



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 08:59 am BST

PDB ID : 8AM9 / pdb_00008am9
EMDB ID : EMD-15523
Title : Cryo-EM structure of the proline-rich antimicrobial peptide drosocin bound to the elongating ribosome
Authors : Koller, T.O.; Morici, M.; Wilson, D.N.
Deposited on : 2022-08-03
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

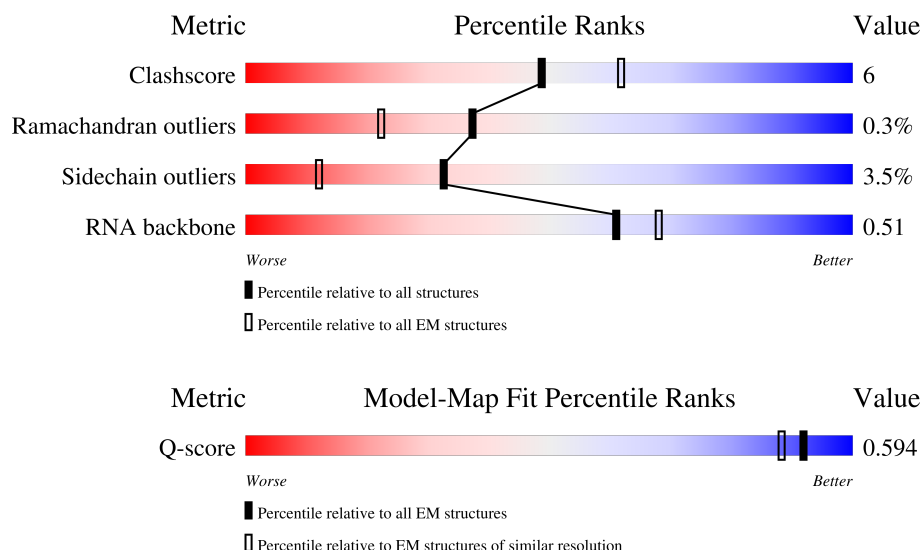
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	0	55	
2	1	46	
3	2	65	

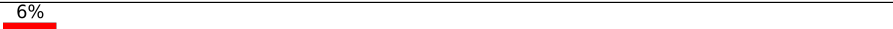
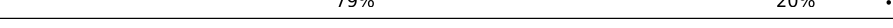
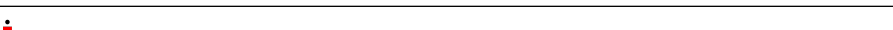
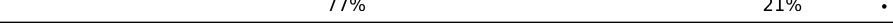
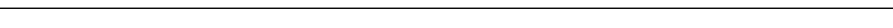
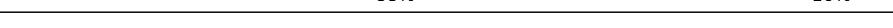
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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	B	1534	
7	C	241	
8	D	233	
9	E	206	
10	F	167	
11	G	135	
12	H	179	
13	I	130	
14	J	130	
15	K	103	
16	L	129	
17	M	124	
18	N	118	
19	O	101	
20	P	89	
21	Q	82	
22	R	84	
23	S	75	
24	T	92	
25	U	87	
26	V	71	
27	a	2903	
28	b	120	

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Mol	Chain	Length	Quality of chain
29	c	273	
30	d	209	
31	e	201	
32	f	179	
33	g	177	
34	h	149	
35	i	142	
36	j	123	
37	k	144	
38	l	136	
39	m	127	
40	n	117	
41	o	115	
42	p	118	
43	q	103	
44	r	110	
45	s	100	
46	t	104	
47	u	94	
48	v	85	
49	w	78	
50	x	63	
51	y	59	
52	z	57	
53	X	12	

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Mol	Chain	Length	Quality of chain
54	Y	76	
55	8	85	
56	A	19	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	A2G	A	101	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 142036 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 protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 7 is a protein called 30S ribosomal protein S2.

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

- Molecule 8 is a protein called 30S ribosomal protein S3.

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

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

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

- Molecule 11 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

- Molecule 12 is a protein called 30S ribosomal protein S7.

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

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S13.

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

- Molecule 19 is a protein called 30S ribosomal protein S14.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S16.

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

- Molecule 22 is a protein called 30S ribosomal protein S17.

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

- Molecule 23 is a protein called 30S ribosomal protein S18.

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

- Molecule 24 is a protein called 30S ribosomal protein S19.

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

- Molecule 25 is a protein called 30S ribosomal protein S20.

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

- Molecule 26 is a protein called 30S ribosomal protein S21.

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

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	2753	Total	C	N	O	P	1	0
			59148	26391	10899	19104	2754		

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

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

- Molecule 31 is a protein called 50S ribosomal protein L4.

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

- Molecule 32 is a protein called 50S ribosomal protein L5.

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

- Molecule 33 is a protein called 50S ribosomal protein L6.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	12	Total	C	N	O	P	0	0
			255	114	42	87	12		

- Molecule 54 is a RNA chain called Initiator tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Y	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 55 is a RNA chain called Leucine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	75	Total	C	N	O	P	0	0
			1602	715	291	521	75		

- Molecule 56 is a protein called Drosocin1.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	A	19	Total	C	N	O	0	0
			155	98	34	23		

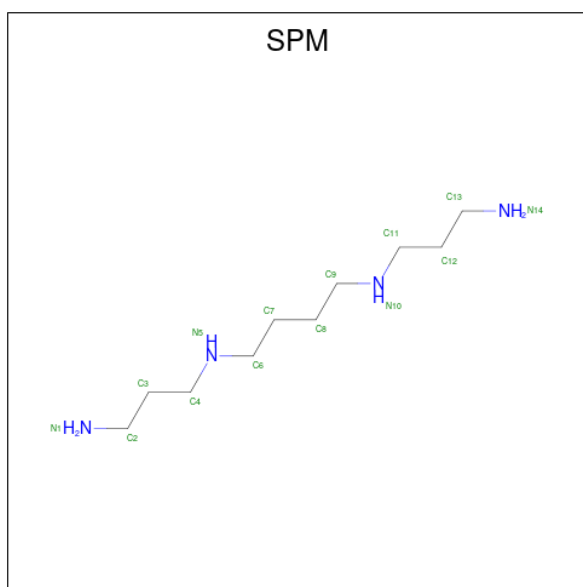
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

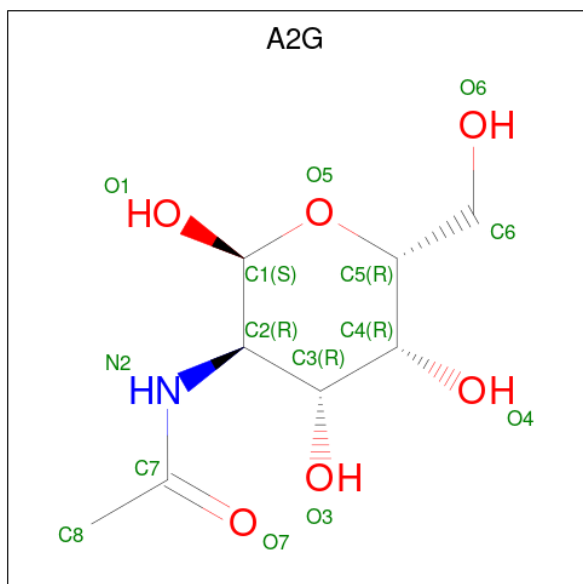
Mol	Chain	Residues	Atoms		AltConf
58	B	75	Total	Mg	0
			75	75	
58	O	1	Total	Mg	0
			1	1	
58	R	1	Total	Mg	0
			1	1	
58	a	208	Total	Mg	0
			208	208	
58	b	5	Total	Mg	0
			5	5	
58	d	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	
58	A	1	Total	Mg	0
			1	1	

- Molecule 59 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
59	a	1	Total	C	N	0
			14	10	4	

- Molecule 60 is 2-acetamido-2-deoxy- α -D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
60	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	a	2	Total	O	0
			2	2	

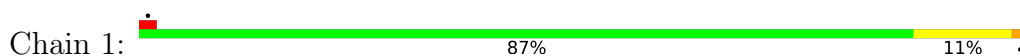
3 Residue-property plots [i](#)

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

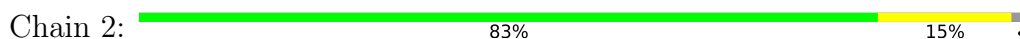
- Molecule 1: 50S ribosomal protein L33



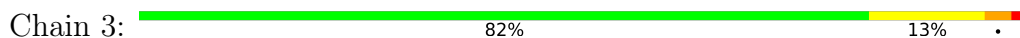
- Molecule 2: 50S ribosomal protein L34



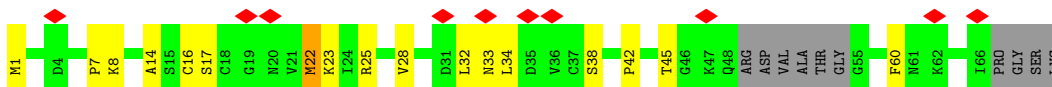
- Molecule 3: 50S ribosomal protein L35



- Molecule 4: 50S ribosomal protein L36

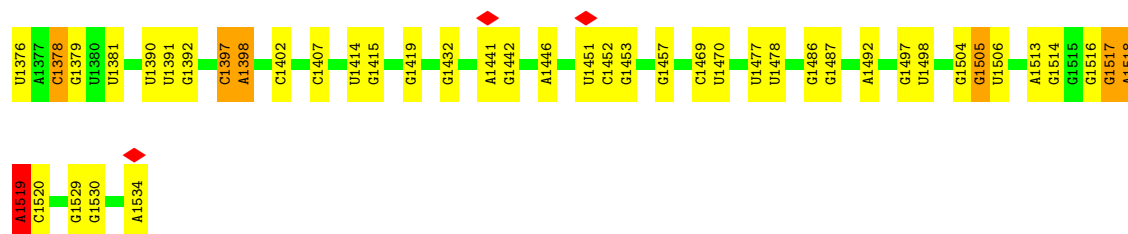


- Molecule 5: 50S ribosomal protein L31

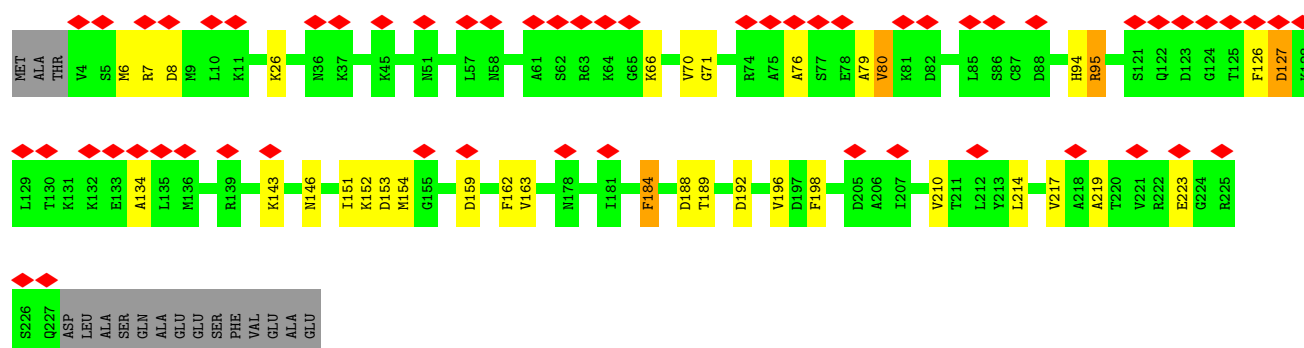
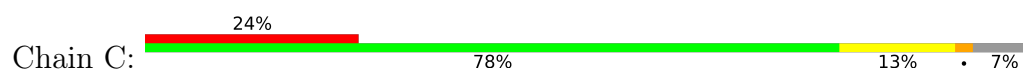


- Molecule 6: 16S ribosomal RNA

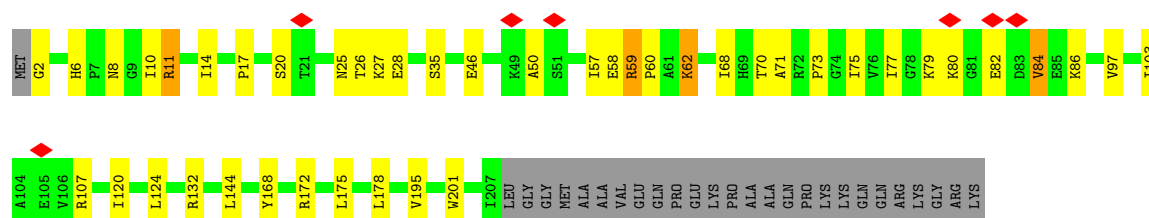




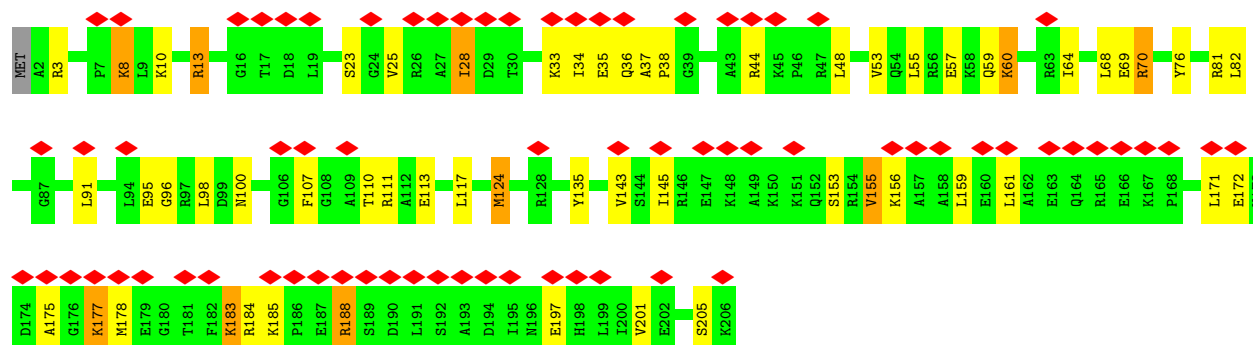
• Molecule 7: 30S ribosomal protein S2



• Molecule 8: 30S ribosomal protein S3



• Molecule 9: 30S ribosomal protein S4



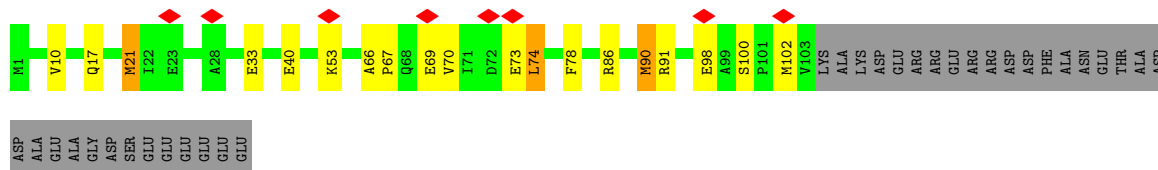
• Molecule 10: 30S ribosomal protein S5

Chain F:  80% 13% 7%



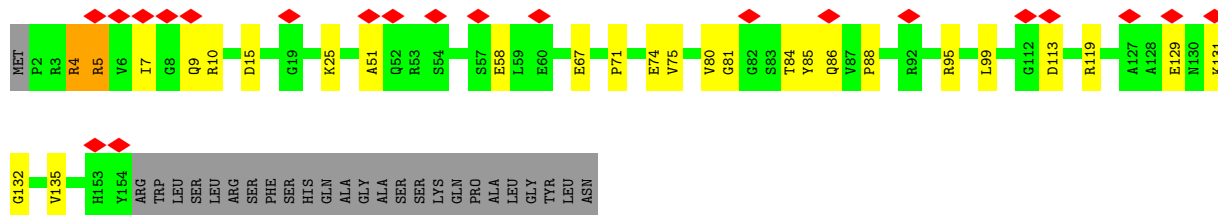
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain G:  6% 62% 12% 24%



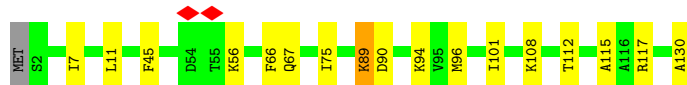
- Molecule 12: 30S ribosomal protein S7

Chain H:  12% 70% 14% 15%



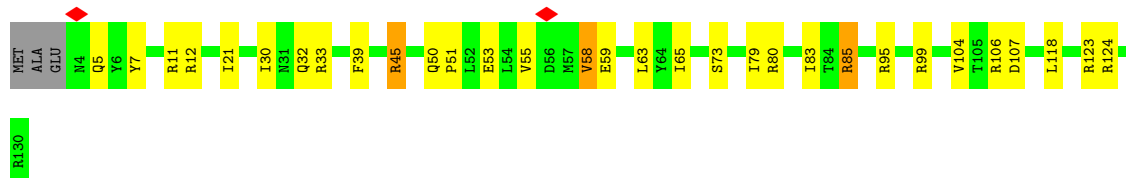
- Molecule 13: 30S ribosomal protein S8

Chain I:  86% 12% ..



