8 (24%)
1	2MG	A	1516	1	23,26,27	2.50	7 (30%)	33,38,41	2.21	13 (39%)
22	OMG	a	2251	22,54	23,26,27	2.52	8 (34%)	32,38,41	1.91	8 (25%)
1	5MC	A	967	1	19,22,23	3.86	9 (47%)	26,32,35	1.02	2 (7%)
1	PSU	A	516	1,56	18,21,22	1.08	2 (11%)	21,30,33	1.88	5 (23%)
22	PSU	a	2457	22	18,21,22	1.21	1 (5%)	21,30,33	2.08	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	V	39	55	18,21,22	1.03	1 (5%)	21,30,33	1.88	4 (19%)
55	2MU	V	54	55	20,23,24	1.42	5 (25%)	27,33,36	2.00	7 (25%)
55	H2U	V	47	55	18,21,22	1.07	2 (11%)	19,30,33	1.19	2 (10%)
22	G7M	a	2069	22	23,26,27	2.64	7 (30%)	34,39,42	1.80	10 (29%)
22	PSU	a	955	22	18,21,22	1.19	1 (5%)	21,30,33	2.01	5 (23%)
22	1MG	a	745	22	23,26,27	2.67	8 (34%)	33,39,42	1.68	8 (24%)
22	PSU	a	2580	22	18,21,22	1.31	3 (16%)	21,30,33	2.18	6 (28%)
1	G7M	A	527	1	23,26,27	2.73	8 (34%)	34,39,42	1.76	9 (26%)
1	4OC	A	1402	1,56	20,23,24	2.78	8 (40%)	25,32,35	1.08	2 (8%)
54	OMC	Z	33	54	19,22,23	2.68	7 (36%)	25,31,34	0.74	0
55	70U	V	34	55,53	22,26,27	1.17	1 (4%)	27,37,40	0.85	1 (3%)
22	PSU	a	746	22,56	18,21,22	1.28	3 (16%)	21,30,33	2.18	5 (23%)
33	4D4	l	81	33	9,11,12	1.53	1 (11%)	7,13,15	2.22	4 (57%)
33	MS6	l	82	33	5,7,8	1.10	1 (20%)	2,7,9	1.33	0
55	G7M	V	46	55	23,26,27	2.81	8 (34%)	34,39,42	1.77	10 (29%)
55	5MC	V	49	55	19,22,23	3.86	9 (47%)	26,32,35	1.13	3 (11%)
22	2MG	a	2445	22	23,26,27	2.47	6 (26%)	33,38,41	2.17	10 (30%)
54	H2U	Z	21	54	18,21,22	1.00	2 (11%)	19,30,33	0.98	1 (5%)
22	2MG	a	1835	22	23,26,27	2.44	7 (30%)	33,38,41	2.35	10 (30%)
22	2MA	a	2503	22,56	22,25,26	3.71	10 (45%)	32,37,40	3.05	10 (31%)
55	5MC	V	48	55	19,22,23	3.79	9 (47%)	26,32,35	1.10	2 (7%)
22	H2U	a	2449	22	18,21,22	1.49	2 (11%)	19,30,33	0.79	0
22	OMC	a	2498	22,56	19,22,23	2.59	7 (36%)	25,31,34	1.02	1 (4%)
11	IAS	K	119	11	6,7,8	1.01	0	3,8,10	1.31	1 (33%)
55	PSU	V	27	55	18,21,22	0.97	1 (5%)	21,30,33	1.76	4 (19%)
1	MA6	A	1518	1	23,26,27	1.59	5 (21%)	33,38,41	2.32	12 (36%)
22	6MZ	a	2030	22	22,25,26	2.65	6 (27%)	29,36,39	2.41	11 (37%)
1	MA6	A	1519	1	23,26,27	1.64	5 (21%)	33,38,41	2.33	12 (36%)
1	2MG	A	1207	1	23,26,27	2.57	7 (30%)	33,38,41	2.16	8 (24%)
22	PSU	a	2604	22	18,21,22	1.15	1 (5%)	21,30,33	2.20	5 (23%)
54	5MU	Z	55	54	19,22,23	4.58	6 (31%)	27,32,35	3.75	9 (33%)
22	5MU	a	1939	22	19,22,23	4.51	7 (36%)	27,32,35	3.78	10 (37%)
22	3TD	a	1915	22	19,22,23	4.05	8 (42%)	23,32,35	1.89	2 (8%)
55	PSU	V	55	55	18,21,22	1.03	2 (11%)	21,30,33	2.09	5 (23%)
54	4SU	Z	8	54	18,21,22	4.19	8 (44%)	25,30,33	2.46	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	Z	56	54	18,21,22	1.11	1 (5%)	21,30,33	1.82	3 (14%)
22	OMU	a	2552	22	19,22,23	2.61	6 (31%)	25,31,34	2.17	5 (20%)
1	2MG	A	966	1	23,26,27	2.54	6 (26%)	33,38,41	2.42	10 (30%)
1	5MC	A	1407	1	19,22,23	3.42	8 (42%)	26,32,35	1.10	3 (11%)
12	D2T	L	89	12	8,9,10	2.32	2 (25%)	6,11,13	1.18	1 (16%)
25	MEQ	d	150	25	8,9,10	1.41	2 (25%)	5,10,12	1.20	1 (20%)
22	5MU	a	747	22	19,22,23	4.60	7 (36%)	27,32,35	3.69	10 (37%)
22	6MZ	a	1618	22	22,25,26	2.60	6 (27%)	29,36,39	2.32	10 (34%)
22	PSU	a	2504	22	18,21,22	1.05	1 (5%)	21,30,33	1.82	3 (14%)
1	UR3	A	1498	1	19,22,23	2.74	6 (31%)	26,32,35	1.67	4 (15%)
55	1MA	V	58	55	21,25,26	0.56	0	30,37,40	0.74	1 (3%)
55	12A	V	37	55,56	33,36,37	0.87	0	46,52,55	1.36	7 (15%)
22	PSU	a	1917	22	18,21,22	1.15	2 (11%)	21,30,33	2.04	5 (23%)
22	PSU	a	2605	22	18,21,22	1.18	1 (5%)	21,30,33	2.14	4 (19%)
22	5MC	a	1962	22	19,22,23	3.60	8 (42%)	26,32,35	1.23	3 (11%)
22	PSU	a	1911	22	18,21,22	0.99	2 (11%)	21,30,33	1.97	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	2MG	V	10	55	–	0/9/27/28	0/3/3/3
55	2MG	V	6	55	–	1/9/27/28	0/3/3/3
1	2MG	A	1516	1	–	0/9/27/28	0/3/3/3
22	OMG	a	2251	22,54	–	1/9/27/28	0/3/3/3
1	5MC	A	967	1	–	0/7/25/26	0/2/2/2
1	PSU	A	516	1,56	–	0/7/25/26	0/2/2/2
22	PSU	a	2457	22	–	0/7/25/26	0/2/2/2
55	PSU	V	39	55	–	0/7/25/26	0/2/2/2
55	2MU	V	54	55	–	0/9/27/28	0/2/2/2
55	H2U	V	47	55	–	6/7/38/39	0/2/2/2
22	G7M	a	2069	22	–	1/7/25/26	0/3/3/3
22	PSU	a	955	22	–	0/7/25/26	0/2/2/2
22	1MG	a	745	22	–	0/7/25/26	0/3/3/3
22	PSU	a	2580	22	–	0/7/25/26	0/2/2/2
1	G7M	A	527	1	–	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	A	1402	1,56	-	0/9/29/30	0/2/2/2
54	OMC	Z	33	54	-	1/9/27/28	0/2/2/2
55	70U	V	34	55,53	-	1/13/31/32	0/2/2/2
22	PSU	a	746	22,56	-	2/7/25/26	0/2/2/2
33	4D4	l	81	33	-	1/11/12/14	-
33	MS6	l	82	33	-	1/4/6/8	-
55	G7M	V	46	55	-	1/7/25/26	0/3/3/3
55	5MC	V	49	55	-	2/7/25/26	0/2/2/2
22	2MG	a	2445	22	-	0/9/27/28	0/3/3/3
54	H2U	Z	21	54	-	2/7/38/39	0/2/2/2
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
22	2MA	a	2503	22,56	-	2/7/25/26	0/3/3/3
55	5MC	V	48	55	-	2/7/25/26	0/2/2/2
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
22	OMC	a	2498	22,56	-	0/9/27/28	0/2/2/2
11	IAS	K	119	11	-	0/7/7/8	-
55	PSU	V	27	55	-	2/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
1	MA6	A	1519	1	-	2/11/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
54	5MU	Z	55	54	-	0/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
55	PSU	V	55	55	-	0/7/25/26	0/2/2/2
54	4SU	Z	8	54	-	0/7/25/26	0/2/2/2
54	PSU	Z	56	54	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
1	2MG	A	966	1	-	2/9/27/28	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
12	D2T	L	89	12	-	1/7/12/14	-
25	MEQ	d	150	25	-	1/8/9/11	-
22	5MU	a	747	22	-	1/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
22	PSU	a	2504	22	-	1/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
55	1MA	V	58	55	-	2/7/25/26	0/3/3/3
55	12A	V	37	55,56	-	4/25/43/44	0/3/3/3
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2

All (271) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C6-C5	12.56	1.49	1.35
22	a	2503	2MA	C4-N3	11.02	1.48	1.34
54	Z	55	5MU	C6-N1	10.45	1.55	1.38
54	Z	55	5MU	C2-N1	10.25	1.54	1.38
22	a	747	5MU	C6-N1	10.22	1.55	1.38
22	a	1618	6MZ	C6-N6	10.01	1.45	1.34
22	a	2030	6MZ	C6-N6	9.99	1.45	1.34
22	a	1939	5MU	C2-N1	9.95	1.54	1.38
22	a	747	5MU	C2-N1	9.93	1.54	1.38
22	a	1939	5MU	C6-N1	9.77	1.54	1.38
54	Z	8	4SU	C4-N3	9.69	1.47	1.37
1	A	967	5MC	C6-C5	9.29	1.49	1.34
22	a	1962	5MC	C6-C5	9.24	1.49	1.34
55	V	48	5MC	C6-C5	9.21	1.49	1.34
22	a	747	5MU	C4-C5	9.11	1.59	1.44
55	V	49	5MC	C6-C5	9.02	1.49	1.34
22	a	1915	3TD	C2-N1	9.02	1.48	1.37
54	Z	55	5MU	C4-C5	8.96	1.59	1.44
1	A	1407	5MC	C6-C5	8.72	1.48	1.34
22	a	1939	5MU	C4-C5	8.28	1.58	1.44
22	a	1939	5MU	C4-N3	-8.24	1.23	1.38
22	a	747	5MU	C4-N3	-7.90	1.24	1.38
55	V	6	2MG	C2-N3	7.77	1.46	1.32
54	Z	8	4SU	C2-N1	7.62	1.50	1.38
55	V	10	2MG	C2-N3	7.53	1.46	1.32
54	Z	55	5MU	C4-N3	-7.46	1.24	1.38
55	V	49	5MC	C4-N3	7.32	1.45	1.34
1	A	966	2MG	C2-N3	7.30	1.45	1.32
1	A	1207	2MG	C2-N3	7.30	1.45	1.32
1	A	967	5MC	C4-N3	7.28	1.45	1.34
1	A	1498	UR3	C2-N1	7.25	1.48	1.38
22	a	2503	2MA	C2-N3	7.22	1.46	1.34
55	V	48	5MC	C4-N3	7.05	1.45	1.34
22	a	2251	OMG	C4-N3	6.99	1.50	1.34
55	V	10	2MG	C4-N3	6.83	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	46	G7M	C2-N2	6.71	1.49	1.34
55	V	6	2MG	C4-N3	6.71	1.49	1.34
1	A	1516	2MG	C4-N3	6.58	1.49	1.34
1	A	1516	2MG	C2-N3	6.54	1.44	1.32
1	A	1207	2MG	C4-N3	6.54	1.49	1.34
1	A	966	2MG	C4-N3	6.53	1.49	1.34
54	Z	8	4SU	C2-N3	6.52	1.49	1.38
22	a	1835	2MG	C2-N3	6.50	1.44	1.32
22	a	2445	2MG	C2-N3	6.48	1.44	1.32
55	V	49	5MC	C5-C4	6.46	1.49	1.44
22	a	745	1MG	C2-N3	6.45	1.43	1.33
1	A	967	5MC	C2-N3	6.41	1.49	1.36
1	A	527	G7M	C4-N3	6.39	1.48	1.34
55	V	46	G7M	C4-N3	6.34	1.48	1.34
55	V	49	5MC	C2-N3	6.32	1.48	1.36
55	V	48	5MC	C2-N3	6.28	1.48	1.36
54	Z	8	4SU	C4-S4	-6.09	1.57	1.68
54	Z	55	5MU	C6-C5	6.08	1.44	1.34
22	a	1962	5MC	C4-N3	6.07	1.43	1.34
1	A	527	G7M	C2-N2	6.05	1.48	1.34
22	a	2069	G7M	C4-N3	6.02	1.48	1.34
22	a	2445	2MG	C4-N3	6.00	1.48	1.34
1	A	1402	4OC	C4-N3	5.99	1.42	1.32
1	A	1407	5MC	C4-N3	5.93	1.43	1.34
1	A	967	5MC	C5-C4	5.88	1.48	1.44
1	A	1402	4OC	C6-C5	5.88	1.48	1.35
1	A	1498	UR3	C6-C5	5.87	1.48	1.35
22	a	1939	5MU	C6-C5	5.79	1.44	1.34
22	a	2503	2MA	C2-N1	5.79	1.44	1.34
22	a	745	1MG	C4-N3	5.79	1.47	1.34
22	a	747	5MU	C6-C5	5.78	1.44	1.34
22	a	2069	G7M	C2-N2	5.75	1.47	1.34
22	a	1835	2MG	C4-N3	5.72	1.47	1.34
54	Z	8	4SU	C6-C5	5.69	1.48	1.35
54	Z	33	OMC	C2-N3	5.65	1.47	1.36
55	V	48	5MC	C5-C4	5.60	1.48	1.44
22	a	2552	OMU	C2-N1	5.58	1.47	1.38
22	a	745	1MG	C2-N2	5.58	1.43	1.34
54	Z	33	OMC	C6-C5	5.55	1.47	1.35
22	a	2498	OMC	C6-C5	5.52	1.47	1.35
22	a	1962	5MC	C2-N3	5.48	1.47	1.36
22	a	1962	5MC	C5-C4	5.42	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C6-N1	5.42	1.45	1.36
1	A	1407	5MC	C2-N3	5.41	1.47	1.36
22	a	2552	OMU	C2-N3	5.40	1.47	1.38
1	A	527	G7M	C2-N3	5.38	1.46	1.33
22	a	2069	G7M	C5-N7	-5.36	1.33	1.39
55	V	46	G7M	C2-N3	5.34	1.46	1.33
22	a	2503	2MA	C6-N6	-5.29	1.20	1.34
54	Z	8	4SU	C5-C4	5.28	1.48	1.42
22	a	2552	OMU	C6-C5	5.27	1.47	1.35
55	V	10	2MG	C2-N1	5.19	1.44	1.36
22	a	2498	OMC	C2-N3	5.07	1.46	1.36
55	V	6	2MG	C2-N1	5.06	1.44	1.36
22	a	2503	2MA	C5-C6	4.92	1.54	1.41
1	A	967	5MC	C6-N1	4.88	1.46	1.38
1	A	1402	4OC	C2-N3	4.85	1.46	1.36
12	L	89	D2T	CB-CA	-4.84	1.53	1.54
55	V	48	5MC	C6-N1	4.78	1.46	1.38
22	a	1962	5MC	C6-N1	4.77	1.46	1.38
55	V	49	5MC	C6-N1	4.75	1.46	1.38
1	A	527	G7M	C5-N7	-4.73	1.33	1.39
1	A	1407	5MC	C5-C4	4.60	1.47	1.44
1	A	1407	5MC	C6-N1	4.58	1.45	1.38
1	A	1207	2MG	C2-N1	4.57	1.44	1.36
22	a	2251	OMG	C2-N3	4.56	1.44	1.33
1	A	1498	UR3	C2-N3	4.56	1.48	1.39
55	V	46	G7M	C5-N7	-4.55	1.33	1.39
22	a	2069	G7M	C2-N3	4.54	1.44	1.33
54	Z	33	OMC	C4-N4	4.40	1.44	1.33
22	a	2251	OMG	C2-N2	4.35	1.44	1.34
22	a	1915	3TD	C2-N3	4.28	1.47	1.38
22	a	1835	2MG	C2-N1	4.23	1.43	1.36
1	A	966	2MG	C2-N1	4.17	1.43	1.36
55	V	49	5MC	C2-N1	4.16	1.48	1.40
55	V	34	70U	C2-S2	-4.16	1.61	1.67
22	a	2498	OMC	C2-N1	4.10	1.48	1.40
1	A	1516	2MG	C2-N1	4.07	1.43	1.36
54	Z	33	OMC	C4-N3	4.07	1.42	1.34
55	V	48	5MC	C2-N1	4.03	1.48	1.40
22	a	2552	OMU	O2-C2	-4.03	1.15	1.23
22	a	2503	2MA	C5-N7	-4.02	1.31	1.39
22	a	2498	OMC	C4-N4	4.00	1.43	1.33
1	A	967	5MC	C4-N4	3.99	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C2-N1	3.99	1.48	1.40
1	A	1402	4OC	O2-C2	-3.94	1.16	1.23
22	a	2251	OMG	C5-N7	-3.92	1.31	1.39
55	V	48	5MC	C4-N4	3.91	1.44	1.34
1	A	1518	MA6	C5-C4	-3.91	1.32	1.39
55	V	49	5MC	C4-N4	3.90	1.44	1.34
22	a	2445	2MG	C5-N7	-3.84	1.31	1.39
54	Z	8	4SU	O2-C2	-3.81	1.16	1.23
1	A	1519	MA6	C5-C4	-3.81	1.32	1.39
22	a	2251	OMG	O6-C6	-3.81	1.16	1.23
22	a	2449	H2U	C2-N3	-3.80	1.31	1.38
1	A	1402	4OC	C4-N4	3.73	1.43	1.36
22	a	2030	6MZ	C5-C4	-3.72	1.32	1.39
22	a	1835	2MG	C5-N7	-3.71	1.31	1.39
22	a	2498	OMC	O2-C2	-3.71	1.16	1.23
22	a	2449	H2U	C4-N3	-3.70	1.31	1.37
22	a	745	1MG	C5-N7	-3.70	1.31	1.39
54	Z	33	OMC	C2-N1	3.67	1.47	1.40
22	a	2552	OMU	O4-C4	-3.63	1.17	1.24
22	a	1962	5MC	C4-N4	3.63	1.43	1.34
22	a	2445	2MG	C2-N1	3.63	1.42	1.36
22	a	2445	2MG	O6-C6	-3.59	1.16	1.23
22	a	1618	6MZ	C5-C4	-3.59	1.32	1.39
22	a	1962	5MC	C2-N1	3.57	1.47	1.40
22	a	2498	OMC	C4-N3	3.57	1.41	1.34
1	A	527	G7M	C5-C6	3.56	1.53	1.43
55	V	46	G7M	C5-C6	3.55	1.53	1.43
1	A	1407	5MC	C4-N4	3.54	1.43	1.34
22	a	2069	G7M	C5-C6	3.51	1.53	1.43
22	a	1939	5MU	O2-C2	-3.50	1.16	1.23
54	Z	56	PSU	C6-C5	3.48	1.39	1.35
1	A	1402	4OC	C2-N1	3.46	1.47	1.40
22	a	2030	6MZ	C8-N9	-3.43	1.31	1.37
54	Z	33	OMC	O2-C2	-3.42	1.17	1.23
22	a	747	5MU	O2-C2	-3.40	1.17	1.23
1	A	1207	2MG	C5-N7	-3.38	1.32	1.39
22	a	2069	G7M	O6-C6	-3.37	1.17	1.23
33	l	81	4D4	OB-CB	-3.37	1.36	1.43
12	L	89	D2T	CB-SB	3.34	1.85	1.82
22	a	1962	5MC	O2-C2	-3.32	1.17	1.23
1	A	966	2MG	C5-N7	-3.31	1.32	1.39
1	A	1519	MA6	C8-N9	-3.30	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1519	MA6	C5-N7	-3.27	1.33	1.39
22	a	2030	6MZ	C5-N7	-3.25	1.33	1.39
1	A	1407	5MC	O2-C2	-3.23	1.17	1.23
1	A	1402	4OC	C5-C4	3.19	1.48	1.41
55	V	6	2MG	C5-N7	-3.19	1.32	1.39
1	A	1407	5MC	C2-N1	3.15	1.46	1.40
22	a	745	1MG	C4-N9	-3.11	1.30	1.38
1	A	1519	MA6	C6-N6	3.09	1.45	1.36
1	A	1516	2MG	O6-C6	-3.08	1.17	1.23
22	a	745	1MG	O6-C6	-3.07	1.16	1.23
1	A	1516	2MG	C5-N7	-3.05	1.32	1.39
55	V	27	PSU	C6-C5	3.04	1.38	1.35
22	a	1835	2MG	O6-C6	-3.02	1.17	1.23
1	A	1518	MA6	C8-N9	-3.01	1.32	1.37
22	a	1618	6MZ	C5-N7	-2.98	1.33	1.39
1	A	966	2MG	O6-C6	-2.98	1.17	1.23
22	a	1618	6MZ	C8-N9	-2.97	1.32	1.37
55	V	47	H2U	C2-N3	-2.96	1.32	1.38
1	A	1518	MA6	C5-N7	-2.95	1.33	1.39
55	V	46	G7M	C2-N1	2.94	1.44	1.37
22	a	1917	PSU	C6-C5	2.92	1.38	1.35
22	a	2445	2MG	C4-N9	-2.91	1.30	1.38
1	A	1498	UR3	O4-C4	-2.89	1.17	1.23
22	a	955	PSU	C6-C5	2.84	1.38	1.35
55	V	46	G7M	C6-N1	2.83	1.44	1.38
55	V	10	2MG	C5-N7	-2.83	1.33	1.39
55	V	39	PSU	C6-C5	2.82	1.38	1.35
55	V	55	PSU	C6-C5	2.82	1.38	1.35
55	V	47	H2U	C4-N3	-2.81	1.32	1.37
1	A	1518	MA6	C6-N6	2.81	1.44	1.36
22	a	1939	5MU	O4-C4	-2.79	1.18	1.23
54	Z	8	4SU	C6-N1	2.78	1.44	1.38
1	A	527	G7M	O6-C6	-2.78	1.18	1.23
55	V	46	G7M	O6-C6	-2.78	1.18	1.23
1	A	1518	MA6	C4-N9	-2.77	1.31	1.37
55	V	54	2MU	C4-N3	-2.77	1.33	1.38
1	A	1498	UR3	C6-N1	2.76	1.44	1.38
22	a	2504	PSU	C6-C5	2.73	1.38	1.35
22	a	745	1MG	C2-N1	2.72	1.42	1.37
22	a	2580	PSU	C6-C5	2.71	1.38	1.35
1	A	1498	UR3	O2-C2	-2.70	1.17	1.22
22	a	2503	2MA	C6-N1	2.67	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1516	2MG	C4-N9	-2.67	1.31	1.38
22	a	2604	PSU	C6-C5	2.67	1.38	1.35
55	V	54	2MU	C2-N1	2.66	1.42	1.38
22	a	1835	2MG	C4-N9	-2.65	1.31	1.38
1	A	516	PSU	C6-C5	2.64	1.38	1.35
22	a	1915	3TD	O4-C4	-2.64	1.17	1.23
22	a	2251	OMG	C4-N9	-2.64	1.31	1.38
1	A	527	G7M	C2-N1	2.63	1.44	1.37
22	a	746	PSU	O4'-C1'	-2.62	1.40	1.43
55	V	10	2MG	O6-C6	-2.61	1.18	1.23
1	A	1402	4OC	C6-N1	2.59	1.44	1.38
1	A	967	5MC	O2-C2	-2.57	1.18	1.23
55	V	10	2MG	C5-C6	2.56	1.53	1.44
22	a	745	1MG	C5-C6	2.55	1.52	1.45
54	Z	21	H2U	C4-N3	-2.54	1.33	1.37
55	V	48	5MC	O2-C2	-2.54	1.19	1.23
22	a	2580	PSU	O4'-C1'	-2.52	1.40	1.43
1	A	1519	MA6	C4-N9	-2.52	1.32	1.37
22	a	2498	OMC	C6-N1	2.52	1.44	1.38
25	d	150	MEQ	CB-CA	2.51	1.57	1.53
22	a	746	PSU	C6-C5	2.51	1.38	1.35
54	Z	33	OMC	C6-N1	2.46	1.43	1.38
55	V	10	2MG	C6-N1	2.45	1.43	1.38
22	a	2552	OMU	C4-N3	2.45	1.42	1.38
22	a	2251	OMG	C8-N9	-2.44	1.32	1.37
22	a	1915	3TD	O2-C2	-2.42	1.18	1.23
1	A	1207	2MG	O6-C6	-2.40	1.19	1.23
1	A	1207	2MG	C5-C6	2.40	1.53	1.44
1	A	1516	2MG	C5-C6	2.38	1.53	1.44
54	Z	21	H2U	C2-N3	-2.38	1.33	1.38
22	a	2503	2MA	C8-N9	-2.38	1.33	1.37
22	a	2503	2MA	C5-C4	-2.37	1.34	1.39
22	a	1835	2MG	C5-C6	2.37	1.53	1.44
22	a	2457	PSU	C4-C5	-2.35	1.37	1.44
22	a	747	5MU	O4-C4	-2.35	1.19	1.23
55	V	6	2MG	C5-C6	2.35	1.53	1.44
33	l	82	MS6	CB-CA	2.35	1.57	1.53
22	a	2605	PSU	C4-C5	-2.34	1.37	1.44
1	A	516	PSU	C4-C5	-2.34	1.37	1.44
54	Z	55	5MU	O2-C2	-2.33	1.18	1.23
55	V	49	5MC	O2-C2	-2.33	1.19	1.23
22	a	1915	3TD	C4-N3	2.29	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	150	MEQ	CE-NE2	-2.29	1.41	1.45
55	V	54	2MU	C6-C5	2.29	1.38	1.34
55	V	49	5MC	CM5-C5	2.27	1.56	1.50
55	V	6	2MG	O6-C6	-2.27	1.19	1.23
22	a	746	PSU	C4-C5	-2.27	1.38	1.44
22	a	2580	PSU	C4-C5	-2.25	1.38	1.44
1	A	527	G7M	C6-N1	2.25	1.43	1.38
22	a	2251	OMG	C5-C6	2.25	1.52	1.44
1	A	966	2MG	C5-C6	2.24	1.52	1.44
22	a	1911	PSU	C6-C5	2.21	1.37	1.35
55	V	54	2MU	C2-N3	-2.21	1.34	1.38
22	a	1917	PSU	C4-C5	-2.19	1.38	1.44
1	A	1207	2MG	C4-N9	-2.17	1.32	1.38
22	a	1618	6MZ	C6-N1	-2.17	1.31	1.35
55	V	54	2MU	C4-C5	2.17	1.48	1.44
55	V	48	5MC	CM5-C5	2.16	1.55	1.50
1	A	967	5MC	CM5-C5	2.16	1.55	1.50
55	V	55	PSU	O4'-C1'	-2.12	1.40	1.43
22	a	2030	6MZ	C4-N9	-2.09	1.33	1.37
22	a	2069	G7M	C2-N1	2.09	1.42	1.37
22	a	2030	6MZ	C6-N1	-2.08	1.31	1.35
22	a	1618	6MZ	C5-C6	-2.06	1.36	1.41
55	V	6	2MG	C6-N1	2.03	1.42	1.38
22	a	2503	2MA	CM2-C2	2.03	1.55	1.49
22	a	1911	PSU	C4-C5	-2.01	1.38	1.44
22	a	1915	3TD	O4'-C1'	-2.01	1.41	1.43