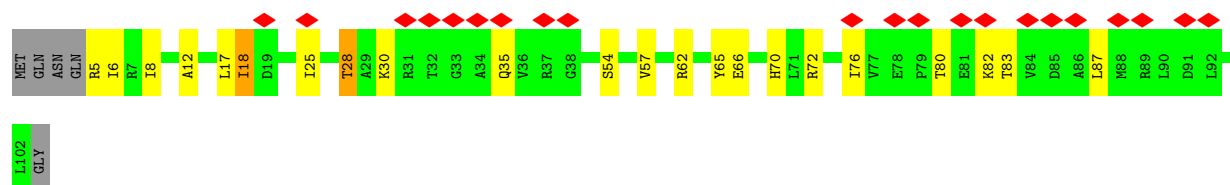
- Molecule 14: 30S ribosomal protein S9

Chain J:  74% 22% ..



- Molecule 15: 30S ribosomal protein S10

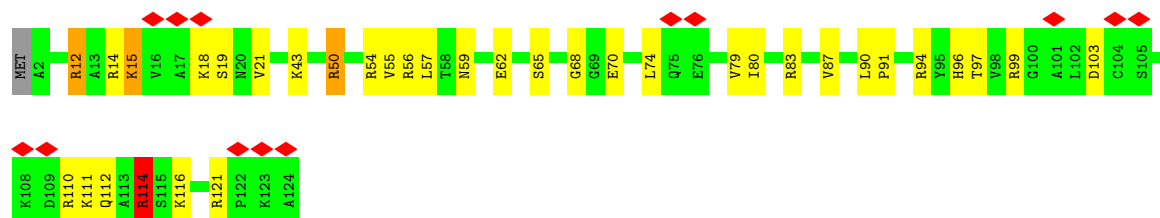
Chain K:  20% 74% 19% 5%



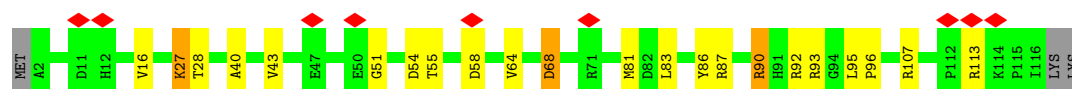
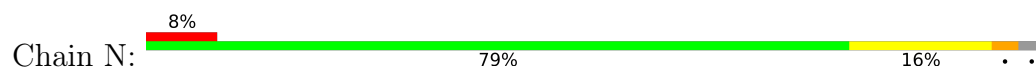
- Molecule 16: 30S ribosomal protein S11



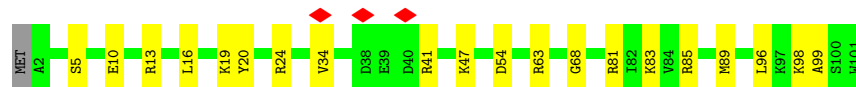
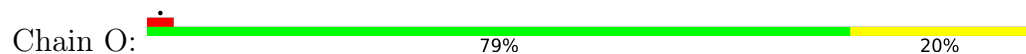
- Molecule 17: 30S ribosomal protein S12



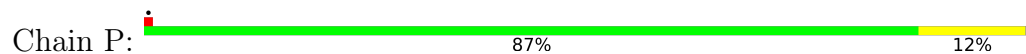
- Molecule 18: 30S ribosomal protein S13



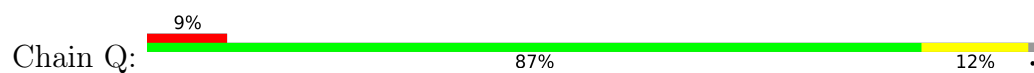
- Molecule 19: 30S ribosomal protein S14



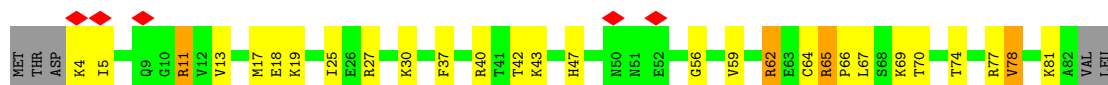
- Molecule 20: 30S ribosomal protein S15



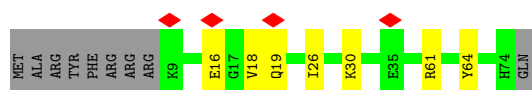
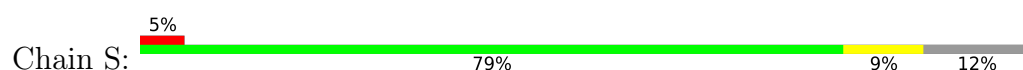
- Molecule 21: 30S ribosomal protein S16



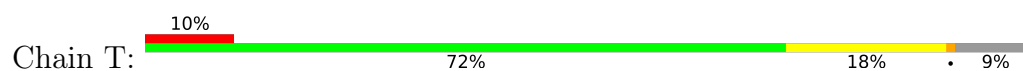
- Molecule 22: 30S ribosomal protein S17



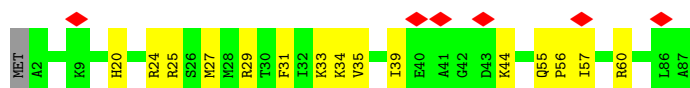
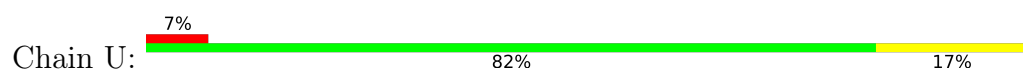
- Molecule 23: 30S ribosomal protein S18



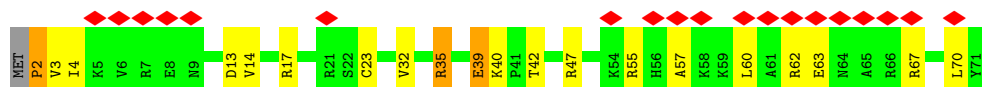
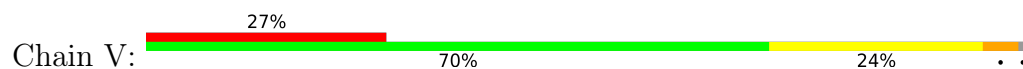
- Molecule 24: 30S ribosomal protein S19



- Molecule 25: 30S ribosomal protein S20



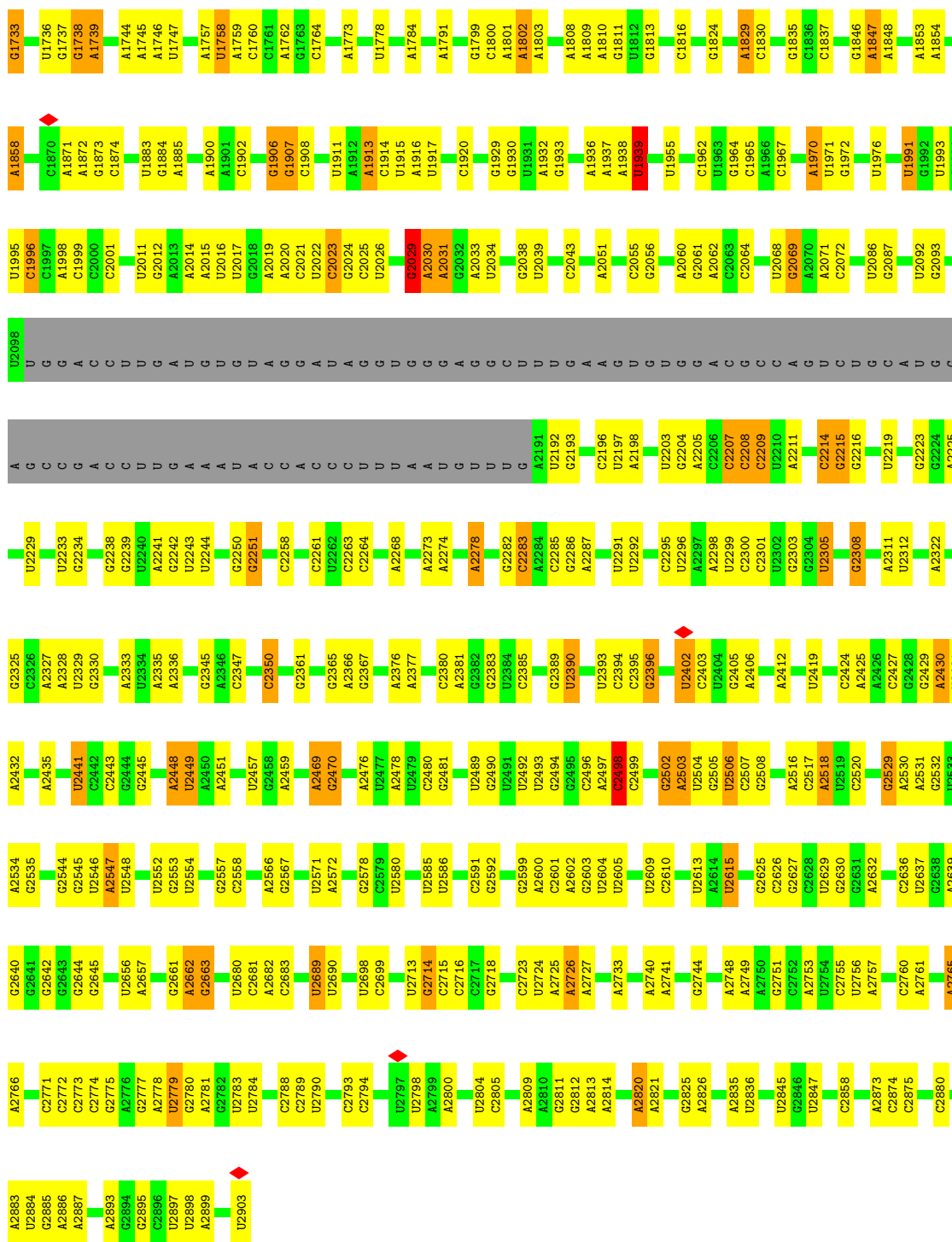
- Molecule 26: 30S ribosomal protein S21



- Molecule 27: 23S ribosomal RNA





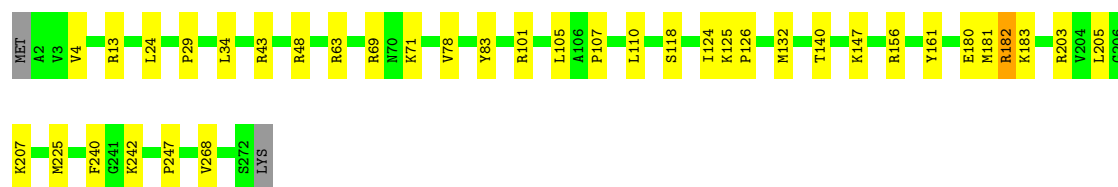


• Molecule 28: 5S ribosomal RNA



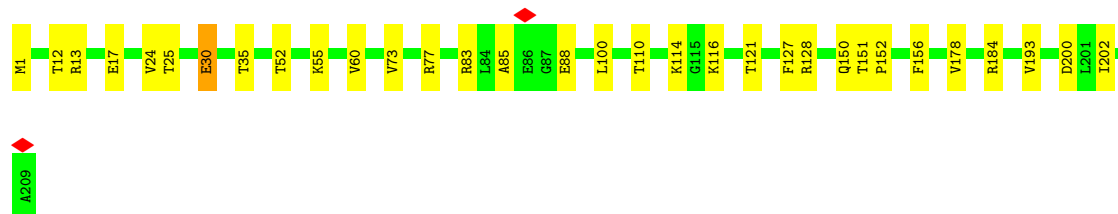
• Molecule 29: 50S ribosomal protein L2

Chain c:  86% 13% .



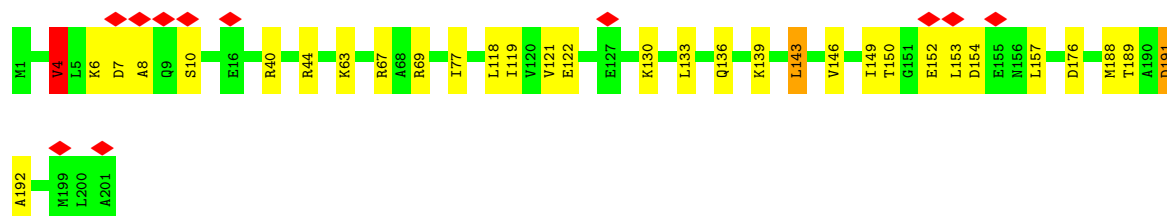
- Molecule 30: 50S ribosomal protein L3

Chain d:  85% 15%



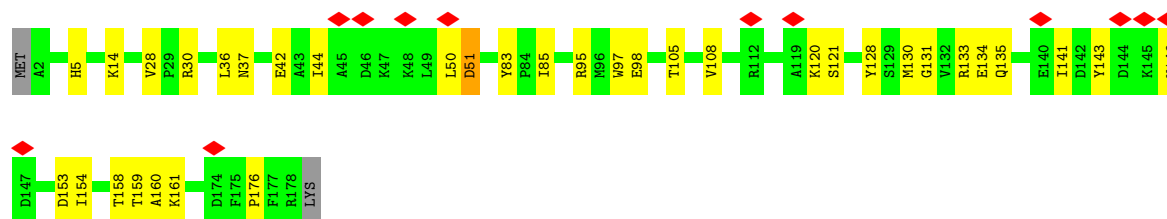
- Molecule 31: 50S ribosomal protein L4

Chain e:  5% 84% 14% .