All (317) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Z	55	5MU	C5-C4-N3	12.46	126.16	115.32
22	a	1939	5MU	C5-C4-N3	12.33	126.04	115.32
22	a	747	5MU	C5-C4-N3	11.50	125.32	115.32
54	Z	55	5MU	C5-C6-N1	-9.99	112.46	123.31
22	a	1939	5MU	C5-C6-N1	-9.99	112.47	123.31
22	a	2503	2MA	C5-C4-N3	-9.92	116.73	127.18
22	a	747	5MU	C5-C6-N1	-9.45	113.05	123.31
54	Z	8	4SU	C4-N3-C2	-8.16	119.50	127.31
22	a	2503	2MA	N3-C4-N9	7.12	136.02	126.99
1	A	966	2MG	C2-N3-C4	7.05	120.82	112.00
22	a	2445	2MG	C2-N3-C4	6.83	120.54	112.00
22	a	2552	OMU	C4-N3-C2	-6.79	118.18	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2030	6MZ	N1-C2-N3	-6.76	118.35	128.58
1	A	1516	2MG	C2-N3-C4	6.71	120.39	112.00
22	a	1835	2MG	C2-N3-C4	6.69	120.37	112.00
55	V	10	2MG	C2-N3-C4	6.66	120.34	112.00
1	A	1207	2MG	C2-N3-C4	6.57	120.22	112.00
22	a	1915	3TD	N1-C2-N3	6.36	120.75	116.13
1	A	1518	MA6	N1-C2-N3	-6.35	118.98	128.58
1	A	966	2MG	C5-C4-N3	-6.32	118.33	128.39
22	a	2503	2MA	C1'-N9-C8	6.28	141.04	127.09
22	a	2503	2MA	C4-N9-C1'	-6.26	112.00	126.63
55	V	6	2MG	C2-N3-C4	6.16	119.71	112.00
22	a	746	PSU	N1-C2-N3	5.97	121.47	115.17
1	A	1519	MA6	N1-C2-N3	-5.96	119.57	128.58
22	a	2604	PSU	N1-C2-N3	5.86	121.35	115.17
54	Z	55	5MU	O4-C4-C5	-5.73	118.36	124.92
22	a	2580	PSU	N1-C2-N3	5.58	121.05	115.17
22	a	955	PSU	N1-C2-N3	5.55	121.02	115.17
22	a	1939	5MU	O4-C4-C5	-5.54	118.58	124.92
22	a	1835	2MG	N1-C2-N2	5.51	122.19	116.56
55	V	6	2MG	C5-C4-N3	-5.50	119.64	128.39
1	A	1498	UR3	C4-N3-C2	-5.49	120.16	124.58
1	A	1207	2MG	C5-C4-N3	-5.48	119.67	128.39
22	a	2605	PSU	C4-N3-C2	-5.42	118.90	126.37
55	V	55	PSU	N1-C2-N3	5.42	120.89	115.17
1	A	966	2MG	C2-N1-C6	-5.41	118.01	124.55
22	a	2457	PSU	N1-C2-N3	5.39	120.86	115.17
22	a	1835	2MG	C5-C4-N3	-5.39	119.81	128.39
22	a	2604	PSU	C4-N3-C2	-5.38	118.97	126.37
22	a	1911	PSU	C4-N3-C2	-5.36	118.99	126.37
22	a	1618	6MZ	N1-C2-N3	-5.34	120.50	128.58
22	a	2457	PSU	C4-N3-C2	-5.33	119.02	126.37
22	a	746	PSU	C4-N3-C2	-5.32	119.04	126.37
22	a	2605	PSU	N1-C2-N3	5.28	120.74	115.17
22	a	2251	OMG	C5-C4-N3	-5.26	120.02	128.39
22	a	1917	PSU	N1-C2-N3	5.25	120.71	115.17
22	a	1939	5MU	C4-N3-C2	-5.22	120.50	127.34
54	Z	8	4SU	C5-C4-N3	5.20	119.59	114.75
22	a	2580	PSU	C4-N3-C2	-5.17	119.25	126.37
22	a	2445	2MG	C5-C4-N3	-5.10	120.27	128.39
1	A	516	PSU	C4-N3-C2	-5.09	119.36	126.37
22	a	955	PSU	C4-N3-C2	-5.09	119.36	126.37
22	a	1618	6MZ	C5-C4-N3	-5.06	119.75	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	1917	PSU	C4-N3-C2	-5.02	119.45	126.37
54	Z	56	PSU	C4-N3-C2	-4.99	119.50	126.37
54	Z	55	5MU	C4-N3-C2	-4.99	120.80	127.34
22	a	2504	PSU	C4-N3-C2	-4.95	119.55	126.37
55	V	55	PSU	C4-N3-C2	-4.93	119.58	126.37
55	V	10	2MG	C5-C4-N3	-4.92	120.56	128.39
22	a	1939	5MU	N3-C2-N1	4.92	121.29	114.89
22	a	747	5MU	N3-C2-N1	4.87	121.23	114.89
54	Z	8	4SU	C5-C4-S4	-4.87	118.75	124.31
22	a	2069	G7M	C2-N3-C4	4.84	120.64	112.30
55	V	54	2MU	N3-C2-N1	4.83	121.18	114.89
22	a	747	5MU	C5M-C5-C4	4.83	123.93	118.78
55	V	39	PSU	C4-N3-C2	-4.81	119.74	126.37
22	a	2552	OMU	N3-C2-N1	4.81	121.15	114.89
55	V	39	PSU	N1-C2-N3	4.79	120.22	115.17
22	a	747	5MU	C4-N3-C2	-4.73	121.14	127.34
22	a	1911	PSU	N1-C2-N3	4.73	120.15	115.17
22	a	747	5MU	O4-C4-C5	-4.70	119.54	124.92
22	a	747	5MU	C5M-C5-C6	-4.67	116.52	122.85
1	A	1518	MA6	C2-N1-C6	4.64	123.17	111.83
22	a	2030	6MZ	N9-C8-N7	-4.63	107.36	113.94
55	V	37	12A	CA-N-CC	-4.63	114.28	121.99
1	A	1519	MA6	C2-N1-C6	4.61	123.08	111.83
22	a	2504	PSU	N1-C2-N3	4.57	119.99	115.17
22	a	1835	2MG	C2-N1-C6	-4.57	119.02	124.55
1	A	1519	MA6	N9-C8-N7	-4.54	107.50	113.94
22	a	1915	3TD	C4-N3-C2	-4.50	119.85	124.61
22	a	1962	5MC	C5-C6-N1	-4.47	118.45	123.31
22	a	1618	6MZ	N9-C8-N7	-4.44	107.64	113.94
1	A	1516	2MG	C5-C4-N3	-4.44	121.33	128.39
55	V	27	PSU	C4-N3-C2	-4.43	120.27	126.37
1	A	1518	MA6	N9-C8-N7	-4.42	107.67	113.94
22	a	745	1MG	C5-C4-N3	-4.40	121.39	128.39
1	A	516	PSU	N1-C2-N3	4.37	119.78	115.17
1	A	1207	2MG	C2-N1-C6	-4.37	119.27	124.55
54	Z	56	PSU	N1-C2-N3	4.36	119.77	115.17
22	a	2030	6MZ	C9-N6-C6	-4.33	118.83	122.85
22	a	2251	OMG	C2-N3-C4	4.33	119.76	112.30
1	A	1519	MA6	C4-C5-C6	4.32	120.38	115.91
55	V	46	G7M	C2-N3-C4	4.32	119.73	112.30
55	V	27	PSU	N1-C2-N3	4.30	119.70	115.17
1	A	966	2MG	N9-C4-N3	4.22	134.39	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Z	55	5MU	N3-C2-N1	4.22	120.38	114.89
55	V	10	2MG	C2-N1-C6	-4.14	119.55	124.55
22	a	2030	6MZ	C5-C4-N3	-4.10	121.06	126.72
55	V	6	2MG	C2-N1-C6	-4.10	119.59	124.55
55	V	46	G7M	C5-C6-N1	4.09	120.29	111.84
55	V	54	2MU	C4-N3-C2	-4.07	122.00	127.34
33	l	81	4D4	NE-CZ-NH2	4.06	127.65	120.67
22	a	2552	OMU	C5-C4-N3	4.06	120.49	114.80
1	A	1519	MA6	C5-C4-N3	-4.04	121.16	126.72
1	A	1518	MA6	C4-C5-C6	4.02	120.07	115.91
54	Z	8	4SU	N3-C2-N1	4.00	120.10	114.89
22	a	2069	G7M	C5-C6-N1	3.98	120.06	111.84
22	a	2069	G7M	C5-C4-N3	-3.97	120.65	128.15
55	V	6	2MG	N9-C4-N3	3.95	133.86	125.95
1	A	1207	2MG	N9-C4-N3	3.95	133.86	125.95
1	A	527	G7M	C2-N3-C4	3.93	119.08	112.30
1	A	527	G7M	C5-C6-N1	3.88	119.86	111.84
1	A	1518	MA6	C5-C4-N3	-3.84	121.43	126.72
22	a	1618	6MZ	C4-C5-C6	3.81	119.94	116.78
1	A	527	G7M	C5-C4-N3	-3.79	120.99	128.15
54	Z	55	5MU	C5M-C5-C4	3.78	122.82	118.78
22	a	1939	5MU	C5M-C5-C6	-3.75	117.77	122.85
55	V	10	2MG	N9-C8-N7	-3.74	106.47	113.40
54	Z	55	5MU	C5M-C5-C6	-3.73	117.80	122.85
1	A	1498	UR3	C5-C4-N3	3.64	119.83	115.04
55	V	48	5MC	C5-C6-N1	-3.60	119.40	123.31
22	a	2030	6MZ	C2-N3-C4	3.60	120.61	111.83
55	V	54	2MU	C5-C4-N3	3.59	118.45	115.32
55	V	46	G7M	O6-C6-C5	-3.58	120.01	128.01
55	V	49	5MC	C5-C6-N1	-3.55	119.46	123.31
22	a	2445	2MG	C2-N1-C6	-3.53	120.28	124.55
1	A	1516	2MG	N9-C8-N7	-3.51	106.88	113.40
22	a	745	1MG	C2-N3-C4	3.51	119.87	111.98
22	a	2251	OMG	N9-C4-N3	3.50	132.95	125.95
1	A	1407	5MC	C5-C6-N1	-3.49	119.52	123.31
22	a	1939	5MU	C5M-C5-C4	3.48	122.50	118.78
22	a	2445	2MG	N9-C4-N3	3.46	132.87	125.95
22	a	2445	2MG	N9-C8-N7	-3.44	107.02	113.40
22	a	2580	PSU	O2-C2-N1	-3.44	119.24	122.79
55	V	46	G7M	C5-C4-N3	-3.41	121.70	128.15
1	A	1519	MA6	C5-N7-C8	3.41	108.81	103.45
55	V	55	PSU	O2-C2-N1	-3.41	119.28	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2552	OMU	O2-C2-N1	-3.38	118.40	122.80
22	a	1618	6MZ	C2-N3-C4	3.34	119.98	111.83
22	a	1618	6MZ	C9-N6-C6	-3.33	119.76	122.85
22	a	2503	2MA	N3-C2-N1	-3.33	119.90	125.77
55	V	54	2MU	O4-C4-C5	-3.32	121.11	124.92
22	a	745	1MG	N9-C8-N7	-3.32	107.25	113.40
22	a	2503	2MA	N9-C8-N7	-3.26	109.31	113.94
22	a	1911	PSU	O2-C2-N1	-3.26	119.42	122.79
1	A	1516	2MG	C2-N1-C6	-3.25	120.62	124.55
22	a	2030	6MZ	C5-N7-C8	3.25	108.56	103.45
1	A	527	G7M	O6-C6-C5	-3.23	120.81	128.01
1	A	1516	2MG	N1-C2-N2	3.22	119.85	116.56
22	a	2503	2MA	C6-C5-C4	3.20	121.54	117.18
1	A	1519	MA6	C4-C5-N7	-3.16	106.97	110.58
22	a	2457	PSU	O2-C2-N1	-3.16	119.53	122.79
22	a	1618	6MZ	C5-N7-C8	3.15	108.41	103.45
55	V	10	2MG	N9-C4-N3	3.15	132.26	125.95
55	V	27	PSU	O2-C2-N1	-3.15	119.54	122.79
1	A	527	G7M	CN7-N7-C5	3.15	130.72	126.80
22	a	2251	OMG	C2-N1-C6	-3.13	119.43	125.11
1	A	1518	MA6	C2-N3-C4	3.12	119.44	111.83
1	A	1518	MA6	C5-N7-C8	3.11	108.33	103.45
22	a	747	5MU	O2-C2-N1	-3.10	118.76	122.80
1	A	966	2MG	C5-C6-N1	3.10	121.14	113.25
55	V	46	G7M	C2-N1-C6	-3.08	119.53	125.11
22	a	1618	6MZ	N3-C4-N9	3.07	132.39	127.17
55	V	47	H2U	C5-C4-N3	-3.07	113.42	116.69
1	A	527	G7M	N9-C4-N3	3.05	132.06	125.95
1	A	527	G7M	C2-N1-C6	-3.05	119.58	125.11
1	A	1519	MA6	C2-N3-C4	3.02	119.21	111.83
55	V	10	2MG	N1-C2-N2	3.00	119.63	116.56
1	A	1518	MA6	C4-C5-N7	-3.00	107.15	110.58
55	V	47	H2U	O4-C4-N3	2.98	124.90	120.30
1	A	1207	2MG	N9-C8-N7	-2.98	107.87	113.40
1	A	966	2MG	N9-C8-N7	-2.98	107.88	113.40
55	V	39	PSU	O2-C2-N1	-2.96	119.73	122.79
22	a	746	PSU	C6-N1-C2	-2.95	119.95	122.69
22	a	2552	OMU	O4-C4-C5	-2.92	120.13	125.16
22	a	1835	2MG	N9-C4-N3	2.92	131.78	125.95
22	a	2251	OMG	C5-C6-N1	2.90	120.63	113.25
22	a	2604	PSU	O2-C2-N1	-2.86	119.84	122.79
55	V	10	2MG	C5-C6-N1	2.86	120.53	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2498	OMC	O2-C2-N3	-2.85	117.83	122.33
1	A	966	2MG	O6-C6-C5	-2.85	119.01	126.53
1	A	1207	2MG	C5-C6-N1	2.85	120.50	113.25
55	V	55	PSU	C6-N1-C2	-2.83	120.06	122.69
1	A	1498	UR3	C6-N1-C2	-2.83	119.49	121.80
22	a	746	PSU	O2-C2-N1	-2.82	119.88	122.79
22	a	2605	PSU	C6-C5-C4	2.82	120.08	118.17
22	a	2251	OMG	N9-C8-N7	-2.82	108.17	113.40
22	a	2030	6MZ	C4-C5-N7	-2.80	107.38	110.58
1	A	966	2MG	N1-C2-N2	2.78	119.39	116.56
1	A	1516	2MG	N1-C2-N3	-2.77	119.01	123.68
55	V	54	2MU	C5M-C5-C4	2.77	121.74	118.78
22	a	2445	2MG	N1-C2-N3	-2.77	119.01	123.68
1	A	1207	2MG	O6-C6-C5	-2.76	119.24	126.53
22	a	955	PSU	C6-N1-C2	-2.76	120.13	122.69
22	a	2445	2MG	C5-C6-N1	2.76	120.27	113.25
55	V	34	70U	C1'-N1-C6	-2.76	116.61	121.15
54	Z	21	H2U	O4-C4-N3	2.75	124.54	120.30
1	A	1516	2MG	C5-C6-N1	2.75	120.24	113.25
22	a	2069	G7M	O6-C6-C5	-2.74	121.89	128.01
22	a	2069	G7M	C2-N1-C6	-2.72	120.18	125.11
55	V	6	2MG	N9-C8-N7	-2.71	108.37	113.40
22	a	2445	2MG	N1-C2-N2	2.71	119.33	116.56
22	a	745	1MG	C5-C6-N1	2.70	120.01	115.02
22	a	2030	6MZ	C4-N9-C8	2.70	108.57	105.74
22	a	2069	G7M	N9-C4-N3	2.69	131.34	125.95
1	A	527	G7M	CN7-N7-C8	-2.66	120.76	124.79
1	A	967	5MC	C5-C6-N1	-2.66	120.43	123.31
22	a	1835	2MG	N9-C8-N7	-2.65	108.50	113.40
22	a	747	5MU	O4-C4-N3	-2.64	115.14	120.11
22	a	1835	2MG	N2-C2-N3	-2.63	117.17	120.51
22	a	1835	2MG	C5-C6-N1	2.62	119.93	113.25
1	A	1498	UR3	C1'-N1-C2	2.62	121.33	117.04
22	a	2503	2MA	C5-N7-C8	2.61	107.55	103.45
22	a	2503	2MA	CM2-C2-N3	2.60	121.02	117.13
22	a	2069	G7M	CN7-N7-C5	2.60	130.04	126.80
1	A	1402	4OC	O2-C2-N3	-2.59	118.24	122.33
22	a	2604	PSU	C6-N1-C2	-2.59	120.29	122.69
22	a	2580	PSU	C6-N1-C2	-2.59	120.29	122.69
54	Z	55	5MU	O2-C2-N1	-2.58	119.43	122.80
55	V	10	2MG	C8-N7-C5	2.58	108.86	104.26
55	V	55	PSU	C6-C5-C4	2.58	119.91	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1516	2MG	C1'-N9-C4	-2.58	118.87	126.49
55	V	6	2MG	C5-C6-N1	2.56	119.77	113.25
1	A	1518	MA6	C5-C4-N9	2.54	108.58	105.81
55	V	6	2MG	O6-C6-C5	-2.53	119.84	126.53
22	a	1939	5MU	O4-C4-N3	-2.53	115.36	120.11
55	V	46	G7M	N9-C8-N7	-2.51	106.38	112.48
33	l	81	4D4	O-C-CA	-2.51	118.32	124.77
12	L	89	D2T	O-C-CA	-2.48	118.39	124.77
55	V	39	PSU	C6-N1-C2	-2.48	120.39	122.69
55	V	54	2MU	C6-N1-C2	-2.47	118.84	121.30
54	Z	55	5MU	O4-C4-N3	-2.46	115.48	120.11
1	A	1519	MA6	C4-N9-C8	2.46	108.32	105.74
22	a	1939	5MU	O2-C2-N1	-2.45	119.61	122.80
55	V	10	2MG	O6-C6-C5	-2.44	120.08	126.53
1	A	1518	MA6	C5-C6-N6	2.44	129.20	125.33
55	V	46	G7M	CN7-N7-C5	2.44	129.84	126.80
1	A	1518	MA6	N1-C6-N6	-2.44	113.89	116.86
22	a	2580	PSU	O4'-C1'-C2'	2.44	108.52	105.15
22	a	1917	PSU	C6-C5-C4	2.44	119.82	118.17
1	A	1519	MA6	C5-C6-N6	2.43	129.18	125.33
55	V	27	PSU	C6-N1-C2	-2.42	120.44	122.69
1	A	1402	4OC	C6-C5-C4	2.42	119.92	117.00
1	A	1516	2MG	C8-N7-C5	2.41	108.56	104.26
55	V	10	2MG	N1-C2-N3	-2.41	119.62	123.68
1	A	1518	MA6	C4-N9-C8	2.41	108.27	105.74
22	a	2605	PSU	C5-C6-N1	-2.40	118.81	122.14
55	V	54	2MU	O2-C2-N3	-2.40	117.07	121.49
33	l	81	4D4	CG-CD-NE	-2.40	105.30	111.88
22	a	2251	OMG	O6-C6-C5	-2.40	120.20	126.53
55	V	6	2MG	N1-C2-N2	2.39	119.00	116.56
22	a	2251	OMG	C1'-N9-C4	-2.39	119.42	126.49
22	a	1618	6MZ	C4-N9-C8	2.39	108.25	105.74
22	a	1618	6MZ	C4-C5-N7	-2.38	107.86	110.58
22	a	746	PSU	C6-C5-C4	2.38	119.78	118.17
54	Z	8	4SU	C1'-N1-C2	2.38	121.86	117.59
55	V	46	G7M	N9-C4-N3	2.38	130.71	125.95
22	a	2069	G7M	CN7-N7-C8	-2.37	121.20	124.79
22	a	1835	2MG	CM2-N2-C2	-2.37	118.55	123.65
22	a	1917	PSU	C6-N1-C2	-2.36	120.50	122.69
22	a	2457	PSU	C6-N1-C2	-2.36	120.50	122.69
1	A	1519	MA6	C5-C4-N9	2.36	108.38	105.81
22	a	1917	PSU	O2-C2-N1	-2.35	120.36	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	V	49	5MC	CM5-C5-C6	-2.33	119.69	122.85
22	a	745	1MG	N9-C4-N3	2.31	130.57	125.95
22	a	1835	2MG	O6-C6-C5	-2.30	120.46	126.53
22	a	2445	2MG	O6-C6-C5	-2.29	120.49	126.53
55	V	37	12A	N3-C4-N9	2.28	129.88	126.99
1	A	966	2MG	C8-N7-C5	2.26	108.28	104.26
1	A	1516	2MG	N9-C4-N3	2.26	130.47	125.95
1	A	1407	5MC	CM5-C5-C6	-2.24	119.82	122.85
22	a	2580	PSU	C6-C5-C4	2.24	119.68	118.17
22	a	2069	G7M	N9-C8-N7	-2.24	107.05	112.48
1	A	516	PSU	O2-C2-N1	-2.23	120.49	122.79
55	V	37	12A	N6-CC-N	2.23	116.83	113.77
1	A	516	PSU	O4'-C1'-C2'	2.23	108.23	105.15
22	a	745	1MG	N2-C2-N1	2.22	120.57	118.79
55	V	37	12A	N6-C6-N1	2.22	124.74	117.62
1	A	527	G7M	N9-C8-N7	-2.22	107.10	112.48
22	a	747	5MU	C1'-N1-C2	2.20	121.54	117.59
1	A	1516	2MG	O6-C6-C5	-2.19	120.75	126.53
1	A	966	2MG	CM2-N2-C2	-2.18	118.97	123.65
1	A	1516	2MG	C6-C5-N7	2.16	134.23	130.29
33	l	81	4D4	NH1-CZ-NE	-2.16	114.36	119.27
1	A	1519	MA6	N1-C6-N6	-2.16	114.23	116.86
25	d	150	MEQ	OE1-CD-CG	2.16	125.93	122.02
22	a	2504	PSU	O2-C2-N1	-2.15	120.57	122.79
22	a	2030	6MZ	N3-C4-N9	2.15	130.82	127.17
22	a	2604	PSU	C6-C5-C4	2.15	119.62	118.17
55	V	46	G7M	CN7-N7-C8	-2.14	121.56	124.79
22	a	2069	G7M	N1-C2-N3	-2.12	119.44	123.32
22	a	1962	5MC	O2-C2-N3	-2.12	118.98	122.33
55	V	58	1MA	C6-C5-N7	-2.12	128.41	132.16
22	a	745	1MG	C8-N7-C5	2.11	108.02	104.26
55	V	48	5MC	CM5-C5-C6	-2.10	120.00	122.85
22	a	2445	2MG	C8-N7-C5	2.10	108.01	104.26
22	a	2030	6MZ	C5-C4-N9	2.10	108.10	105.81
22	a	2503	2MA	C2-N3-C4	2.10	122.22	115.02
55	V	37	12A	OG1-CB-CA	2.10	113.30	109.07
55	V	37	12A	O-C-CA	-2.10	114.91	121.86
1	A	516	PSU	C5-C4-N3	2.09	121.15	116.55
1	A	1516	2MG	C4-C5-N7	-2.08	107.37	110.67
55	V	46	G7M	N2-C2-N1	2.07	121.14	116.76
22	a	1939	5MU	C6-C5-C4	2.07	119.73	118.02
1	A	1407	5MC	C5-C4-N3	-2.06	119.64	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2030	6MZ	C4-C5-C6	2.05	118.48	116.78
55	V	49	5MC	O2-C2-N3	-2.04	119.11	122.33
22	a	955	PSU	O2-C2-N1	-2.04	120.68	122.79
22	a	1962	5MC	CM5-C5-C6	-2.03	120.10	122.85
1	A	1207	2MG	N1-C2-N3	-2.03	120.25	123.68
55	V	37	12A	C4-N9-C8	2.02	107.86	105.74
1	A	967	5MC	CM5-C5-C6	-2.02	120.12	122.85
54	Z	56	PSU	C5-C4-N3	2.01	120.97	116.55
22	a	955	PSU	O2-C2-N3	-2.01	118.30	121.86
22	a	745	1MG	C1'-N9-C8	-2.00	121.04	126.73
11	K	119	IAS	OXT-C-O	-2.00	119.54	124.08

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	Z	21	H2U	O4'-C1'-N1-C2
54	Z	21	H2U	O4'-C1'-N1-C6
22	a	2251	OMG	C1'-C2'-O2'-CM2
55	V	47	H2U	O4'-C1'-N1-C6
55	V	47	H2U	C2'-C1'-N1-C2
55	V	47	H2U	C2'-C1'-N1-C6
55	V	49	5MC	O4'-C4'-C5'-O5'
55	V	49	5MC	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
55	V	47	H2U	O4'-C4'-C5'-O5'
55	V	47	H2U	C3'-C4'-C5'-O5'
22	a	2030	6MZ	O4'-C4'-C5'-O5'
55	V	48	5MC	O4'-C4'-C5'-O5'
55	V	58	1MA	O4'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
55	V	48	5MC	C3'-C4'-C5'-O5'
55	V	37	12A	OXT-C-CA-N
55	V	27	PSU	O4'-C4'-C5'-O5'
55	V	37	12A	C-CA-CB-OG1
55	V	37	12A	C-CA-CB-CG2
55	V	58	1MA	C3'-C4'-C5'-O5'
1	A	966	2MG	C3'-C4'-C5'-O5'
55	V	6	2MG	C3'-C4'-C5'-O5'
25	d	150	MEQ	C-CA-CB-CG
1	A	527	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	V	46	G7M	O4'-C4'-C5'-O5'
55	V	47	H2U	O4'-C1'-N1-C2
55	V	37	12A	O-C-CA-N
1	A	966	2MG	O4'-C4'-C5'-O5'
22	a	747	5MU	C3'-C4'-C5'-O5'
22	a	746	PSU	O4'-C1'-C5-C6
54	Z	33	OMC	C3'-C2'-O2'-CM2
22	a	2504	PSU	O4'-C4'-C5'-O5'
12	L	89	D2T	CG-CB-SB-CB1
22	a	746	PSU	C2'-C1'-C5-C6
55	V	27	PSU	C3'-C4'-C5'-O5'
22	a	2069	G7M	C4'-C5'-O5'-P
22	a	2503	2MA	C4'-C5'-O5'-P
33	l	82	MS6	CB-CG-SD-CE
33	l	81	4D4	O-C-CA-CB
55	V	34	70U	C5-C5M-C8-O9
1	A	527	G7M	C4'-C5'-O5'-P
22	a	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