- Molecule 32: 50S ribosomal protein L5

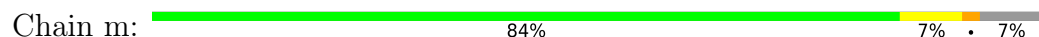
Chain f:  7% 79% 19% ..



- Molecule 33: 50S ribosomal protein L6

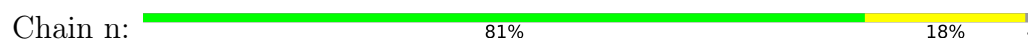
Chain g:  6% 79% 20% ..



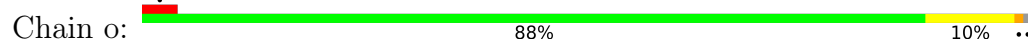




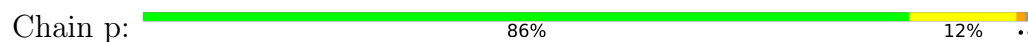
- Molecule 40: 50S ribosomal protein L18



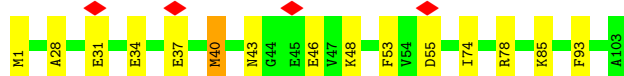
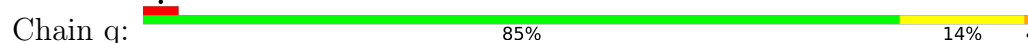
- Molecule 41: 50S ribosomal protein L19



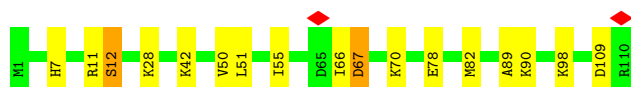
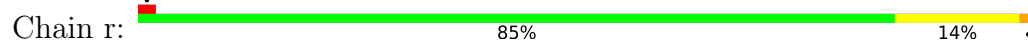
- Molecule 42: 50S ribosomal protein L20



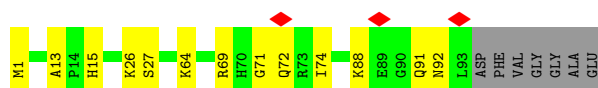
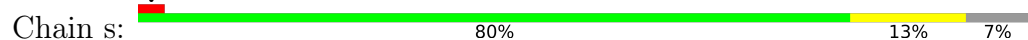
- Molecule 43: 50S ribosomal protein L21



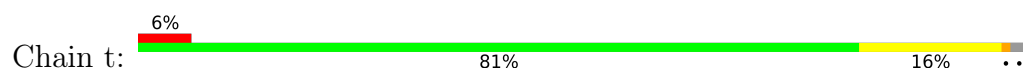
- Molecule 44: 50S ribosomal protein L22



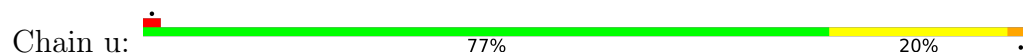
- Molecule 45: 50S ribosomal protein L23



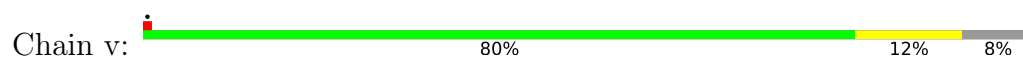
- Molecule 46: 50S ribosomal protein L24



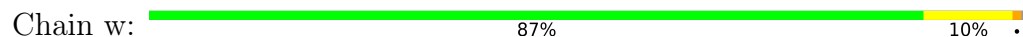
- Molecule 47: 50S ribosomal protein L25



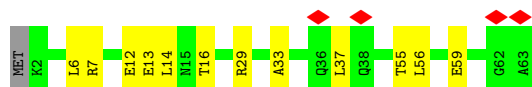
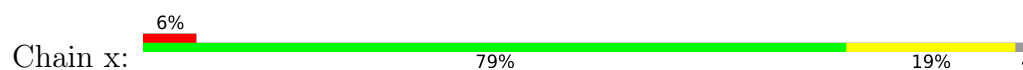
- Molecule 48: 50S ribosomal protein L27



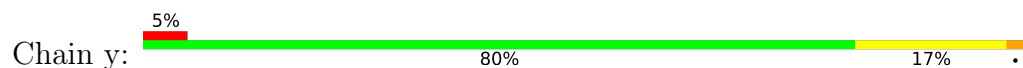
- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29



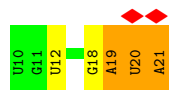
- Molecule 51: 50S ribosomal protein L30



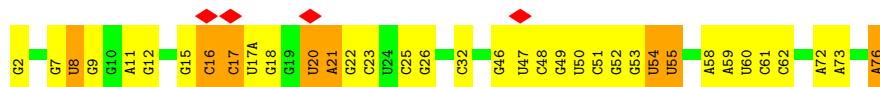
- Molecule 52: 50S ribosomal protein L32



- Molecule 53: mRNA



- Molecule 54: Initiator tRNA



- Molecule 55: Leucine tRNA



- Molecule 56: Drosocin1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84697	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2G, MEQ, ZN, H2U, SPM, 2MG, 2MA, MG, 1MG, PSU, 5MU, 6MZ, 5MC, UR3, MA6, OMG, 4SU, OMU, OMC, G7M, 4OC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.24	0/424	0.46	0/565
2	1	0.31	0/380	0.50	0/498
3	2	0.28	0/513	0.51	0/676
4	3	0.28	0/303	0.49	0/397
5	4	0.20	0/488	0.43	0/649
6	B	0.32	0/36236	0.63	0/56520
7	C	0.19	0/1784	0.43	0/2403
8	D	0.22	0/1651	0.45	0/2225
9	E	0.19	0/1665	0.46	0/2227
10	F	0.24	0/1165	0.44	0/1568
11	G	0.20	0/858	0.43	0/1160
12	H	0.20	0/1219	0.46	0/1635
13	I	0.22	0/989	0.44	0/1326
14	J	0.22	0/1034	0.45	0/1375
15	K	0.23	0/796	0.48	0/1077
16	L	0.22	0/893	0.45	0/1205
17	M	0.22	0/969	0.47	0/1300
18	N	0.20	0/900	0.44	0/1204
19	O	0.24	0/817	0.43	0/1088
20	P	0.20	0/722	0.41	0/964
21	Q	0.20	0/653	0.47	0/877
22	R	0.20	0/650	0.46	0/871
23	S	0.21	0/553	0.42	0/742
24	T	0.22	0/685	0.43	0/922
25	U	0.19	0/676	0.43	0/895
26	V	0.20	0/597	0.45	0/792
27	a	0.39	0/65722	0.63	13/102528 (0.0%)
28	b	0.33	0/2850	0.62	0/4444
29	c	0.28	0/2121	0.48	1/2852 (0.0%)
30	d	0.28	0/1576	0.45	0/2119
31	e	0.26	0/1571	0.41	0/2113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	f	0.20	0/1434	0.42	0/1926
33	g	0.20	0/1343	0.45	0/1816
34	h	0.22	0/306	0.43	0/413
35	i	0.26	0/1152	0.41	0/1551
36	j	0.27	0/955	0.46	0/1279
37	k	0.25	0/1062	0.46	0/1413
38	l	0.27	0/1093	0.47	0/1460
39	m	0.28	0/958	0.47	0/1281
40	n	0.24	0/902	0.44	0/1209
41	o	0.25	0/929	0.41	0/1242
42	p	0.27	0/960	0.46	0/1278
43	q	0.25	0/829	0.47	0/1107
44	r	0.24	0/864	0.43	0/1156
45	s	0.22	0/744	0.43	0/994
46	t	0.21	0/787	0.46	0/1051
47	u	0.25	0/766	0.49	0/1025
48	v	0.26	0/593	0.45	0/785
49	w	0.24	0/635	0.46	0/848
50	x	0.21	0/502	0.45	0/667
51	y	0.24	0/453	0.43	0/605
52	z	0.28	0/450	0.50	0/599
53	X	0.38	0/284	0.63	0/440
54	Y	0.30	0/1725	0.65	0/2689
55	8	0.26	0/1790	0.65	0/2786
56	A	0.56	0/162	0.95	1/221 (0.5%)
All	All	0.33	0/153138	0.59	15/229058 (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
3	2	0	2
4	3	0	1
7	C	0	2
8	D	0	3
9	E	0	7
10	F	0	1
12	H	0	1
14	J	0	4
15	K	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	M	0	5
18	N	0	5
19	O	0	1
21	Q	0	1
22	R	0	5
25	U	0	2
26	V	0	3
29	c	0	6
30	d	0	3
31	e	0	1
32	f	0	1
33	g	0	1
35	i	0	1
36	j	0	3
37	k	0	1
38	l	0	2
39	m	0	3
42	p	0	1
43	q	0	1
47	u	0	1
48	v	0	2
50	x	0	1
51	y	0	1
52	z	0	1
56	A	0	1
All	All	0	77

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	168	G	P-O3'-C3'	-9.00	106.69	120.20
27	a	160	A	P-O3'-C3'	-8.75	107.07	120.20
27	a	2216	G	P-O3'-C3'	-8.65	107.22	120.20
27	a	2208	C	P-O3'-C3'	-8.44	107.54	120.20
27	a	167	A	P-O3'-C3'	-8.43	107.56	120.20
27	a	2207	C	P-O3'-C3'	-7.89	108.37	120.20
27	a	166	U	P-O3'-C3'	-7.72	108.61	120.20
27	a	2215	G	P-O3'-C3'	-7.41	109.09	120.20
27	a	2209	C	P-O3'-C3'	-7.17	109.44	120.20
27	a	159	G	P-O3'-C3'	-6.95	109.78	120.20
27	a	2214	C	P-O3'-C3'	-6.23	110.85	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A	12	SER	N-CA-C	5.98	117.79	111.28
27	a	2029	G	C2'-C3'-O3'	5.49	121.94	113.70
27	a	165	A	P-O3'-C3'	-5.39	112.12	120.20
29	c	124	ILE	N-CA-C	5.09	111.66	106.21

There are no chirality outliers.

All (77) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	30	ARG	Sidechain
3	2	40	ARG	Sidechain
4	3	36	ARG	Sidechain
56	A	9	ARG	Sidechain
7	C	7	ARG	Sidechain
7	C	95	ARG	Sidechain
8	D	107	ARG	Sidechain
8	D	11	ARG	Sidechain
8	D	59	ARG	Sidechain
9	E	111	ARG	Sidechain
9	E	13	ARG	Sidechain
9	E	184	ARG	Sidechain
9	E	188	ARG	Sidechain
9	E	3	ARG	Sidechain
9	E	44	ARG	Sidechain
9	E	70	ARG	Sidechain
10	F	112	ARG	Sidechain
12	H	4	ARG	Sidechain
14	J	12	ARG	Sidechain
14	J	45	ARG	Sidechain
14	J	85	ARG	Sidechain
14	J	95	ARG	Sidechain
15	K	5	ARG	Sidechain
15	K	62	ARG	Sidechain
15	K	72	ARG	Sidechain
17	M	114	ARG	Sidechain
17	M	12	ARG	Sidechain
17	M	14	ARG	Sidechain
17	M	56	ARG	Sidechain
17	M	94	ARG	Sidechain
18	N	107	ARG	Sidechain
18	N	113	ARG	Sidechain
18	N	87	ARG	Sidechain

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Mol	Chain	Res	Type	Group
18	N	90	ARG	Sidechain
18	N	93	ARG	Sidechain
19	O	85	ARG	Sidechain
21	Q	28	ARG	Sidechain
22	R	11	ARG	Sidechain
22	R	40	ARG	Sidechain
22	R	62	ARG	Sidechain
22	R	65	ARG	Sidechain
22	R	77	ARG	Sidechain
25	U	25	ARG	Sidechain
25	U	60	ARG	Sidechain
26	V	17	ARG	Sidechain
26	V	35	ARG	Sidechain
26	V	62	ARG	Sidechain
29	c	101	ARG	Sidechain
29	c	156	ARG	Sidechain
29	c	182	ARG	Sidechain
29	c	48	ARG	Sidechain
29	c	63	ARG	Sidechain
29	c	69	ARG	Sidechain
30	d	128	ARG	Sidechain
30	d	184	ARG	Sidechain
30	d	83	ARG	Sidechain
31	e	40	ARG	Sidechain
32	f	95	ARG	Sidechain
33	g	35	ARG	Sidechain
35	i	116	ARG	Sidechain
36	j	18	ARG	Sidechain
36	j	49	ARG	Sidechain
36	j	64	ARG	Sidechain
37	k	123	ARG	Sidechain
38	l	10	ARG	Sidechain
38	l	6	ARG	Sidechain
39	m	2	ARG	Sidechain
39	m	8	ARG	Sidechain
39	m	86	ARG	Sidechain
42	p	13	ARG	Sidechain
43	q	78	ARG	Sidechain
47	u	93	ARG	Sidechain
48	v	25	ARG	Sidechain
48	v	55	ARG	Sidechain
50	x	29	ARG	Sidechain

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Mol	Chain	Res	Type	Group
51	y	30	ARG	Sidechain
52	z	13	ARG	Sidechain

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	0	417	0	451	7	0
2	1	377	0	418	6	0
3	2	504	0	572	5	0
4	3	302	0	340	5	0
5	4	480	0	478	10	0
6	B	32612	0	16431	335	0
7	C	1753	0	1780	20	0
8	D	1624	0	1696	21	0
9	E	1643	0	1707	36	0
10	F	1152	0	1196	12	0
11	G	839	0	833	11	0
12	H	1203	0	1254	13	0
13	I	979	0	1031	9	0
14	J	1022	0	1070	19	0
15	K	786	0	828	11	0
16	L	877	0	887	21	0
17	M	955	0	1016	18	0
18	N	891	0	952	10	0
19	O	805	0	844	17	0
20	P	714	0	734	7	0
21	Q	643	0	661	5	0
22	R	641	0	682	14	0
23	S	544	0	565	3	0
24	T	668	0	693	11	0
25	U	670	0	719	7	0
26	V	589	0	629	10	0
27	a	59148	0	29771	486	0
28	b	2549	0	1291	13	0
29	c	2082	0	2154	21	0
30	d	1566	0	1618	17	0
31	e	1552	0	1619	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	f	1410	0	1444	23	0
33	g	1323	0	1371	24	0
34	h	303	0	327	5	0
35	i	1129	0	1162	17	0
36	j	946	0	1023	16	0
37	k	1053	0	1129	17	0
38	l	1074	0	1157	19	0
39	m	945	0	989	6	0
40	n	892	0	923	14	0
41	o	917	0	962	10	0
42	p	947	0	1019	12	0
43	q	816	0	839	10	0
44	r	857	0	922	10	0
45	s	738	0	807	9	0
46	t	779	0	831	14	0
47	u	753	0	780	12	0
48	v	586	0	596	4	0
49	w	625	0	652	6	0
50	x	501	0	531	6	0
51	y	449	0	488	7	0
52	z	444	0	458	8	0
53	X	255	0	127	4	0
54	Y	1625	0	828	23	0
55	8	1602	0	813	17	0
56	A	155	0	164	14	0
57	3	1	0	0	0	0
57	4	1	0	0	0	0
58	A	1	0	0	0	0
58	B	75	0	0	0	0
58	O	1	0	0	0	0
58	R	1	0	0	0	0
58	a	208	0	0	0	0
58	b	5	0	0	0	0
58	d	1	0	0	0	0
58	z	1	0	0	0	0
59	a	14	0	26	1	0
60	A	14	0	12	14	0
61	a	2	0	0	0	0
All	All	142036	0	95300	1337	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 6.

All (1337) 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)
27:a:747:5MU:C5	27:a:747:5MU:C4	1.80	1.67
54:Y:54:5MU:C5	54:Y:54:5MU:C4	1.79	1.64
27:a:1939:5MU:C4	27:a:1939:5MU:C5	1.80	1.59
27:a:2609[B]:U:N3	60:A:101:A2G:O3	1.80	1.13
27:a:2609[B]:U:C2	60:A:101:A2G:O3	2.08	1.02
55:8:18:G:O2'	55:8:66:G:N2	2.06	0.87
6:B:407:U:O2'	9:E:113:GLU:OE1	1.95	0.83
27:a:2609[A]:U:O2'	60:A:101:A2G:O7	1.97	0.81
27:a:1385:A:O2'	27:a:1396:U:O2	2.02	0.77
27:a:1259:G:N7	56:A:1:GLY:N	2.31	0.74
6:B:201:G:HO2'	6:B:469:C:HO2'	1.37	0.73
17:M:68:GLY:O	17:M:99:ARG:NH1	2.23	0.71
2:1:7:PRO:HB2	27:a:1309:G:H4'	1.73	0.71
5:4:25:ARG:NE	32:f:98:GLU:OE2	2.23	0.71
27:a:309:A:N3	27:a:329:G:O2'	2.23	0.71
39:m:69:ARG:O	39:m:71:ARG:N	2.22	0.70
6:B:79:G:N2	6:B:91:U:O2	2.25	0.70
6:B:55:A:OP2	6:B:352:C:N4	2.25	0.69
27:a:2609[B]:U:O2'	56:A:14:PRO:HG3	1.93	0.69
27:a:2609[B]:U:C6	56:A:14:PRO:HB3	2.28	0.69
6:B:717:U:H4'	16:L:119:ASN:HD22	1.58	0.68
6:B:215:C:O2'	6:B:216:U:O4'	2.12	0.67
6:B:5:U:H4'	6:B:6:G:H5'	1.76	0.67
8:D:35:SER:OG	8:D:59:ARG:NH2	2.29	0.66
1:0:6:ARG:NH1	27:a:2285:C:OP2	2.26	0.66
3:2:12:LYS:NZ	27:a:249:C:O2	2.30	0.65
27:a:855:G:H2'	27:a:856:G:H5''	1.79	0.64
54:Y:76:A:H3'	56:A:19:VAL:C	2.22	0.64
18:N:68:ASP:OD1	18:N:68:ASP:N	2.22	0.64
6:B:769:G:H4'	6:B:1513:A:H4'	1.82	0.62
27:a:158:U:H2'	27:a:159:G:C8	2.35	0.62
8:D:11:ARG:NH2	8:D:175:LEU:O	2.32	0.62
9:E:172:GLU:N	9:E:172:GLU:OE1	2.33	0.62
27:a:870:U:OP1	38:l:6:ARG:NH2	2.33	0.61
19:O:83:LYS:HA	19:O:83:LYS:HE2	1.83	0.61
37:k:91:ASP:OD1	37:k:92:LEU:N	2.33	0.61
27:a:644:A:H2'	27:a:645:C:O4'	2.01	0.61
6:B:1356:G:H2'	6:B:1357:A:C8	2.36	0.60
38:l:53:MET:HG3	38:l:120:ALA:HB2	1.83	0.60
8:D:50:ALA:HA	8:D:75:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:30:LYS:HA	22:R:37:PHE:HA	1.82	0.60
27:a:2609[A]:U:HO2'	56:A:14:PRO:HD3	1.67	0.60
6:B:575:G:O2'	6:B:821:G:OP2	2.15	0.60
6:B:273:U:O4	6:B:274:A:N6	2.34	0.59
24:T:28:LYS:HG2	24:T:29:LYS:H	1.67	0.59
6:B:362:G:N2	6:B:365:U:OP2	2.32	0.59
15:K:54:SER:O	19:O:81:ARG:NH1	2.31	0.59
27:a:2609[A]:U:O2'	60:A:101:A2G:H8	2.02	0.59
27:a:1394:U:H4'	27:a:1603:A:H4'	1.85	0.59
6:B:573:A:H5'	6:B:573:A:H8	1.67	0.59
46:t:7:ARG:NE	46:t:26:LYS:O	2.35	0.59
6:B:98:A:H2'	6:B:99:C:C6	2.38	0.59
28:b:30:C:H2'	28:b:31:C:H5'	1.84	0.58
6:B:86:G:H4'	6:B:86:G:OP1	2.04	0.58
6:B:754:C:O5'	20:P:72:ARG:NH2	2.36	0.58
27:a:160:A:H2'	27:a:161:A:C8	2.39	0.58
27:a:2609[A]:U:C2'	60:A:101:A2G:O7	2.50	0.58
33:g:55:ARG:HG2	33:g:56:ASP:H	1.69	0.58
6:B:781:A:H2'	6:B:782:A:H5'	1.86	0.58
27:a:768:G:O6	59:a:3209:SPM:N14	2.37	0.58
6:B:95:C:H5'	6:B:95:C:H6	1.69	0.58
6:B:1053:G:H4'	6:B:1054:C:H5''	1.86	0.57
28:b:20:G:H2'	28:b:21:G:O4'	2.04	0.57
30:d:35:THR:HG22	30:d:73:VAL:HG21	1.85	0.57
35:i:31:GLU:OE2	35:i:35:ARG:NE	2.37	0.57
55:8:15:A:N6	55:8:16:U:O4	2.38	0.57
6:B:718:A:H5'	16:L:119:ASN:CG	2.30	0.57
6:B:1007:U:OP1	19:O:19:LYS:NZ	2.38	0.57
27:a:876:C:H2'	27:a:877:A:O4'	2.04	0.57
27:a:931:U:OP1	51:y:30:ARG:NH2	2.37	0.57
53:X:18:G:C5	53:X:19:A:H1'	2.38	0.57
9:E:95:GLU:OE1	9:E:100:ASN:ND2	2.37	0.57
27:a:612:G:C2	27:a:614:A:H5''	2.40	0.57
27:a:931:U:O4	27:a:1166:G:N2	2.37	0.57
6:B:174:A:C8	6:B:174:A:H5'	2.40	0.57
6:B:380:G:N2	6:B:382:A:OP2	2.38	0.56
6:B:521:G:H4'	17:M:70:GLU:HG2	1.87	0.56
27:a:2609[A]:U:C2	60:A:101:A2G:H8B	2.40	0.56
33:g:9:VAL:HG11	33:g:73:ASN:HB2	1.88	0.56
47:u:75:GLN:HB2	47:u:92:VAL:HG23	1.87	0.56
54:Y:52:G:H2'	54:Y:53:G:O4'	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:q:43:ASN:N	43:q:46:GLU:OE1	2.38	0.56
27:a:2609[A]:U:HO2'	60:A:101:A2G:C7	2.12	0.56
6:B:869:G:H8	6:B:869:G:H5''	1.71	0.56
1:0:22:THR:HG21	27:a:2419:U:H4'	1.88	0.56
17:M:15:LYS:H	17:M:15:LYS:HD3	1.70	0.56
36:j:1:MET:SD	36:j:67:LYS:NZ	2.78	0.56
9:E:35:GLU:N	9:E:35:GLU:OE1	2.38	0.56
27:a:1597:A:H5''	27:a:1598:A:H5'	1.88	0.56
54:Y:20:U:H2'	54:Y:59:A:N6	2.21	0.56
55:8:9:G:OP2	55:8:13:A:N6	2.32	0.56
7:C:94:HIS:O	7:C:95:ARG:C	2.49	0.55
27:a:527:C:O2'	27:a:2779:U:O2'	2.23	0.55
27:a:857:G:H2'	27:a:858:G:O4'	2.05	0.55
27:a:2640:G:OP1	35:i:96:ARG:NH1	2.39	0.55
50:x:6:LEU:HB3	50:x:56:LEU:HD22	1.87	0.55
6:B:1376:U:O4	12:H:10:ARG:NH1	2.36	0.55
54:Y:76:A:H3'	56:A:19:VAL:HG13	1.87	0.55
6:B:94:G:N2	6:B:96:U:O4	2.39	0.55
6:B:401:C:OP1	9:E:70:ARG:NH1	2.39	0.55
6:B:1019:A:H2'	6:B:1020:G:O4'	2.06	0.55
27:a:1906:G:H2'	27:a:1907:G:H5''	1.88	0.55
6:B:380:G:N2	6:B:382:A:O5'	2.39	0.55
44:r:82:MET:HB2	44:r:98:LYS:HB2	1.89	0.55
54:Y:76:A:H5'	56:A:19:VAL:HG13	1.88	0.55
6:B:269:C:H2'	6:B:270:A:C8	2.42	0.55
9:E:95:GLU:HA	9:E:100:ASN:ND2	2.22	0.55
2:1:29:GLN:NE2	27:a:210:C:OP1	2.38	0.55
6:B:430:A:OP2	9:E:8:LYS:NZ	2.40	0.55
27:a:2051:A:H5'	27:a:2578:G:O4'	2.07	0.55
28:b:29:A:H2'	28:b:30:C:O4'	2.06	0.55
18:N:81:MET:O	18:N:92:ARG:NH2	2.37	0.55
6:B:675:A:O2'	16:L:116:ILE:O	2.25	0.55
27:a:2014:A:H2'	27:a:2015:A:C8	2.42	0.55
6:B:201:G:O2'	6:B:469:C:O2'	2.12	0.54
6:B:414:A:H2'	6:B:415:A:O4'	2.07	0.54
6:B:113:G:N3	6:B:353:A:O2'	2.41	0.54
15:K:12:ALA:HB3	15:K:18:ILE:HG12	1.90	0.54
27:a:1914:C:H2'	27:a:1915:U:O4'	2.08	0.54
6:B:1002:G:H2'	6:B:1003:G:O4'	2.08	0.54
31:e:67:ARG:HD3	56:A:5:PRO:HD3	1.89	0.54
6:B:346:G:OP1	41:o:39:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:1759:A:O2'	27:a:2714:G:O2'	2.22	0.54
27:a:2291:U:H2'	27:a:2292:U:C6	2.43	0.54
6:B:383:A:N7	6:B:384:G:H1'	2.23	0.54
12:H:80:VAL:HG12	12:H:81:GLY:H	1.72	0.54
27:a:1357:C:H2'	27:a:1358:G:O4'	2.08	0.54
27:a:2233:U:H2'	27:a:2234:G:C8	2.41	0.54
30:d:12:THR:HG22	30:d:13:ARG:H	1.73	0.54
6:B:1033:G:H2'	6:B:1034:G:O4'	2.08	0.54
11:G:66:ALA:HB1	11:G:67:PRO:HD2	1.90	0.54
27:a:2780:G:O6	35:i:99:ARG:NH1	2.41	0.54
27:a:856:G:H2'	27:a:857:G:C8	2.42	0.53
31:e:152:GLU:O	31:e:153:LEU:C	2.50	0.53
27:a:2609[A]:U:C5	60:A:101:A2G:O3	2.55	0.53
56:A:9:ARG:HB3	56:A:10:PRO:HD2	1.91	0.53
17:M:57:LEU:HB2	17:M:59:ASN:OD1	2.09	0.53
27:a:114:U:H2'	27:a:115:C:C6	2.44	0.53
27:a:166:U:H2'	27:a:167:A:H8	1.74	0.53
6:B:121:U:H5''	6:B:121:U:H6	1.73	0.53
6:B:468:A:C8	6:B:468:A:H5''	2.44	0.53
27:a:166:U:H2'	27:a:167:A:C8	2.42	0.53
29:c:181:MET:HB3	29:c:268:VAL:HB	1.91	0.53
6:B:900:A:H2'	6:B:901:A:C8	2.44	0.53
27:a:1496:A:N3	27:a:1577:C:O2'	2.40	0.53
6:B:299:G:N2	6:B:565:U:O2	2.41	0.53
22:R:47:HIS:HB3	22:R:74:THR:HG22	1.91	0.53
27:a:1469:A:H2'	27:a:1470:A:C8	2.44	0.53
45:s:88:LYS:O	45:s:91:GLN:HG2	2.09	0.53
27:a:281:C:H5''	27:a:281:C:H6	1.72	0.53
6:B:225:C:H2'	6:B:226:G:H5''	1.91	0.53
6:B:38:G:H22	6:B:397:A:H5'	1.74	0.52
6:B:373:A:O2'	6:B:451:A:N6	2.34	0.52
27:a:577:G:O2'	27:a:1254:A:OP1	2.25	0.52
44:r:11:ARG:O	44:r:12:SER:HB2	2.09	0.52
6:B:381:C:H2'	6:B:382:A:C8	2.44	0.52
6:B:980:C:O3'	19:O:13:ARG:NH2	2.42	0.52
27:a:2273:A:H2'	27:a:2274:A:C8	2.45	0.52
33:g:102:VAL:HG23	33:g:116:GLN:HA	1.91	0.52
46:t:86:ARG:HG3	46:t:95:PHE:CD2	2.44	0.52
51:y:41:THR:HG22	51:y:43:ALA:H	1.74	0.52
54:Y:72:A:H2'	54:Y:73:A:C8	2.44	0.52
27:a:956:G:H4'	38:l:82:MET:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:1733:G:H5'	27:a:1733:G:H8	1.74	0.52
27:a:2845:U:H5''	41:o:52:ASN:O	2.09	0.52
5:4:28:VAL:HG21	5:4:32:LEU:HD21	1.92	0.52
6:B:481:G:O2'	6:B:483:C:N4	2.42	0.52
6:B:1040:U:H2'	6:B:1041:G:C8	2.44	0.52
6:B:486:U:H2'	6:B:487:A:H8	1.75	0.52
19:O:16:LEU:HD12	19:O:54:ASP:HB2	1.91	0.52
27:a:2:G:H2'	27:a:3:U:C6	2.43	0.52
6:B:616:G:H2'	6:B:617:G:H5'	1.92	0.52
5:4:38:SER:HB2	32:f:105:THR:HA	1.92	0.52
6:B:19:A:H4'	6:B:864:A:O4'	2.10	0.52
6:B:78:A:H2'	6:B:79:G:C8	2.44	0.52
6:B:995:C:H2'	6:B:996:A:H5''	1.92	0.52
27:a:357:C:H2'	27:a:358:U:C6	2.45	0.52
27:a:1667:G:O2'	27:a:1991:U:O4	2.24	0.52
33:g:61:GLY:O	33:g:62:TRP:HB2	2.09	0.52
6:B:1373:G:OP2	14:J:73:SER:OG	2.27	0.52