14 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	V	10	2MG	4	0
1	A	1516	2MG	1	0
1	A	967	5MC	1	0
54	Z	33	OMC	1	0
54	Z	21	H2U	1	0
22	a	2503	2MA	1	0
22	a	2498	OMC	1	0
11	K	119	IAS	1	0
22	a	2030	6MZ	2	0
1	A	1519	MA6	1	0
1	A	1207	2MG	1	0
22	a	1939	5MU	1	0
55	V	58	1MA	1	0
55	V	37	12A	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 393 ligands modelled in this entry, 393 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

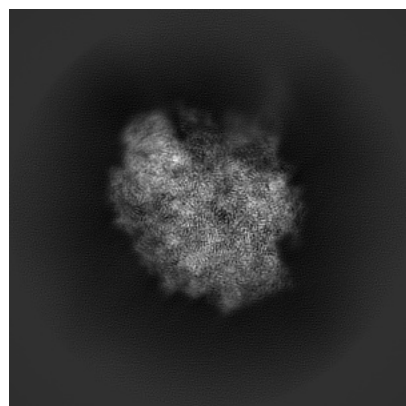
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61706. These allow visual inspection of the internal detail of the map and identification of artifacts.

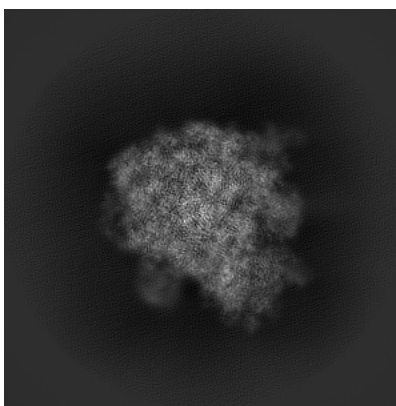
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

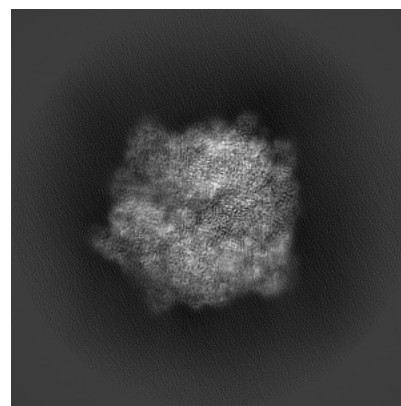
6.1.1 Primary map



X

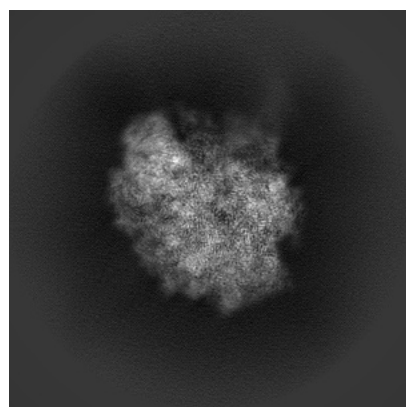


Y

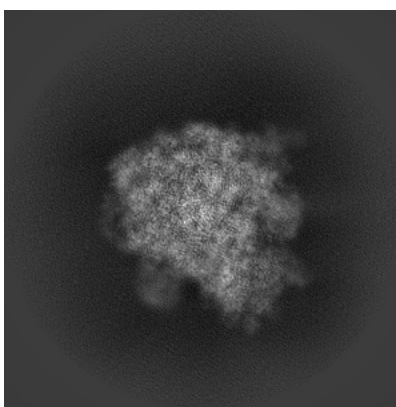


Z

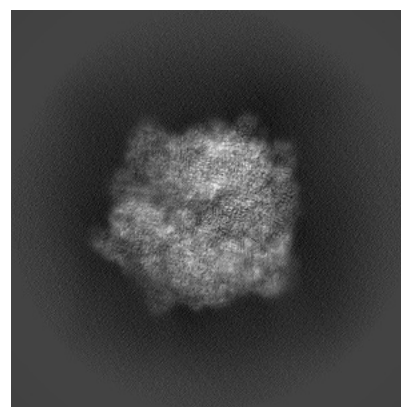
6.1.2 Raw map



X



Y

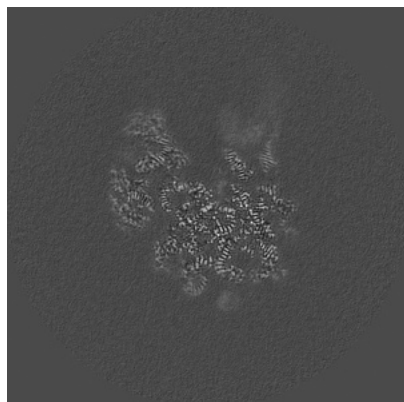


Z

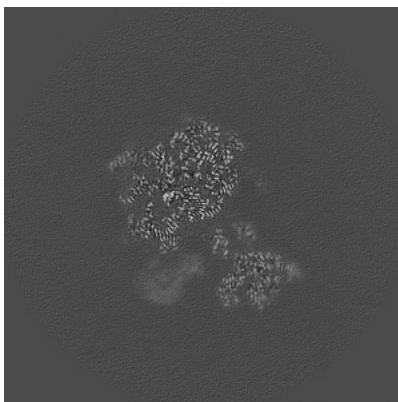
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

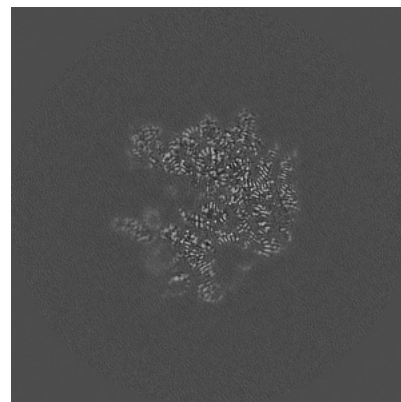
6.2.1 Primary map



X Index: 265

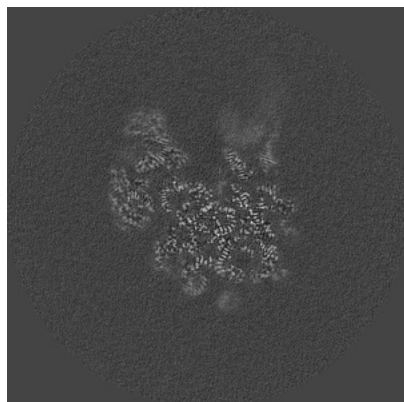


Y Index: 265

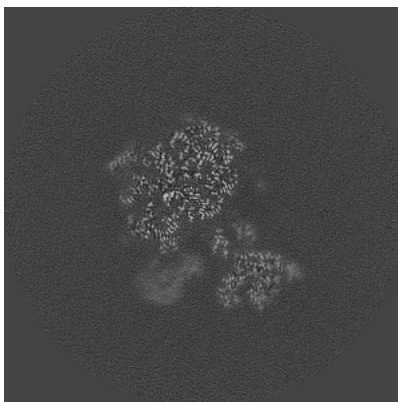


Z Index: 265

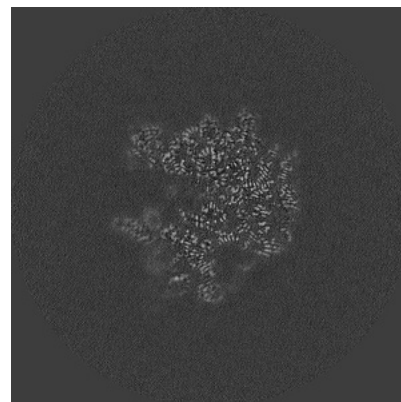
6.2.2 Raw map



X Index: 265



Y Index: 265

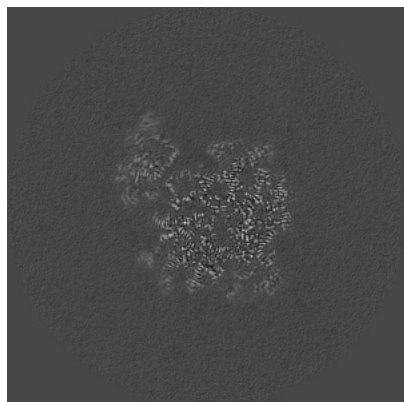


Z Index: 265

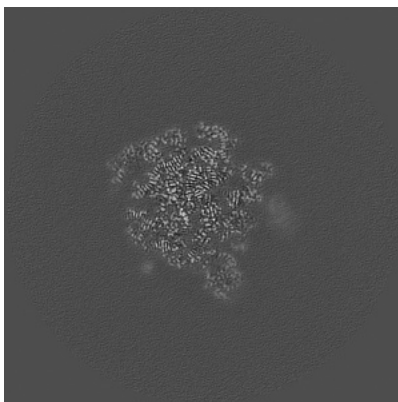
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