22:R:64:CYS:SG	22:R:74:THR:HG23	2.50	0.52
27:a:2698:U:H2'	27:a:2699:C:C6	2.45	0.52
6:B:379:C:H3'	6:B:380:G:H8	1.75	0.52
28:b:30:C:H2'	28:b:31:C:C5'	2.40	0.52
28:b:40:U:N3	28:b:44:G:OP2	2.37	0.52
55:8:23:A:N3	55:8:23:A:H2'	2.25	0.52
7:C:188:ASP:OD1	7:C:189:THR:N	2.39	0.52
14:J:50:GLN:OE1	14:J:80:ARG:NH1	2.39	0.52
19:O:10:GLU:HG3	19:O:63:ARG:HD2	1.92	0.52
6:B:673:A:H2'	6:B:674:G:C8	2.45	0.51
6:B:1323:G:H2'	6:B:1324:A:C8	2.45	0.51
12:H:5:ARG:HE	12:H:7:ILE:H	1.58	0.51
20:P:18:ASP:OD1	20:P:19:ALA:N	2.41	0.51
27:a:250:G:H2'	27:a:251:A:C8	2.45	0.51
27:a:910:A:H2'	27:a:911:A:C8	2.45	0.51
6:B:56:U:H2'	6:B:57:G:C8	2.45	0.51
6:B:350:G:H2'	6:B:351:G:C8	2.45	0.51
6:B:718:A:O2'	26:V:35:ARG:NH2	2.44	0.51
27:a:2609[B]:U:C4	60:A:101:A2G:O3	2.60	0.51
33:g:22:GLN:NE2	33:g:41:VAL:O	2.31	0.51
27:a:479:A:N3	27:a:481:G:H5''	2.26	0.51
27:a:1183:U:H2'	27:a:1184:U:C6	2.45	0.51
40:n:43:ASN:OD1	40:n:44:GLY:N	2.43	0.51
6:B:1035:A:H4'	6:B:1036:A:OP1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:897:C:OP1	55:8:65:C:C2	2.63	0.51
37:k:108:ALA:HB3	37:k:125:LEU:HD22	1.93	0.51
6:B:562:U:H1'	17:M:12:ARG:HB3	1.92	0.51
27:a:1028:A:H2'	27:a:1029:A:C8	2.46	0.51
56:A:15:ARG:HH21	56:A:17:ILE:HG12	1.74	0.51
6:B:172:A:C5	6:B:174:A:N7	2.79	0.51
15:K:80:THR:HG22	15:K:82:LYS:H	1.75	0.51
27:a:12:U:H2'	27:a:12:U:O2	2.10	0.51
27:a:340:A:H2'	27:a:341:C:O4'	2.11	0.51
27:a:2532:G:O2'	27:a:2657:A:N1	2.41	0.51
27:a:160:A:N6	27:a:167:A:H1'	2.26	0.51
6:B:820:U:H4'	6:B:821:G:OP2	2.11	0.51
6:B:946:A:H2'	6:B:947:G:C8	2.46	0.51
27:a:1746:A:H2'	27:a:1747:U:C6	2.45	0.51
27:a:1915:U:H2'	27:a:1916:A:C8	2.46	0.51
27:a:2395:C:H2'	27:a:2396:G:O4'	2.11	0.51
46:t:54:GLN:HB2	46:t:55:PRO:HD3	1.91	0.51
55:8:42:A:H2'	55:8:43:A:C8	2.45	0.51
6:B:1068:G:N7	6:B:1094:G:H2'	2.26	0.51
6:B:1391:U:H2'	6:B:1392:G:C8	2.45	0.51
14:J:21:ILE:HG12	14:J:63:LEU:HD22	1.93	0.51
16:L:29:ASN:OD1	16:L:30:THR:N	2.44	0.51
47:u:9:ARG:HG2	47:u:41:GLU:HG2	1.93	0.51
11:G:86:ARG:NH1	23:S:64:TYR:O	2.37	0.51
20:P:44:ALA:O	20:P:47:LYS:NZ	2.42	0.51
27:a:2615:U:H1'	52:z:4:GLN:HB3	1.93	0.51
5:4:1:MET:HG2	28:b:43:C:H5''	1.93	0.50
6:B:97:G:H3'	6:B:98:A:O4'	2.10	0.50
32:f:161:LYS:H	32:f:161:LYS:HD2	1.77	0.50
43:q:93:PHE:CD1	43:q:93:PHE:C	2.89	0.50
6:B:51:A:N7	6:B:114:U:O2'	2.44	0.50
6:B:1278:G:H4'	6:B:1279:G:C4	2.46	0.50
10:F:13:GLU:HG2	10:F:39:VAL:HG12	1.93	0.50
10:F:108:GLY:O	10:F:109:GLY:C	2.54	0.50
14:J:32:GLN:O	14:J:33:ARG:HG3	2.12	0.50
46:t:86:ARG:NH1	46:t:100:SER:OG	2.44	0.50
27:a:540:C:H2'	27:a:541:A:C8	2.46	0.50
48:v:38:VAL:HG12	48:v:59:LEU:HB2	1.93	0.50
6:B:188:C:H2'	6:B:189:A:O4'	2.12	0.50
6:B:1287:A:H2'	6:B:1288:A:C8	2.47	0.50
24:T:66:MET:HG2	24:T:74:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:537:G:H5''	35:i:5:THR:HG21	1.93	0.50
6:B:193:C:H2'	6:B:194:C:C6	2.47	0.50
6:B:593:U:H2'	6:B:594:U:H6	1.75	0.50
6:B:1266:G:N2	6:B:1269:A:OP2	2.35	0.50
30:d:156:PHE:CE1	35:i:81:ILE:HD13	2.47	0.50
9:E:37:ALA:HB1	9:E:38:PRO:HD2	1.94	0.50
27:a:308:G:H2'	27:a:309:A:C8	2.47	0.50
38:l:64:TRP:HB2	38:l:104:GLU:HB2	1.93	0.50
7:C:126:PHE:HB3	7:C:134:ALA:HB1	1.93	0.50
22:R:69:LYS:HG3	22:R:70:THR:HG23	1.94	0.50
27:a:276:U:H2'	27:a:277:G:C8	2.46	0.50
27:a:588:U:H2'	27:a:589:U:C6	2.46	0.50
36:j:43:ILE:HD12	36:j:56:ASP:HB2	1.94	0.50
47:u:31:TYR:CE1	47:u:92:VAL:HG22	2.46	0.50
6:B:539:A:H2'	6:B:540:G:C8	2.47	0.50
27:a:1507:C:H2'	27:a:1508:A:H4'	1.94	0.50
27:a:1544:A:H2'	27:a:1545:A:C8	2.46	0.50
6:B:309:A:O2'	6:B:607:A:N1	2.41	0.49
6:B:545:C:H5'	9:E:69:GLU:HB2	1.93	0.49
6:B:1121:U:H2'	6:B:1122:U:C6	2.46	0.49
6:B:1152:A:OP1	15:K:70:HIS:ND1	2.44	0.49
9:E:110:THR:H	9:E:113:GLU:HB3	1.77	0.49
18:N:86:TYR:CZ	18:N:90:ARG:HD2	2.47	0.49
19:O:20:TYR:O	19:O:24:ARG:HG3	2.12	0.49
25:U:29:ARG:O	25:U:33:LYS:HG3	2.12	0.49
27:a:1932:A:H2'	27:a:1933:G:O4'	2.12	0.49
43:q:37:GLU:HB3	43:q:53:PHE:CE1	2.47	0.49
9:E:76:TYR:CD1	9:E:76:TYR:C	2.90	0.49
27:a:807:U:OP2	37:k:41:ARG:NH2	2.45	0.49
47:u:2:PHE:HB2	47:u:61:LEU:HD12	1.94	0.49
47:u:31:TYR:O	47:u:92:VAL:HA	2.11	0.49
52:z:36:GLU:OE2	52:z:46:ASP:HB3	2.13	0.49
6:B:253:A:O2'	22:R:17:MET:SD	2.69	0.49
27:a:2393:U:H5'	37:k:60:ARG:O	2.12	0.49
45:s:13:ALA:HB1	50:x:33:ALA:HB1	1.93	0.49
7:C:94:HIS:ND1	7:C:146:ASN:O	2.41	0.49
27:a:2303:G:O2'	32:f:121:SER:O	2.29	0.49
27:a:2875:C:O3'	41:o:2:SER:N	2.45	0.49
36:j:4:GLU:O	36:j:5:GLN:HB2	2.11	0.49
55:8:11:C:H2'	55:8:12:G:H8	1.77	0.49
6:B:723:U:OP1	26:V:55:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1053:G:N7	6:B:1200:C:H5''	2.28	0.49
8:D:62:LYS:O	8:D:97:VAL:HB	2.12	0.49
27:a:811:U:H2'	37:k:21:ARG:HA	1.95	0.49
27:a:1995:U:H3'	27:a:1996:C:H2'	1.95	0.49
27:a:2627:G:O2'	27:a:2781:A:N1	2.38	0.49
54:Y:76:A:O3'	56:A:19:VAL:HG22	2.13	0.49
6:B:131:A:H2'	6:B:132:C:C6	2.47	0.49
10:F:16:ILE:HD11	10:F:38:VAL:HG22	1.95	0.49
27:a:828:U:H4'	27:a:831:G:N1	2.27	0.49
17:M:79:VAL:N	17:M:103:ASP:OD2	2.38	0.49
27:a:1637:A:H5'	27:a:1760:C:O2'	2.12	0.49
1:O:11:LEU:N	1:O:21:TYR:O	2.43	0.49
6:B:519:C:H2'	6:B:520:A:C8	2.48	0.49
6:B:521:G:N7	17:M:50:ARG:NH2	2.58	0.49
16:L:35:THR:HG22	16:L:41:ALA:HA	1.94	0.49
27:a:191:A:H2'	27:a:192:C:C6	2.48	0.49
27:a:366:C:H2'	27:a:367:G:O4'	2.13	0.49
27:a:2609[A]:U:H1'	60:A:101:A2G:H8	1.94	0.49
38:l:66:ARG:NH1	38:l:104:GLU:OE2	2.45	0.49
6:B:1218:C:H2'	6:B:1219:A:C8	2.48	0.49
17:M:55:VAL:HG21	17:M:80:ILE:HD11	1.94	0.49
27:a:2627:G:N2	27:a:2777:G:OP2	2.45	0.49
6:B:171:A:H2'	6:B:172:A:C8	2.48	0.48
6:B:551:U:H2'	6:B:552:U:C6	2.48	0.48
6:B:860:A:H2'	6:B:861:G:O4'	2.12	0.48
6:B:1106:G:H5''	8:D:172:ARG:HG2	1.93	0.48
6:B:1169:A:H2'	6:B:1170:A:C8	2.48	0.48
6:B:1179:A:OP2	14:J:99:ARG:NH2	2.46	0.48
14:J:59:GLU:OE1	14:J:59:GLU:N	2.46	0.48
27:a:1902:C:H4'	29:c:242:LYS:O	2.13	0.48
32:f:36:LEU:HD22	32:f:154:ILE:HG12	1.95	0.48
6:B:426:U:H5''	9:E:36:GLN:NE2	2.28	0.48
6:B:1004:A:H2'	6:B:1005:A:O4'	2.13	0.48
7:C:184:PHE:CD1	7:C:184:PHE:N	2.81	0.48
27:a:120:U:H5''	27:a:122:G:OP2	2.14	0.48
27:a:167:A:C2	27:a:168:G:H1'	2.48	0.48
27:a:1156:A:C8	42:p:51:ARG:HG2	2.48	0.48
27:a:1268:A:H2'	27:a:1269:A:O4'	2.14	0.48
27:a:1415:U:H1'	27:a:1588:G:N2	2.28	0.48
27:a:1737:G:H2'	27:a:1738:G:C1'	2.43	0.48
27:a:2327:A:H2'	27:a:2328:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:2591:C:H2'	27:a:2592:G:C8	2.48	0.48
32:f:161:LYS:HD2	32:f:161:LYS:N	2.28	0.48
15:K:66:GLU:HB2	19:O:99:ALA:HB2	1.96	0.48
27:a:914:G:H5'	27:a:915:C:OP2	2.13	0.48
29:c:29:PRO:HG2	29:c:34:LEU:HD11	1.95	0.48
33:g:52:PHE:N	33:g:52:PHE:CD1	2.81	0.48
6:B:323:U:H2'	6:B:324:G:O4'	2.12	0.48
6:B:1193:G:O6	8:D:2:GLY:N	2.46	0.48
27:a:78:U:OP1	50:x:7:ARG:NH2	2.44	0.48
27:a:121:G:H4'	27:a:149:A:H5'	1.96	0.48
27:a:2233:U:H2'	27:a:2234:G:H8	1.79	0.48
31:e:7:ASP:OD2	31:e:122:GLU:N	2.43	0.48
46:t:49:VAL:HB	46:t:52:LEU:O	2.12	0.48
6:B:266:G:N3	6:B:266:G:H2'	2.29	0.48
16:L:17:SER:HA	16:L:79:ILE:HA	1.93	0.48
27:a:893:C:H5''	27:a:893:C:H6	1.78	0.48
27:a:958:U:O2	28:b:89:U:H1'	2.13	0.48
27:a:2600:A:H2'	27:a:2601:C:C6	2.48	0.48
39:m:114:GLU:OE1	39:m:118:ARG:NH2	2.46	0.48
6:B:392:C:OP1	21:Q:13:LYS:N	2.40	0.48
6:B:1062:U:H2'	6:B:1063:C:C6	2.49	0.48
6:B:1304:G:C6	6:B:1305:G:N1	2.81	0.48
11:G:67:PRO:O	11:G:70:VAL:HG22	2.14	0.48
14:J:123:ARG:NH1	14:J:124:ARG:O	2.43	0.48
27:a:2443:C:OP1	31:e:63:LYS:HD3	2.13	0.48
37:k:77:ILE:HD13	37:k:108:ALA:HB1	1.95	0.48
47:u:20:LEU:HD22	47:u:25:LYS:HB2	1.95	0.48
52:z:53:LYS:HE2	52:z:56:ALA:HA	1.96	0.48
6:B:182:A:N1	6:B:223:A:O2'	2.47	0.48
6:B:502:A:H2'	6:B:503:C:O4'	2.14	0.48
22:R:25:ILE:HB	22:R:42:THR:HG23	1.94	0.48
25:U:20:HIS:O	25:U:24:ARG:HG2	2.14	0.48
27:a:1421:G:N2	27:a:1495:A:N1	2.59	0.48
27:a:2489:U:O2'	27:a:2490:G:H5'	2.14	0.48