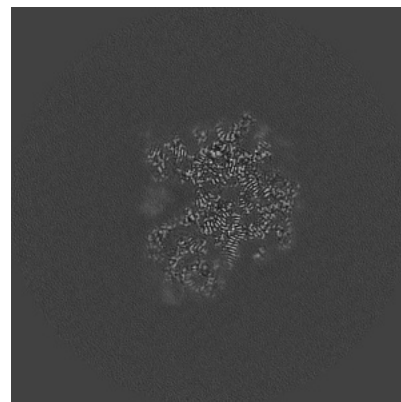
6.3.1 Primary map



X Index: 294

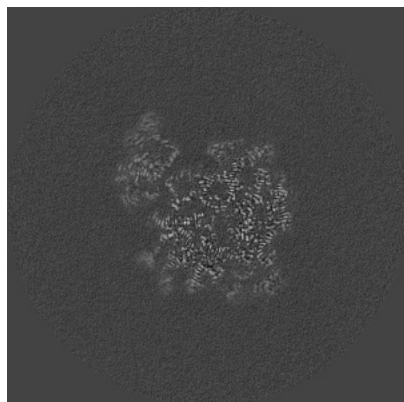


Y Index: 318

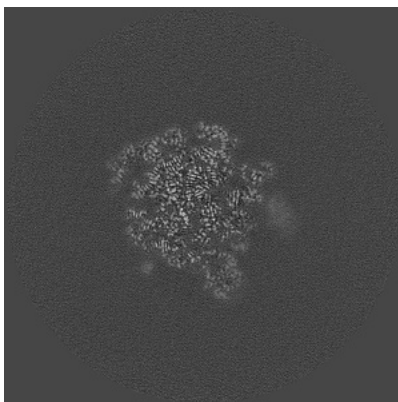


Z Index: 244

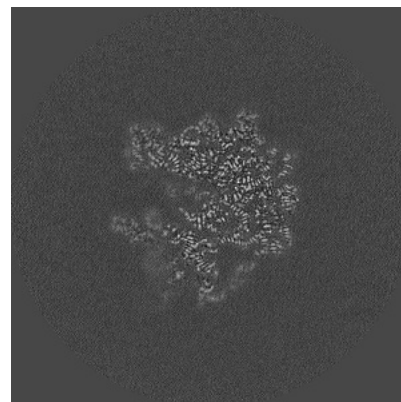
6.3.2 Raw map



X Index: 294



Y Index: 318

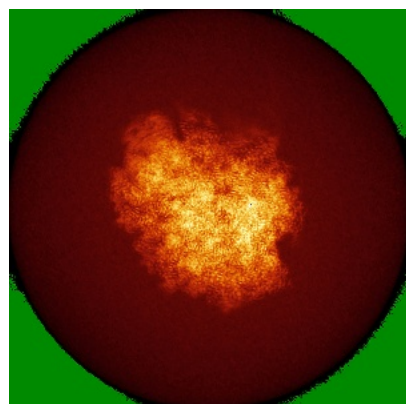


Z Index: 268

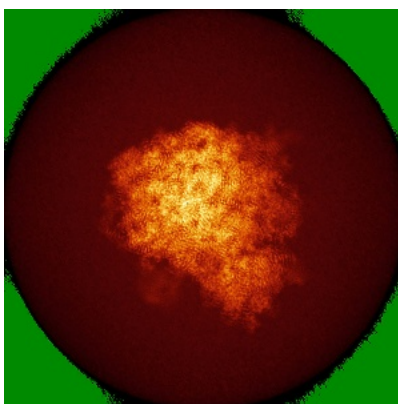
The images above show the largest variance slices of the map in three orthogonal directions.

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

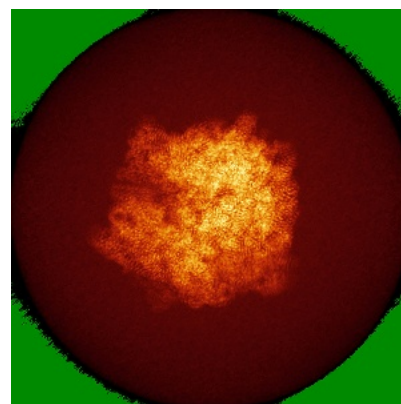
6.4.1 Primary map



X

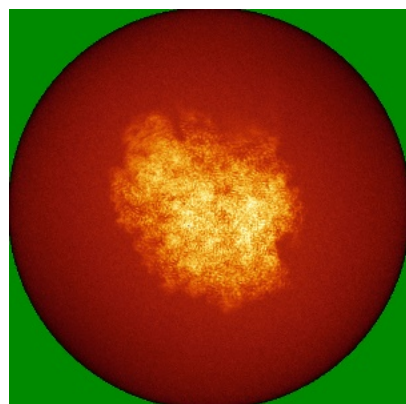


Y

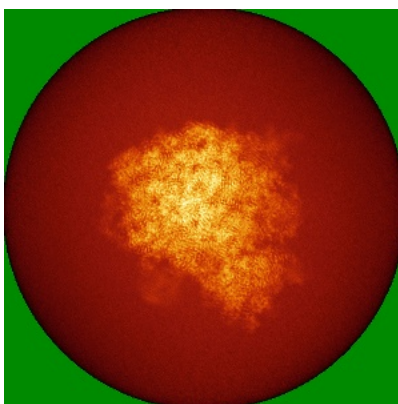


Z

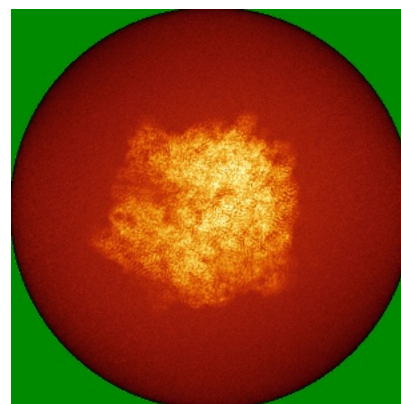
6.4.2 Raw map



X



Y

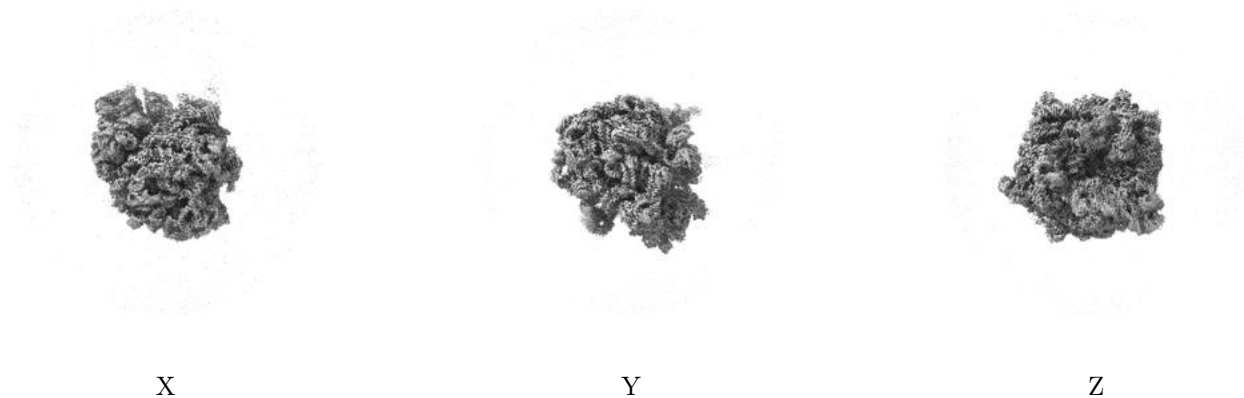


Z

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

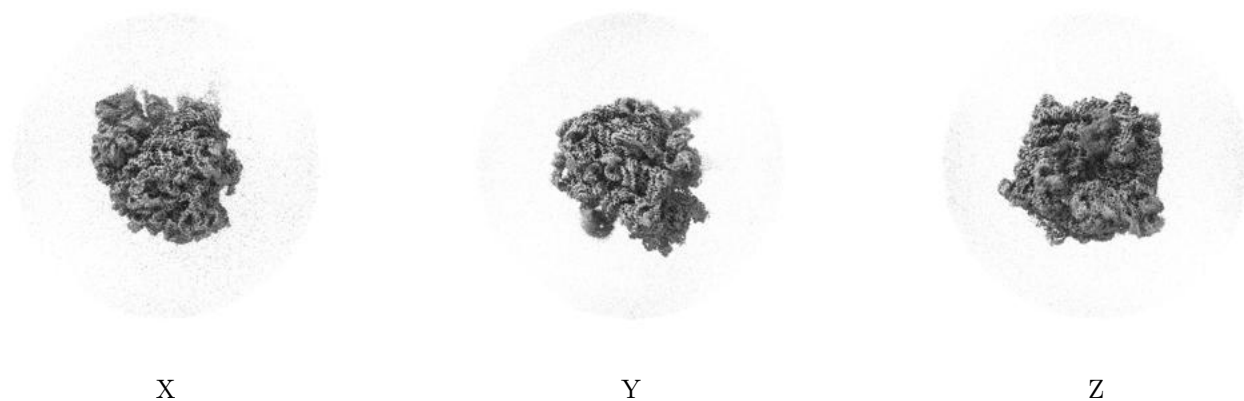
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0107. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

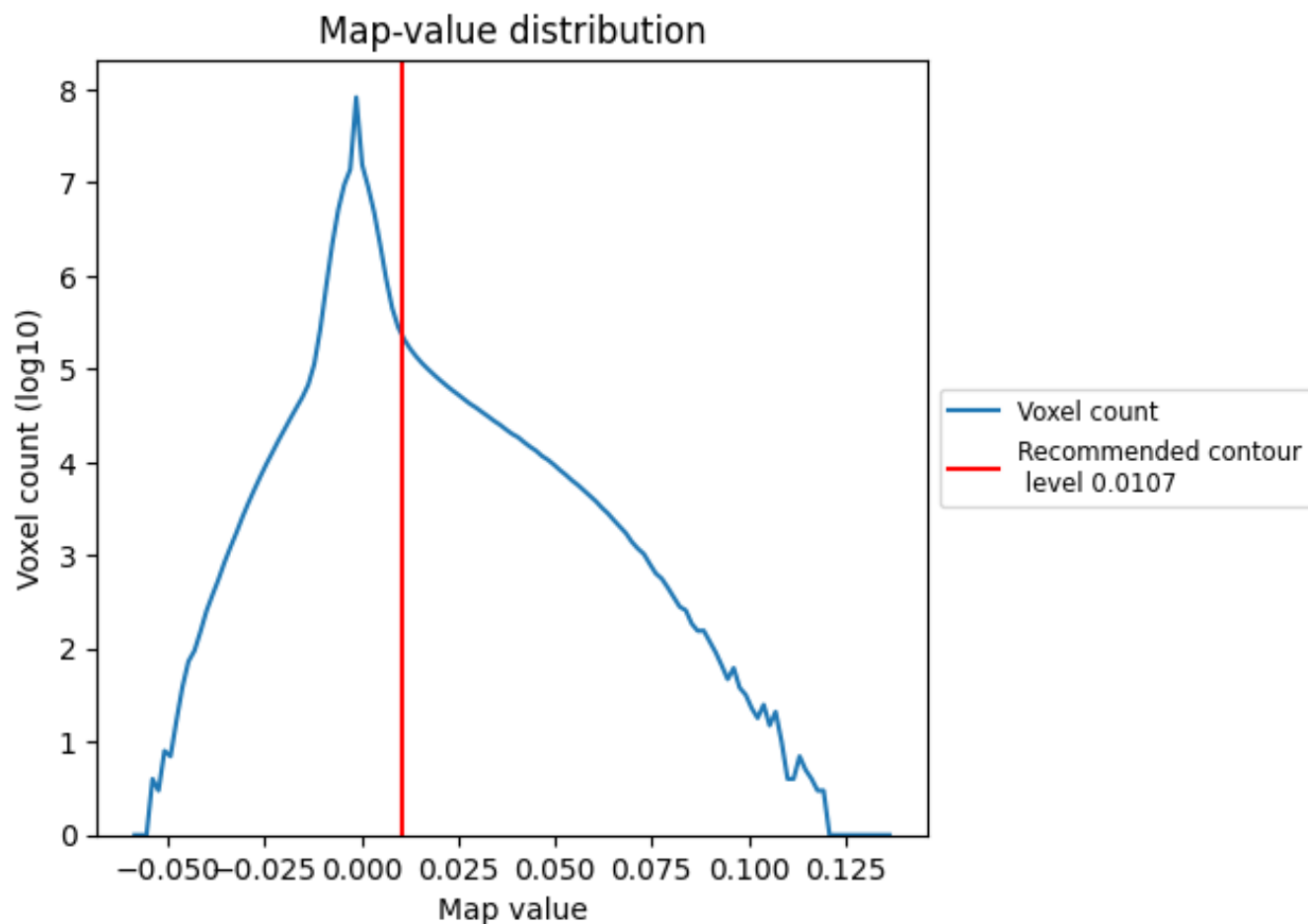
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

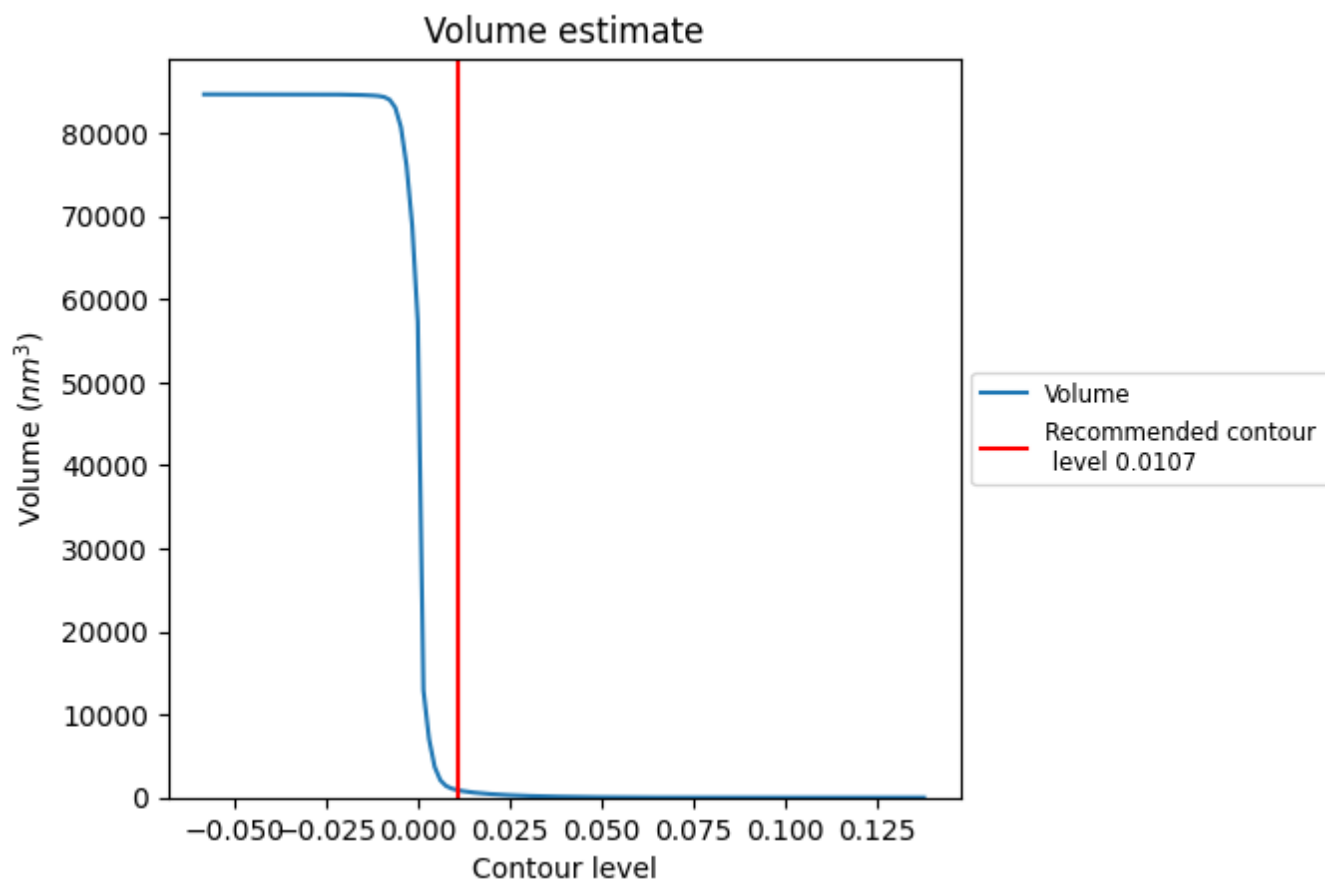
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

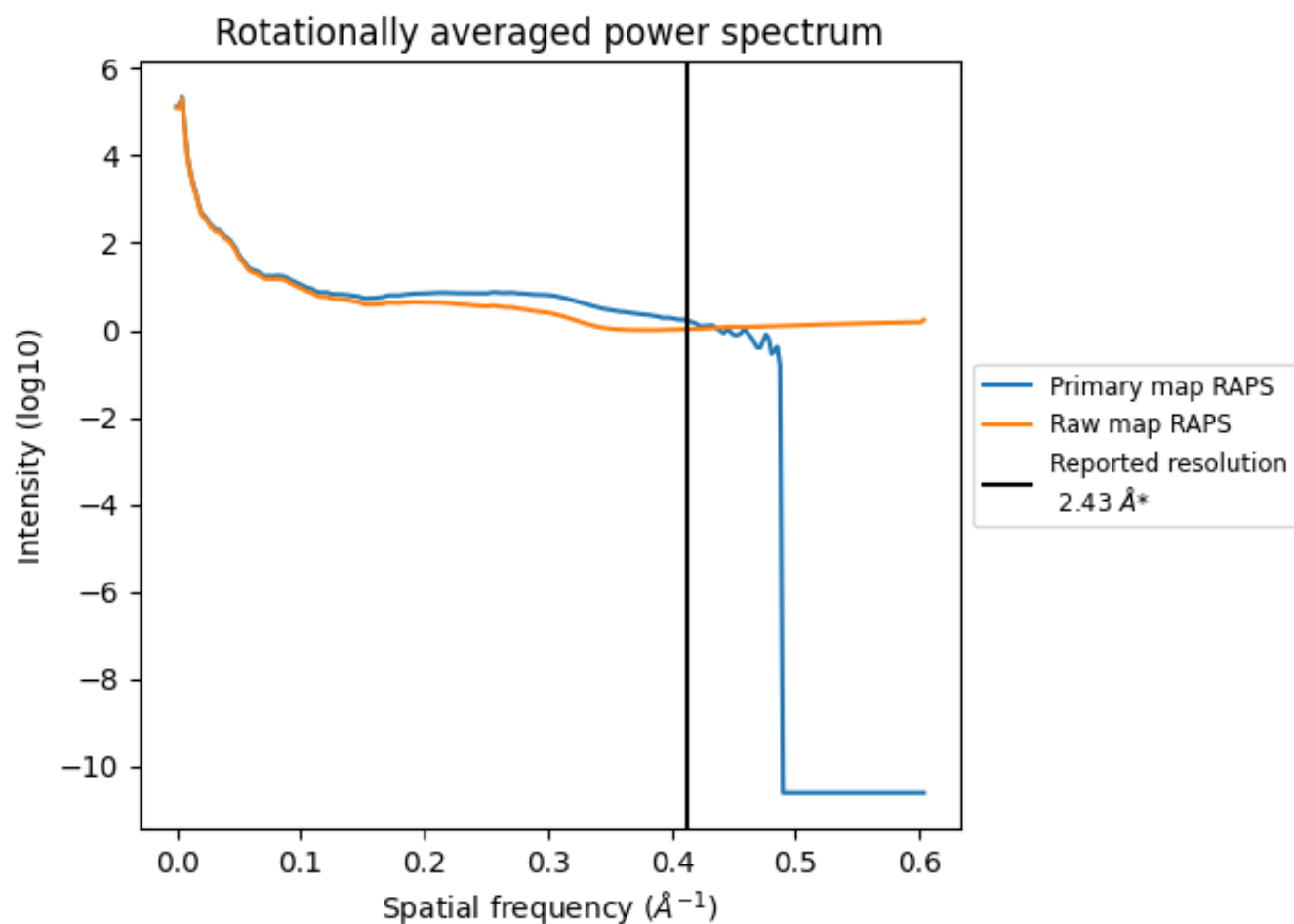
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 896 nm^3 ; this corresponds to an approximate mass of 809 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