30:d:121:THR:HB	30:d:127:PHE:CD2	2.48	0.48
6:B:382:A:H2'	6:B:383:A:H8	1.78	0.48
6:B:701:U:OP1	6:B:702:A:O2'	2.25	0.48
6:B:1305:G:N2	6:B:1331:G:H1'	2.28	0.48
15:K:6:ILE:HB	15:K:76:ILE:HB	1.96	0.48
27:a:1433:A:H2'	27:a:1434:A:C1'	2.43	0.48
27:a:2430:A:N3	27:a:2430:A:H2'	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:48:U:H4'	40:n:100:HIS:HD2	1.79	0.48
40:n:56:LYS:HD2	40:n:56:LYS:N	2.28	0.48
6:B:373:A:H1'	6:B:481:G:O4'	2.14	0.48
9:E:107:PHE:CG	9:E:145:ILE:HD11	2.49	0.48
26:V:13:ASP:OD1	26:V:14:VAL:N	2.46	0.48
31:e:121:VAL:O	31:e:189:THR:HA	2.13	0.48
33:g:69:ARG:HG3	33:g:69:ARG:HH11	1.78	0.48
6:B:479:U:O2	6:B:479:U:H2'	2.13	0.48
27:a:1180:U:H2'	27:a:1181:U:C6	2.49	0.48
27:a:2609[A]:U:O2'	60:A:101:A2G:C7	2.61	0.48
27:a:2788:C:H2'	27:a:2789:C:C6	2.49	0.48
32:f:44:ILE:HA	32:f:83:TYR:HE2	1.79	0.48
33:g:2:SER:O	33:g:6:LYS:HG2	2.14	0.48
37:k:141:LYS:HE3	37:k:143:GLU:HB3	1.96	0.48
5:4:14:ALA:N	5:4:22:MET:O	2.47	0.47
6:B:492:C:H2'	6:B:493:A:C8	2.49	0.47
27:a:2092:U:H4'	27:a:2093:G:O5'	2.14	0.47
32:f:5:HIS:HB2	32:f:97:TRP:CG	2.49	0.47
6:B:1130:A:O2'	14:J:5:GLN:NE2	2.45	0.47
7:C:196:VAL:HG12	7:C:198:PHE:H	1.79	0.47
27:a:493:G:H2'	27:a:494:G:O4'	2.14	0.47
27:a:729:G:C6	29:c:207:LYS:HB2	2.49	0.47
27:a:1314:C:H2'	27:a:1314:C:O2	2.14	0.47
27:a:1720:U:H2'	27:a:1721:G:O4'	2.14	0.47
27:a:2086:U:H2'	27:a:2087:G:C8	2.49	0.47
27:a:2376:A:H2'	27:a:2377:A:O4'	2.14	0.47
40:n:4:LYS:O	40:n:8:ILE:HG12	2.14	0.47
55:8:20:U:N3	55:8:68:G:OP2	2.47	0.47
9:E:96:GLY:HA3	9:E:185:LYS:NZ	2.29	0.47
27:a:703:U:H2'	27:a:704:G:O4'	2.14	0.47
27:a:1433:A:H2'	27:a:1434:A:O4'	2.14	0.47
4:3:2:LYS:HG3	4:3:35:GLN:HG2	1.96	0.47
6:B:184:G:O4'	6:B:224:U:H4'	2.14	0.47
6:B:607:A:H2'	6:B:608:A:C8	2.49	0.47
14:J:53:GLU:HA	14:J:58:VAL:HG22	1.94	0.47
27:a:248:G:N3	27:a:2431:U:H4'	2.30	0.47
27:a:2019:A:H4'	42:p:34:VAL:HG21	1.96	0.47
42:p:112:LYS:HZ2	42:p:112:LYS:HB2	1.79	0.47
55:8:19:G:H4'	55:8:20:U:H5''	1.95	0.47
6:B:224:U:H2'	6:B:225:C:C6	2.50	0.47
18:N:27:LYS:HA	18:N:27:LYS:HZ3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:165:A:H2'	27:a:166:U:O4'	2.13	0.47
27:a:751:A:H5'	44:r:90:LYS:HA	1.97	0.47
29:c:107:PRO:HD2	29:c:110:LEU:HD22	1.97	0.47
41:o:18:PRO:HG3	41:o:84:ILE:O	2.13	0.47
6:B:530:G:H1'	55:8:36:A:O2'	2.14	0.47
29:c:24:LEU:HD13	29:c:83:TYR:HB2	1.96	0.47
44:r:28:LYS:HA	44:r:70:LYS:HG2	1.97	0.47
6:B:97:G:N7	6:B:98:A:C4	2.83	0.47
6:B:782:A:OP1	6:B:1514:G:N2	2.43	0.47
6:B:1414:U:H2'	6:B:1415:G:H8	1.80	0.47
14:J:11:ARG:HB2	14:J:106:ARG:HE	1.80	0.47
18:N:40:ALA:HB3	18:N:43:VAL:HG23	1.97	0.47
27:a:84:A:H4'	27:a:85:G:O5'	2.15	0.47
27:a:483:A:H5''	46:t:47:LYS:HD2	1.97	0.47
27:a:653:U:O5'	27:a:653:U:H6	1.98	0.47
27:a:871:U:H2'	27:a:872:U:C6	2.50	0.47
27:a:2016:U:H2'	27:a:2017:U:C6	2.50	0.47
33:g:102:VAL:HG22	33:g:114:ASP:OD1	2.15	0.47
34:h:29:PHE:C	34:h:32:PRO:HD2	2.40	0.47
37:k:77:ILE:HD12	37:k:77:ILE:N	2.29	0.47
40:n:63:LYS:HD3	40:n:63:LYS:C	2.39	0.47
43:q:55:ASP:N	43:q:55:ASP:OD1	2.46	0.47
48:v:33:ALA:N	48:v:64:ASP:OD1	2.47	0.47
1:0:33:LYS:HG3	1:0:51:GLU:HB3	1.97	0.47
6:B:490:C:C2	6:B:491:G:C8	3.02	0.47
9:E:76:TYR:HE2	9:E:201:VAL:HA	1.79	0.47
13:I:90:ASP:OD1	13:I:90:ASP:N	2.46	0.47
27:a:728:G:H4'	29:c:13:ARG:HD3	1.95	0.47
27:a:1684:G:H2'	27:a:1685:C:C6	2.49	0.47
27:a:2029:G:C8	27:a:2029:G:H3'	2.50	0.47
30:d:110:THR:CG2	30:d:202:ILE:HB	2.45	0.47
6:B:80:A:N6	6:B:81:A:N3	2.63	0.47
6:B:1289:A:H2'	6:B:1290:G:H5'	1.96	0.47
25:U:31:PHE:CD2	25:U:57:ILE:HD13	2.49	0.47
27:a:412:A:N6	27:a:2412:A:O4'	2.48	0.47
27:a:959:A:H2'	27:a:960:A:C8	2.49	0.47
27:a:1028:A:N6	27:a:1125:G:H2'	2.30	0.47
27:a:1188:U:O2'	27:a:1189:A:H5'	2.15	0.47
27:a:2017:U:H4'	52:z:5:GLN:O	2.15	0.47
27:a:2547:A:H8	27:a:2547:A:H5''	1.80	0.47
40:n:43:ASN:HD21	40:n:46:GLU:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:175:C:H2'	6:B:176:C:C6	2.50	0.47
6:B:337:G:H2'	6:B:338:A:C8	2.51	0.47
6:B:1147:C:H4'	14:J:7:TYR:CE2	2.50	0.47
7:C:79:ALA:HB1	7:C:214:LEU:HD12	1.97	0.47
8:D:79:LYS:H	8:D:79:LYS:HD2	1.79	0.47
9:E:177:LYS:O	9:E:178:MET:HB2	2.14	0.47
16:L:21:ALA:HB2	16:L:82:LEU:HD13	1.97	0.47
27:a:156:A:H2'	27:a:157:C:O4'	2.14	0.47
27:a:501:A:H2'	27:a:502:A:C8	2.50	0.47
27:a:893:C:H2'	27:a:894:U:O4'	2.15	0.47
32:f:42:GLU:H	32:f:42:GLU:CD	2.23	0.47
6:B:94:G:N2	6:B:98:A:C2	2.84	0.46
6:B:144:G:H5'	6:B:144:G:H8	1.80	0.46
6:B:993:G:H2'	6:B:993:G:N3	2.30	0.46
24:T:32:ARG:HG3	24:T:57:HIS:ND1	2.30	0.46
27:a:324:A:H8	27:a:324:A:H5''	1.79	0.46
27:a:1824:G:O3'	29:c:247:PRO:HD3	2.14	0.46
27:a:2553:G:H2'	27:a:2554:U:O4'	2.15	0.46
6:B:664:G:H22	6:B:741:G:H1	1.62	0.46
6:B:1060:U:H2'	6:B:1061:G:H8	1.79	0.46
6:B:1518:MA6:O5'	6:B:1518:MA6:H8	2.15	0.46
27:a:559:G:N2	42:p:49:ASP:OD1	2.48	0.46
6:B:160:A:H2'	6:B:161:A:O4'	2.15	0.46
6:B:163:C:H2'	6:B:164:G:O4'	2.15	0.46
6:B:407:U:H2'	6:B:408:A:C8	2.51	0.46
6:B:859:G:H2'	6:B:860:A:C8	2.51	0.46
6:B:1352:C:H2'	6:B:1353:G:C8	2.50	0.46
27:a:1050:A:C2	27:a:2751:G:C4	3.03	0.46
27:a:2571:U:O2'	30:d:151:THR:O	2.30	0.46
27:a:2740:A:H2'	27:a:2741:A:C8	2.51	0.46
54:Y:11:A:H2'	54:Y:12:G:C8	2.50	0.46
6:B:1178:G:N2	6:B:1181:G:OP2	2.47	0.46
11:G:69:GLU:O	11:G:73:GLU:HG3	2.15	0.46
27:a:441:U:H2'	27:a:442:G:C8	2.50	0.46
27:a:609:A:H2'	27:a:610:C:O4'	2.15	0.46
27:a:1187:G:OP1	43:q:85:LYS:NZ	2.40	0.46
27:a:2557:G:H2'	27:a:2558:C:C6	2.50	0.46
32:f:51:ASP:OD1	32:f:51:ASP:N	2.49	0.46
34:h:31:VAL:HB	34:h:32:PRO:HD3	1.98	0.46
35:i:110:PRO:O	35:i:115:GLY:HA3	2.15	0.46
6:B:555:U:H2'	6:B:556:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:619:U:H5'	6:B:619:U:C6	2.50	0.46
6:B:1189:U:OP1	19:O:98:LYS:NZ	2.49	0.46
9:E:60:LYS:O	9:E:64:ILE:HG13	2.15	0.46
24:T:51:VAL:HG21	24:T:71:LEU:HB3	1.97	0.46
27:a:353:C:H2'	27:a:354:A:O4'	2.14	0.46
27:a:693:A:O2'	27:a:1353:A:N3	2.46	0.46
27:a:1108:U:C6	27:a:1109:C:H5	2.34	0.46
27:a:2024:G:OP2	27:a:2034:U:H4'	2.16	0.46
27:a:2502:G:H5''	27:a:2503:2MA:H5''	1.97	0.46
27:a:2506:U:C2	27:a:2585:U:O4	2.68	0.46
39:m:114:GLU:OE1	39:m:118:ARG:NE	2.47	0.46
41:o:114:LEU:O	41:o:115:ASN:ND2	2.49	0.46
45:s:64:LYS:HD2	45:s:64:LYS:N	2.30	0.46
2:l:1:MET:SD	27:a:752:A:H3'	2.55	0.46
6:B:663:A:H5'	6:B:836:G:OP1	2.15	0.46
10:F:156:LYS:HG3	10:F:157:ARG:HG3	1.97	0.46
12:H:74:GLU:OE2	12:H:95:ARG:NE	2.42	0.46
16:L:67:ALA:HB2	16:L:96:THR:HG23	1.97	0.46
27:a:1437:C:H2'	27:a:1438:U:C6	2.51	0.46
27:a:2207:C:H2'	27:a:2208:C:C6	2.51	0.46
6:B:782:A:H4'	6:B:1514:G:O2'	2.16	0.46
12:H:129:GLU:HB2	12:H:131:LYS:HE2	1.98	0.46
27:a:308:G:O4'	27:a:501:A:H5'	2.15	0.46
27:a:1495:A:H1'	27:a:1579:A:H5'	1.97	0.46
27:a:2300:C:H2'	27:a:2301:C:C6	2.51	0.46
33:g:17:VAL:HG11	33:g:50:LEU:HD21	1.98	0.46
44:r:7:HIS:HB2	44:r:50:VAL:HG22	1.98	0.46
6:B:616:G:C2'	6:B:617:G:H5'	2.46	0.46
6:B:790:A:H2'	6:B:791:G:C8	2.51	0.46
27:a:655:A:H4'	27:a:656:G:H5'	1.98	0.46
27:a:910:A:N3	27:a:2264:C:O2'	2.46	0.46
27:a:1682:G:C2	27:a:1757:A:O4'	2.69	0.46
27:a:2376:A:N3	40:n:111:ARG:NH2	2.61	0.46
55:8:21:A:C6	55:8:22:G:H1'	2.51	0.46
6:B:722:G:H2'	6:B:722:G:N3	2.31	0.46
6:B:911:U:H2'	6:B:912:C:C6	2.50	0.46
7:C:151:ILE:HG23	7:C:154:MET:HE2	1.98	0.46
27:a:577:G:H2'	27:a:578:G:C8	2.51	0.46
27:a:812:C:H6	27:a:812:C:H5'	1.81	0.46
27:a:1688:U:O2	27:a:1700:A:H5''	2.16	0.46
6:B:1158:C:C2	6:B:1160:G:C8	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:118:A:OP2	27:a:119:A:H2'	2.16	0.46
27:a:975:A:H1'	27:a:990:A:N1	2.30	0.46
27:a:1778:U:H2'	27:a:1784:A:N6	2.31	0.46
27:a:1999:C:H5''	27:a:2723:C:O2'	2.16	0.46
27:a:2038:G:H2'	27:a:2039:U:O4'	2.16	0.46
32:f:14:LYS:N	32:f:14:LYS:HD2	2.30	0.46
32:f:108:VAL:HG11	32:f:176:PRO:HG3	1.98	0.46
36:j:114:LYS:HE2	36:j:114:LYS:H	1.81	0.46
6:B:672:U:H2'	6:B:673:A:C8	2.51	0.45
7:C:70:VAL:HB	7:C:163:VAL:HG22	1.97	0.45
27:a:103:A:H2'	27:a:104:A:O4'	2.16	0.45
27:a:891:G:H2'	27:a:891:G:N3	2.30	0.45
35:i:76:HIS:CE1	35:i:85:LYS:HB2	2.51	0.45
51:y:41:THR:HB	51:y:44:ILE:HD13	1.98	0.45
52:z:29:SER:OG	52:z:40:ARG:NH1	2.48	0.45
6:B:76:G:N2	6:B:95:C:O2	2.50	0.45
6:B:84:U:H3'	6:B:85:U:H4'	1.99	0.45
6:B:101:A:H5''	6:B:101:A:H8	1.82	0.45
6:B:301:G:H5''	6:B:301:G:H8	1.82	0.45
6:B:420:U:H2'	6:B:421:U:H5''	1.98	0.45
6:B:1317:C:H5''	19:O:24:ARG:NH2	2.31	0.45
9:E:55:LEU:O	9:E:59:GLN:HG2	2.16	0.45
11:G:10:VAL:HG11	11:G:21:MET:HE1	1.98	0.45
18:N:64:VAL:HG13	18:N:68:ASP:HB2	1.98	0.45
27:a:396:G:OP2	49:w:10:LYS:NZ	2.44	0.45
27:a:569:U:O2'	27:a:983:A:N1	2.49	0.45
27:a:641:U:O2'	27:a:2350:C:OP1	2.34	0.45
27:a:1858:A:H1'	27:a:1885:A:C2	2.51	0.45
27:a:2243:U:H2'	27:a:2244:U:C6	2.51	0.45
27:a:2451:A:H1'	54:Y:76:A:O2'	2.16	0.45
27:a:2897:U:H2'	27:a:2898:U:C6	2.51	0.45
3:2:14:PHE:C	3:2:15:LYS:HD2	2.42	0.45
6:B:168:G:H2'	6:B:169:C:O4'	2.16	0.45
6:B:493:A:H2'	6:B:494:G:C8	2.51	0.45
6:B:499:A:C6	6:B:547:A:C8	3.05	0.45
6:B:595:A:C2	6:B:641:U:C2	3.05	0.45
6:B:932:C:H5''	12:H:4:ARG:HD2	1.98	0.45
6:B:959:A:H2'	6:B:960:U:O4'	2.17	0.45
15:K:8:ILE:HD11	15:K:87:LEU:HD13	1.98	0.45
24:T:18:LYS:HB3	24:T:31:LEU:HD23	1.97	0.45
27:a:580:U:H2'	27:a:581:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:2547:A:H2'	27:a:2548:U:C6	2.51	0.45
27:a:2609[A]:U:O2'	56:A:14:PRO:HD3	2.15	0.45
32:f:37:ASN:HB3	32:f:153:ASP:OD1	2.16	0.45
32:f:135:GLN:HG2	32:f:141:ILE:HG21	1.99	0.45
33:g:89:LEU:HD22	33:g:162:VAL:HG22	1.97	0.45
36:j:121:GLU:OE1	41:o:65:SER:OG	2.27	0.45
46:t:86:ARG:HG3	46:t:95:PHE:CE2	2.51	0.45
50:x:13:GLU:O	50:x:16:THR:HG22	2.16	0.45
54:Y:8:4SU:O2'	54:Y:21:A:N1	2.41	0.45
6:B:320:A:H2'	6:B:321:A:O4'	2.17	0.45
6:B:604:G:H2'	6:B:605:U:O4'	2.16	0.45
25:U:35:VAL:O	25:U:39:ILE:HG13	2.17	0.45
27:a:593:U:H2'	27:a:594:U:C6	2.51	0.45
27:a:969:G:O3'	51:y:15:GLY:HA2	2.16	0.45
27:a:2071:A:H2'	27:a:2072:C:C6	2.52	0.45
27:a:2642:G:N2	27:a:2773:C:C2	2.84	0.45
27:a:2804:U:H2'	27:a:2805:C:C6	2.51	0.45
29:c:71:LYS:O	29:c:118:SER:OG	2.34	0.45
38:l:82:MET:HA	38:l:82:MET:HE3	1.98	0.45
6:B:713:G:H2'	6:B:714:G:C8	2.52	0.45
6:B:992:U:H4'	6:B:993:G:H5''	1.99	0.45
6:B:1026:G:N3	6:B:1026:G:H2'	2.31	0.45
7:C:76:ALA:HB2	7:C:210:VAL:HG11	1.99	0.45
17:M:114:ARG:NH1	17:M:114:ARG:HB2	2.31	0.45
18:N:90:ARG:HD3	18:N:96:PRO:O	2.16	0.45
27:a:545:U:O2'	27:a:548:G:N2	2.50	0.45
27:a:639:U:H2'	27:a:640:C:C6	2.51	0.45
27:a:2064:C:O2'	27:a:2251:OMG:N2	2.48	0.45
6:B:1226:C:H4'	24:T:80:TYR:CZ	2.52	0.45
12:H:71:PRO:HG3	12:H:99:LEU:HD12	1.99	0.45
27:a:24:G:O2'	44:r:78:GLU:O	2.34	0.45
27:a:94:A:H2'	27:a:95:A:C8	2.51	0.45
27:a:144:A:H2'	27:a:145:C:C6	2.51	0.45
27:a:1853:A:H2'	27:a:1854:A:C8	2.52	0.45
27:a:2001:C:H4'	27:a:2689:U:H2'	1.99	0.45
30:d:55:LYS:HD3	30:d:60:VAL:HG22	1.99	0.45
39:m:8:ARG:HH11	39:m:8:ARG:HG3	1.81	0.45
44:r:67:ASP:N	44:r:67:ASP:OD1	2.49	0.45
6:B:40:C:H2'	6:B:41:G:O4'	2.16	0.45
6:B:97:G:C8	6:B:98:A:H1'	2.52	0.45
6:B:1148:U:H2'	6:B:1149:C:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1236:A:H4'	6:B:1304:G:H4'	1.99	0.45
22:R:78:VAL:HG21	22:R:81:LYS:HD3	1.98	0.45
27:a:2298:A:H2'	27:a:2299:U:O4'	2.16	0.45
31:e:130:LYS:HB2	31:e:133:LEU:HG	1.97	0.45
38:l:50:ARG:HA	38:l:53:MET:HE2	1.99	0.45
45:s:71:GLY:O	45:s:72:GLN:HG2	2.17	0.45
6:B:502:A:H4'	6:B:550:G:O2'	2.16	0.45
6:B:509:A:H2'	6:B:510:A:C8	2.52	0.45
6:B:573:A:H5'	6:B:573:A:C8	2.50	0.45
6:B:651:C:H2'	6:B:652:U:C6	2.51	0.45
27:a:193:U:O3'	27:a:803:U:H4'	2.17	0.45
27:a:642:U:O2'	27:a:644:A:N7	2.43	0.45
27:a:2390:U:O2	27:a:2390:U:H2'	2.17	0.45
27:a:2718:G:O2'	27:a:2847:U:OP1	2.24	0.45
43:q:43:ASN:HB2	43:q:46:GLU:HB3	1.99	0.45
6:B:104:G:H4'	6:B:174:A:O4'	2.17	0.45
9:E:48:LEU:HD23	9:E:53:VAL:HG22	1.98	0.45
10:F:115:LEU:HD13	10:F:123:VAL:HG11	1.98	0.45
15:K:66:GLU:CB	19:O:99:ALA:HB2	2.47	0.45
27:a:674:G:O2'	31:e:69:ARG:HD2	2.16	0.45
27:a:784:G:H5'	27:a:785:G:OP1	2.16	0.45
27:a:2021:C:OP1	42:p:25:TYR:OH	2.34	0.45
29:c:78:VAL:HG21	29:c:110:LEU:HD11	1.99	0.45
29:c:240:PHE:O	29:c:242:LYS:HG3	2.17	0.45
31:e:6:LYS:HD3	31:e:119:ILE:HG23	1.98	0.45
31:e:7:ASP:OD1	31:e:8:ALA:N	2.47	0.45
46:t:38:GLY:HA2	46:t:41:LEU:HD21	1.99	0.45
56:A:14:PRO:HA	60:A:101:A2G:O4	2.16	0.45
6:B:299:G:H2'	6:B:300:A:C8	2.51	0.45
8:D:10:ILE:HG23	8:D:11:ARG:HG3	1.99	0.45
27:a:527:C:N4	27:a:2779:U:OP2	2.49	0.45
27:a:1182:G:H2'	27:a:1183:U:O4'	2.17	0.45
27:a:1407:G:O2'	27:a:1408:G:H5'	2.17	0.45
30:d:30:GLU:OE1	30:d:30:GLU:N	2.50	0.45
32:f:121:SER:HB2	32:f:128:TYR:CE1	2.52	0.45
32:f:158:THR:HG22	32:f:160:ALA:H	1.82	0.45
33:g:9:VAL:CG2	33:g:50:LEU:HB2	2.47	0.45
33:g:45:HIS:HA	33:g:50:LEU:HA	1.98	0.45
56:A:15:ARG:NH2	56:A:17:ILE:HG12	2.33	0.45
6:B:120:A:H4'	6:B:121:U:O5'	2.17	0.44
6:B:499:A:H4'	6:B:500:G:OP1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:596:A:H5'	6:B:596:A:H8	1.82	0.44
6:B:1225:A:HO2'	6:B:1226:C:P	2.41	0.44
7:C:66:LYS:N	7:C:159:ASP:OD1	2.49	0.44
8:D:71:ALA:C	8:D:73:PRO:HD3	2.42	0.44
16:L:52:PHE:O	16:L:53:ARG:HD2	2.17	0.44
20:P:72:ARG:HG3	20:P:72:ARG:HH11	1.81	0.44
27:a:522:A:H2'	27:a:523:C:C6	2.52	0.44
27:a:880:G:H2'	27:a:881:G:O4'	2.17	0.44
27:a:1570:A:H2'	27:a:1571:A:C8	2.52	0.44
27:a:1652:A:H2'	27:a:1653:G:O4'	2.17	0.44
27:a:2258:C:O2'	27:a:2427:C:OP2	2.34	0.44
2:1:5:PHE:CE2	2:1:7:PRO:HG3	2.52	0.44
6:B:203:G:H2'	6:B:465:A:N6	2.32	0.44
6:B:1102:A:H2'	6:B:1103:C:C6	2.52	0.44
6:B:1206:G:H2'	6:B:1207:2MG:O4'	2.16	0.44
15:K:65:TYR:HB3	19:O:96:LEU:HD11	1.98	0.44
27:a:657:U:H2'	27:a:658:U:C6	2.53	0.44
27:a:2820:A:N3	27:a:2820:A:H2'	2.32	0.44
35:i:11:VAL:HG21	35:i:50:THR:HA	1.98	0.44
41:o:114:LEU:O	41:o:115:ASN:C	2.60	0.44
47:u:48:MET:O	47:u:51:GLN:HG3	2.17	0.44
49:w:78:TYR:CD1	49:w:78:TYR:C	2.95	0.44
6:B:67:C:H2'	6:B:68:G:C8	2.52	0.44
6:B:420:U:C2'	6:B:421:U:H5''	2.47	0.44
6:B:757:U:OP1	6:B:822:U:O2'	2.33	0.44
6:B:1486:G:H2'	6:B:1487:G:O4'	2.17	0.44
27:a:851:C:H2'	27:a:852:U:C6	2.52	0.44
27:a:2308:G:H2'	27:a:2308:G:N3	2.32	0.44
32:f:14:LYS:HD2	32:f:14:LYS:H	1.82	0.44
40:n:25:ARG:HD2	40:n:93:ASP:OD2	2.16	0.44
6:B:1092:A:C4	6:B:1183:U:C4	3.05	0.44
8:D:6:HIS:CE1	8:D:8:ASN:HB3	2.52	0.44
27:a:532:A:N3	27:a:532:A:H2'	2.33	0.44
27:a:878:A:H2'	27:a:879:G:O4'	2.18	0.44
27:a:1239:G:H2'	27:a:1240:U:O4'	2.17	0.44
27:a:1387:A:H5'	27:a:1469:A:H1'	1.99	0.44
29:c:105:LEU:O	29:c:107:PRO:HD3	2.17	0.44
52:z:32:LYS:CE	52:z:32:LYS:H	2.31	0.44
6:B:570:G:H1'	6:B:820:U:C4	2.52	0.44
6:B:579:A:H2'	6:B:580:C:C6	2.52	0.44
6:B:613:C:O2	6:B:628:G:N2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:90:MET:SD	23:S:61:ARG:NE	2.91	0.44
27:a:632:A:H2'	27:a:633:A:C8	2.52	0.44
27:a:891:G:H4'	27:a:891:G:OP1	2.17	0.44
27:a:929:U:H1'	51:y:26:GLY:O	2.18	0.44
27:a:2286:G:N3	27:a:2286:G:H2'	2.32	0.44
34:h:9:VAL:HG13	34:h:12:LEU:HB3	1.98	0.44
48:v:68:LYS:NZ	48:v:69:PHE:O	2.51	0.44
6:B:46:G:H2'	6:B:366:A:N7	2.33	0.44
6:B:718:A:C1'	16:L:118:HIS:HA	2.48	0.44
7:C:151:ILE:O	7:C:151:ILE:HG22	2.18	0.44
7:C:162:PHE:HE2	7:C:214:LEU:HD23	1.82	0.44
27:a:328:U:O3'	46:t:66:GLN:HG3	2.17	0.44
27:a:547:A:H1'	27:a:548:G:C8	2.53	0.44
27:a:2328:A:H2'	27:a:2329:U:C6	2.52	0.44
27:a:2780:G:N1	35:i:102:GLU:OE1	2.47	0.44
27:a:2813:A:H2'	27:a:2814:A:C8	2.53	0.44
28:b:106:G:H2'	28:b:107:G:O4'	2.18	0.44
29:c:203:ARG:HH12	29:c:205:LEU:HD21	1.82	0.44
31:e:143:LEU:HD13	31:e:146:VAL:HG11	1.98	0.44
31:e:154:ASP:OD2	31:e:157:LEU:N	2.45	0.44
36:j:88:ASN:OD1	36:j:90:ASN:N	2.43	0.44
6:B:82:G:N3	6:B:82:G:H2'	2.33	0.44
6:B:165:G:H2'	6:B:166:U:C6	2.53	0.44
6:B:288:A:H2'	6:B:289:G:H4'	1.99	0.44