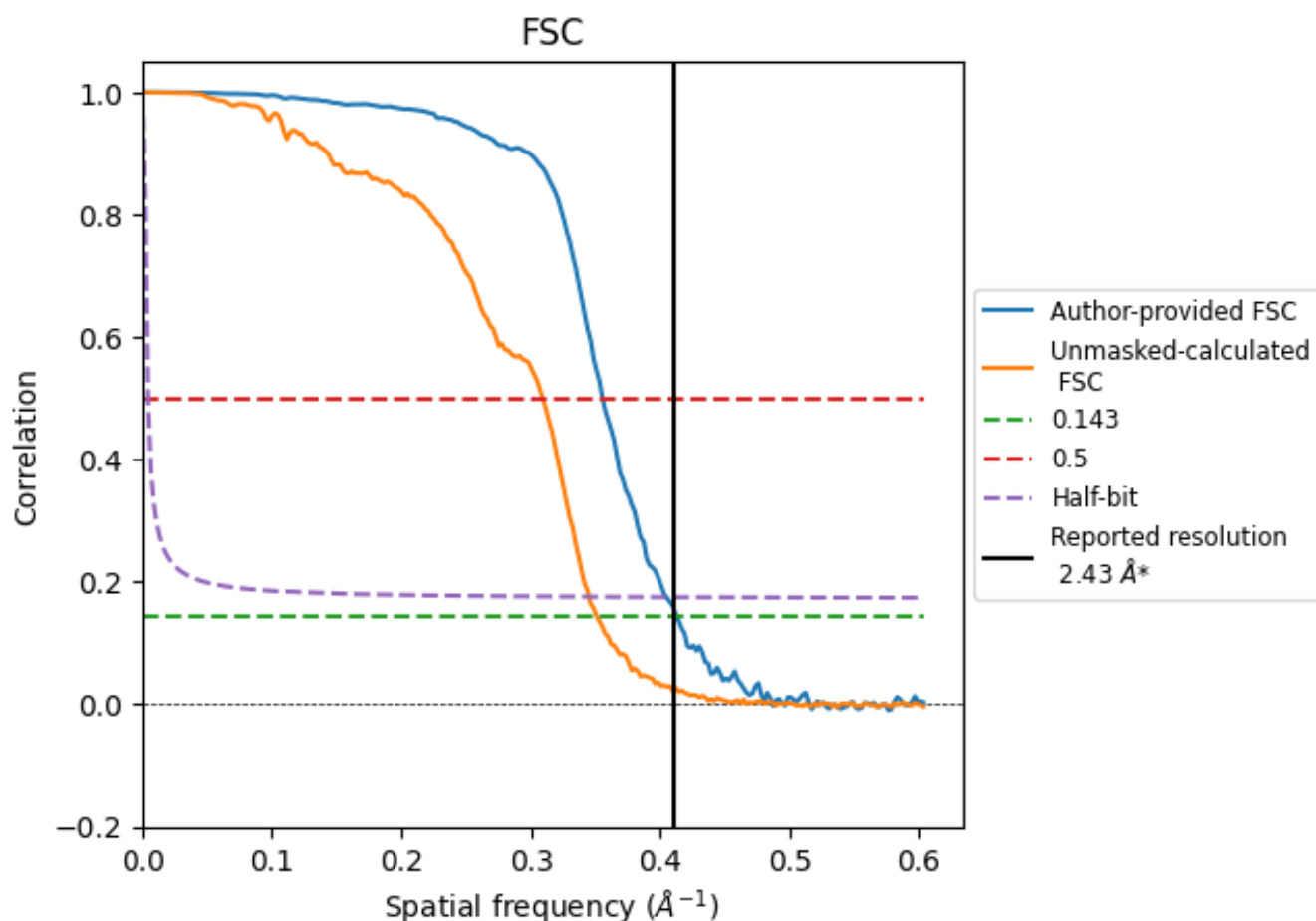


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.412 \AA^{-1}

8.2 Resolution estimates [i](#)

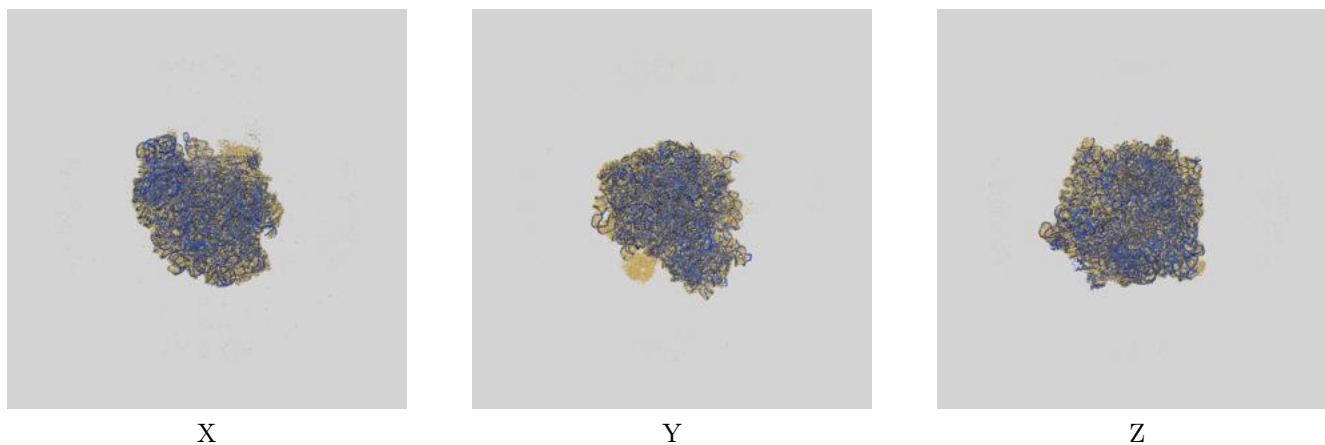
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.42	2.81	2.47
Unmasked-calculated*	2.85	3.23	2.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.85 differs from the reported value 2.43 by more than 10 %

9 Map-model fit [i](#)

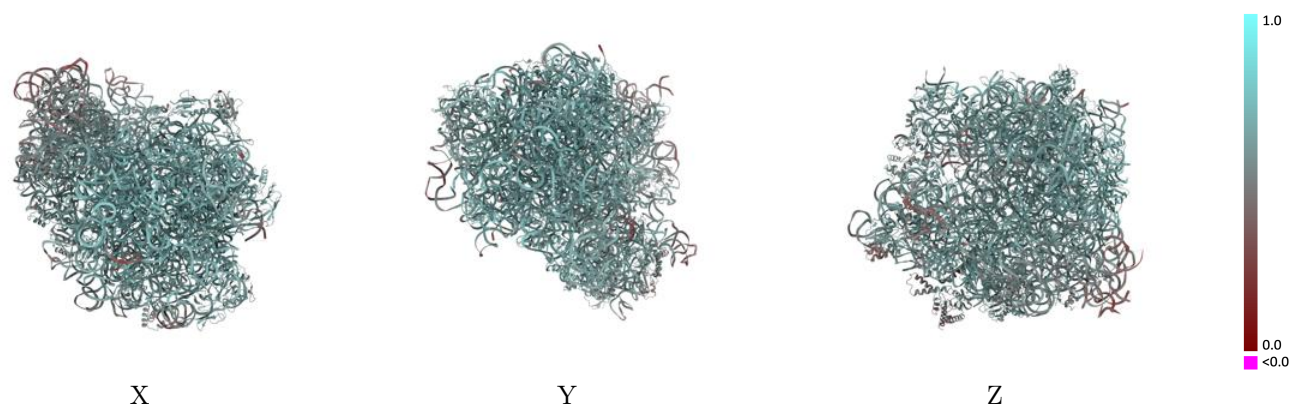
This section contains information regarding the fit between EMDB map EMD-61706 and PDB model 9JPM. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



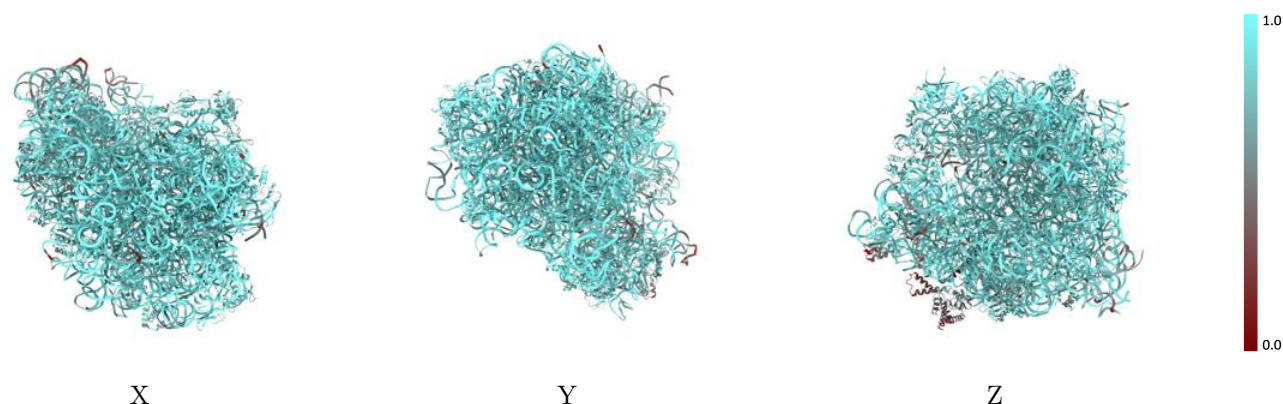
The images above show the 3D surface view of the map at the recommended contour level 0.0107 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



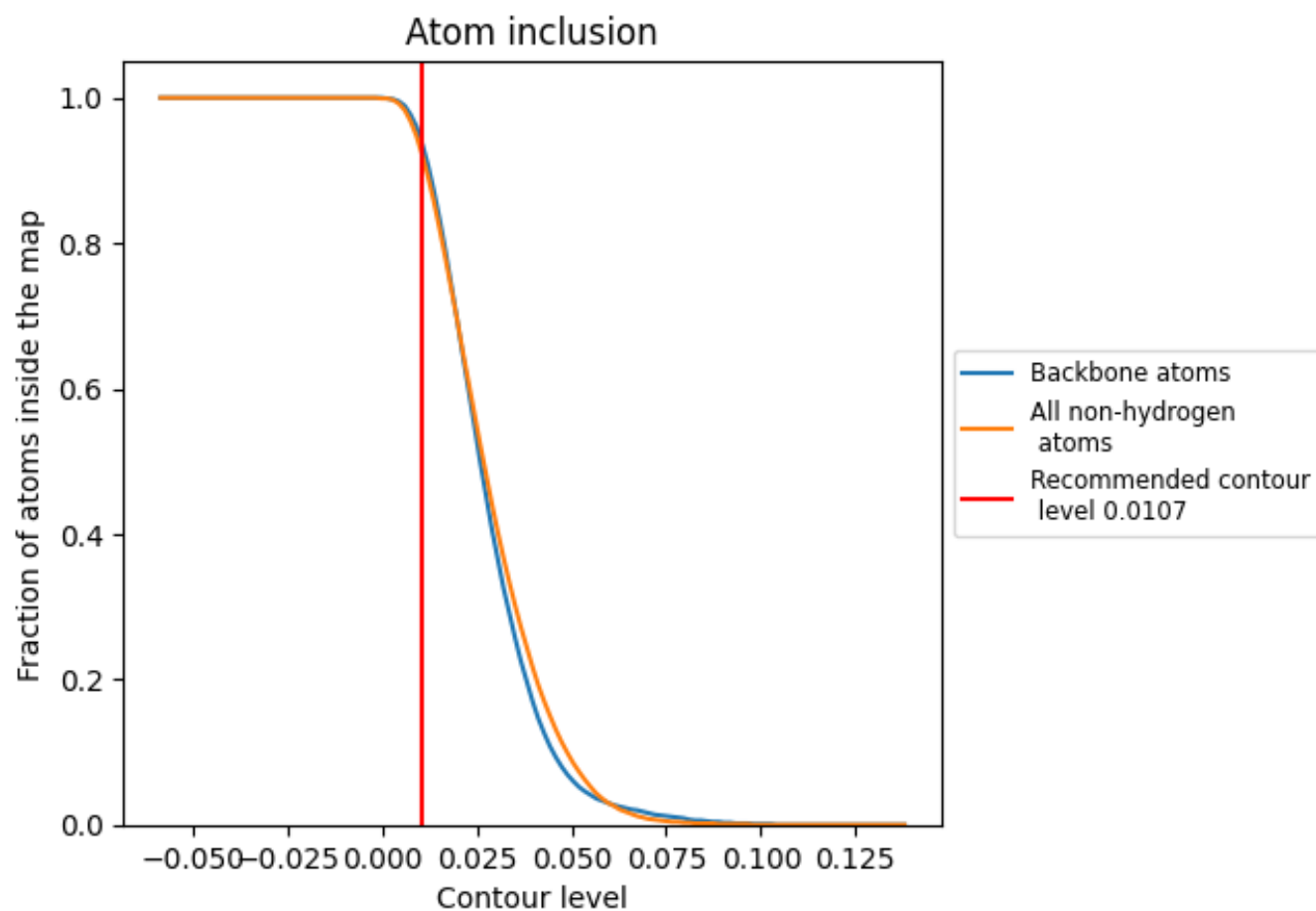
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0107).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% 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 (0.0107) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.6260
0	 0.9270	 0.6660
1	 0.9750	 0.6960
2	 0.9800	 0.7020
3	 0.9390	 0.6460
4	 0.7160	 0.5280
A	 0.9260	 0.5990
B	 0.4300	 0.5060
C	 0.8330	 0.5890
D	 0.6670	 0.5190
E	 0.8790	 0.6190
F	 0.8020	 0.5550
G	 0.8080	 0.5970
H	 0.8880	 0.6110
I	 0.8520	 0.5980
J	 0.6570	 0.5320
K	 0.8750	 0.6180
L	 0.8940	 0.6380
M	 0.8620	 0.5980
N	 0.8510	 0.5910
O	 0.8750	 0.6050
P	 0.7330	 0.5140
Q	 0.8100	 0.5980
R	 0.8260	 0.5880
S	 0.8620	 0.5890
T	 0.7590	 0.5410
U	 0.5080	 0.5250
V	 0.8770	 0.5850
X	 0.9190	 0.6290
Z	 0.8730	 0.5970
a	 0.9680	 0.6520
b	 0.9600	 0.6210
c	 0.9660	 0.6790
d	 0.9360	 0.6770
e	 0.8750	 0.6240



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Chain	Atom inclusion	Q-score
f	 0.8180	 0.5910
g	 0.7810	 0.5690
h	 0.7800	 0.5690
i	 0.9410	 0.6660
j	 0.9450	 0.6810
k	 0.9310	 0.6600
l	 0.9340	 0.6610
m	 0.9810	 0.6920
n	 0.9110	 0.6250
o	 0.9090	 0.6670
p	 0.9680	 0.6740
q	 0.9070	 0.6310
r	 0.9320	 0.6670
s	 0.8520	 0.5920
t	 0.8540	 0.5710
u	 0.8560	 0.6080
v	 0.9320	 0.6830
w	 0.9320	 0.6430
x	 0.7610	 0.5350
y	 0.9290	 0.6460
z	 0.9320	 0.6680