6:B:710:G:OP1	11:G:53:LYS:HE3	2.18	0.44
9:E:33:LYS:NZ	9:E:33:LYS:HB3	2.33	0.44
17:M:43:LYS:HE3	17:M:91:PRO:HD3	1.99	0.44
17:M:110:ARG:NH1	17:M:112:GLN:O	2.51	0.44
28:b:30:C:C2'	28:b:31:C:H5'	2.48	0.44
44:r:51:LEU:O	44:r:55:ILE:HG13	2.18	0.44
6:B:380:G:N3	6:B:380:G:H2'	2.33	0.44
27:a:693:A:H2'	27:a:694:U:C6	2.53	0.44
27:a:748:G:C8	44:r:89:ALA:HB1	2.53	0.44
27:a:1853:A:H1'	27:a:2234:G:O4'	2.17	0.44
27:a:2812:G:H2'	27:a:2813:A:C8	2.53	0.44
31:e:191:ASP:OD1	31:e:191:ASP:N	2.51	0.44
35:i:4:PHE:CD1	35:i:4:PHE:C	2.94	0.44
42:p:91:ASP:OD1	42:p:94:ILE:HG12	2.18	0.44
46:t:96:PHE:HB2	46:t:99:ASN:OD1	2.18	0.44
47:u:56:PHE:CD1	47:u:56:PHE:C	2.96	0.44
6:B:268:U:H2'	6:B:269:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:718:A:H1'	16:L:118:HIS:HA	2.00	0.44
6:B:831:A:H2'	6:B:832:G:O4'	2.17	0.44
14:J:51:PRO:HD3	14:J:80:ARG:HG3	2.00	0.44
16:L:72:ASP:N	16:L:72:ASP:OD1	2.50	0.44
23:S:26:ILE:O	23:S:30:LYS:HG3	2.17	0.44
27:a:1509:A:O2'	27:a:1510:G:OP2	2.20	0.44
27:a:1744:A:H3'	27:a:1745:A:H8	1.83	0.44
27:a:1799:G:O2'	29:c:180:GLU:OE2	2.31	0.44
27:a:1802:A:H2'	27:a:1803:A:C8	2.52	0.44
27:a:2749:A:OP1	33:g:2:SER:OG	2.31	0.44
29:c:125:LYS:NZ	29:c:126:PRO:O	2.49	0.44
32:f:133:ARG:HG3	32:f:134:GLU:HG3	2.00	0.44
40:n:64:TYR:HB3	40:n:67:ASN:HD22	1.82	0.44
6:B:538:G:H5''	17:M:111:LYS:HG2	1.99	0.43
6:B:751:U:H2'	6:B:752:G:O4'	2.18	0.43
8:D:68:ILE:HB	8:D:103:ILE:HD13	2.00	0.43
9:E:159:LEU:HD13	9:E:175:ALA:HB1	2.00	0.43
10:F:151:GLU:H	10:F:151:GLU:CD	2.25	0.43
16:L:20:VAL:HG13	16:L:85:MET:HG2	2.00	0.43
27:a:1141:U:H4'	27:a:1142:A:O4'	2.18	0.43
27:a:1248:G:OP1	31:e:44:ARG:NH1	2.50	0.43
27:a:1506:U:H2'	27:a:1507:C:C6	2.53	0.43
27:a:1846:G:H2'	27:a:1847:A:O4'	2.18	0.43
27:a:2516:A:H2'	27:a:2517:C:C6	2.53	0.43
27:a:2531:A:OP1	33:g:175:LYS:HE2	2.18	0.43
29:c:140:THR:HG23	29:c:161:TYR:HB2	2.00	0.43
33:g:166:ASP:O	33:g:167:GLU:C	2.61	0.43
47:u:51:GLN:HG2	47:u:86:LEU:HD11	2.00	0.43
6:B:80:A:C6	6:B:81:A:H1'	2.52	0.43
6:B:274:A:H1'	6:B:275:G:C8	2.54	0.43
6:B:579:A:H5'	6:B:728:A:H1'	2.00	0.43
6:B:1023:U:H2'	6:B:1024:G:O4'	2.18	0.43
6:B:1517:G:H2'	6:B:1518:MA6:H8	2.00	0.43
14:J:30:ILE:HA	14:J:65:ILE:O	2.18	0.43
27:a:231:A:H2'	27:a:232:G:O4'	2.18	0.43
27:a:830:G:O4'	27:a:2448:A:C2	2.71	0.43
27:a:878:A:C4	27:a:879:G:H1'	2.52	0.43
27:a:1125:G:C6	27:a:1126:A:N6	2.87	0.43
27:a:1668:A:O2'	27:a:1674:G:N7	2.46	0.43
30:d:25:THR:HG21	30:d:193:VAL:HG22	2.00	0.43
33:g:19:ILE:HG23	33:g:24:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Y:25:C:H2'	54:Y:26:G:O4'	2.18	0.43
6:B:169:C:C4	6:B:170:U:C5	3.06	0.43
6:B:477:C:H2'	6:B:478:A:H8	1.82	0.43
7:C:127:ASP:OD1	7:C:127:ASP:N	2.49	0.43
9:E:124:MET:O	9:E:143:VAL:HA	2.18	0.43
10:F:72:ILE:HD12	10:F:145:GLU:HB3	2.00	0.43
27:a:170:U:H2'	27:a:171:U:C6	2.52	0.43
27:a:576:U:H2'	27:a:577:G:C8	2.54	0.43
27:a:782:A:N3	29:c:225:MET:HG2	2.32	0.43
27:a:901:C:H2'	27:a:902:C:C6	2.53	0.43
27:a:2250:G:C5	38:l:82:MET:HB3	2.53	0.43
36:j:43:ILE:CD1	36:j:52:VAL:HB	2.48	0.43
6:B:28:A:O2'	6:B:296:U:OP1	2.32	0.43
6:B:453:G:C8	6:B:453:G:H5''	2.53	0.43
6:B:1273:C:H2'	6:B:1274:A:O4'	2.19	0.43
26:V:39:GLU:CD	26:V:47:ARG:HE	2.26	0.43
27:a:356:G:H2'	27:a:357:C:C6	2.53	0.43
27:a:1434:A:H2'	27:a:1435:G:C8	2.53	0.43
27:a:1681:G:N3	27:a:1762:A:H2'	2.33	0.43
30:d:152:PRO:HG3	30:d:156:PHE:CZ	2.53	0.43
55:8:8:U:H2'	55:8:13:A:N6	2.34	0.43
1:0:7:GLU:HG2	1:0:27:LYS:HE3	1.99	0.43
6:B:784:A:H4'	27:a:1837:C:OP1	2.19	0.43
6:B:1222:G:OP2	6:B:1322:C:N4	2.39	0.43
8:D:27:LYS:HG3	8:D:28:GLU:CD	2.42	0.43
8:D:168:TYR:OH	10:F:55:GLU:OE2	2.18	0.43
27:a:849:A:H2'	27:a:850:U:C6	2.53	0.43
27:a:1738:G:H8	27:a:1738:G:H5''	1.83	0.43
27:a:1900:A:H5'	27:a:1970:A:H5'	2.01	0.43
27:a:2725:A:O2'	27:a:2726:A:H2'	2.19	0.43
28:b:65:U:C4	28:b:108:A:C4	3.07	0.43
33:g:17:VAL:HG13	33:g:26:ILE:HG12	2.00	0.43
38:l:77:PRO:HG2	38:l:80:VAL:HG21	2.00	0.43
6:B:17:U:H2'	6:B:18:C:C6	2.53	0.43
6:B:718:A:H5'	16:L:119:ASN:ND2	2.34	0.43
6:B:1338:G:H2'	6:B:1339:A:C8	2.53	0.43
6:B:1519:MA6:H5''	6:B:1519:MA6:H8	2.00	0.43
13:I:94:LYS:HG2	13:I:117:ARG:HH22	1.82	0.43
27:a:78:U:H2'	27:a:79:C:C6	2.53	0.43
27:a:1022:G:N7	35:i:68:LYS:HD3	2.34	0.43
27:a:1025:G:H4'	27:a:1026:G:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:1408:G:H2'	27:a:1409:U:C6	2.53	0.43
27:a:2489:U:C4	27:a:2490:G:C6	3.06	0.43
27:a:2609[B]:U:H3	60:A:101:A2G:HO3	1.59	0.43
37:k:109:LYS:HA	37:k:126:ARG:O	2.17	0.43
4:3:33:HIS:O	4:3:35:GLN:HG3	2.19	0.43
6:B:96:U:H2'	6:B:97:G:H8	1.83	0.43
6:B:227:G:H2'	6:B:228:A:C8	2.54	0.43
6:B:524:G:H2'	6:B:525:C:C6	2.53	0.43
6:B:626:G:OP1	21:Q:18:GLN:NE2	2.49	0.43
6:B:737:C:H2'	6:B:738:C:C6	2.54	0.43
7:C:219:ALA:O	7:C:223:GLU:HG2	2.19	0.43
9:E:98:LEU:HB2	9:E:135:TYR:HB3	1.99	0.43
16:L:87:LYS:HB2	16:L:113:VAL:HG23	2.00	0.43
21:Q:4:ILE:HG12	21:Q:21:VAL:HG22	2.00	0.43
22:R:4:LYS:HD3	22:R:5:ILE:N	2.32	0.43
26:V:2:PRO:HG2	26:V:23:CYS:HA	2.01	0.43
27:a:196:A:H2'	27:a:2068:U:H5	1.83	0.43
27:a:1733:G:H5'	27:a:1733:G:C8	2.53	0.43
27:a:1813:G:H4'	29:c:43:ARG:O	2.19	0.43
31:e:118:LEU:HD11	31:e:188:MET:SD	2.58	0.43
38:l:20:LEU:HD13	47:u:81:PRO:HG2	2.00	0.43
6:B:240:G:H4'	6:B:240:G:OP1	2.19	0.43
6:B:346:G:OP1	41:o:39:ARG:NH2	2.52	0.43
6:B:426:U:H5''	9:E:36:GLN:HE22	1.82	0.43
6:B:551:U:H5'	17:M:116:LYS:HE2	2.01	0.43
6:B:992:U:H4'	6:B:993:G:C5'	2.49	0.43
6:B:1328:C:H5''	18:N:28:THR:HG21	2.00	0.43
7:C:26:LYS:HD2	7:C:192:ASP:OD1	2.19	0.43
12:H:75:VAL:HA	12:H:88:PRO:HA	2.00	0.43
27:a:1348:C:H2'	27:a:1349:C:H5'	2.01	0.43
27:a:2263:C:H4'	27:a:2329:U:H4'	2.00	0.43
35:i:4:PHE:O	42:p:64:ARG:NH1	2.52	0.43
37:k:124:GLY:O	37:k:125:LEU:HD23	2.18	0.43
53:X:20:U:H2'	53:X:20:U:O2	2.19	0.43
6:B:68:G:C4	6:B:69:G:H1'	2.53	0.43
6:B:503:C:O2	6:B:510:A:H2	2.02	0.43
6:B:563:A:H2'	6:B:563:A:N3	2.33	0.43
27:a:278:A:N3	27:a:278:A:H3'	2.34	0.43
27:a:365:U:H2'	27:a:366:C:C6	2.53	0.43
27:a:480:A:N3	27:a:480:A:H2'	2.34	0.43
27:a:2196:C:H2'	27:a:2197:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:2305:U:H5''	32:f:131:GLY:HA3	2.01	0.43
45:s:91:GLN:O	45:s:92:ASN:HB2	2.19	0.43
6:B:244:U:O4	6:B:906:A:H1'	2.18	0.43
6:B:763:G:H2'	6:B:764:C:C6	2.54	0.43
6:B:920:U:H2'	6:B:921:U:C6	2.54	0.43
27:a:529:A:O2'	27:a:2023:C:N4	2.42	0.43
27:a:1531:C:H6	27:a:1531:C:O5'	2.02	0.43
27:a:1721:G:H1'	27:a:1739:A:H61	1.83	0.43
27:a:1920:C:O5'	27:a:1920:C:H6	2.01	0.43
6:B:545:C:O2'	6:B:549:C:H5''	2.19	0.42
12:H:51:ALA:HB2	12:H:58:GLU:HG3	2.01	0.42
16:L:29:ASN:HD22	16:L:57:LYS:HD2	1.83	0.42
17:M:83:ARG:HG2	17:M:96:HIS:O	2.18	0.42
27:a:167:A:H3'	27:a:168:G:H8	1.84	0.42
27:a:782:A:C2	29:c:225:MET:HG2	2.54	0.42
27:a:1263:U:H2'	27:a:1264:A:C8	2.54	0.42
27:a:1680:U:H2'	27:a:1681:G:O4'	2.19	0.42
27:a:2025:C:H2'	27:a:2026:U:C6	2.54	0.42
27:a:2312:U:H5'	32:f:85:ILE:HD11	2.01	0.42
27:a:2507:C:H2'	27:a:2508:G:O4'	2.19	0.42
37:k:129:LYS:HE3	37:k:129:LYS:HA	2.01	0.42
38:l:17:ASN:OD1	38:l:97:GLN:NE2	2.52	0.42
38:l:41:LEU:HG	38:l:96:ILE:HG13	2.01	0.42
40:n:85:LYS:NZ	40:n:85:LYS:HB3	2.34	0.42
43:q:74:ILE:N	43:q:74:ILE:HD12	2.34	0.42
3:2:45:ARG:N	3:2:46:PRO:HD2	2.34	0.42
5:4:7:PRO:O	5:4:8:LYS:C	2.62	0.42
6:B:380:G:N2	6:B:382:A:P	2.92	0.42
6:B:562:U:H5'	6:B:563:A:C4	2.53	0.42
6:B:634:C:H2'	6:B:635:A:H8	1.83	0.42
9:E:153:SER:O	9:E:155:VAL:N	2.44	0.42
14:J:79:ILE:O	14:J:83:ILE:HG13	2.19	0.42
24:T:64:ASP:OD1	24:T:64:ASP:N	2.52	0.42
27:a:380:G:H4'	49:w:16:ASN:O	2.19	0.42
27:a:565:C:H4'	27:a:1253:A:N6	2.34	0.42
27:a:1011:G:OP2	42:p:66:ASN:ND2	2.51	0.42
27:a:2208:C:H2'	27:a:2209:C:C6	2.54	0.42
27:a:2534:A:H2'	27:a:2535:G:O4'	2.18	0.42
36:j:51:LYS:HD3	36:j:95:ILE:HG22	2.01	0.42
38:l:106:ASP:OD1	38:l:107:GLY:N	2.51	0.42
1:0:25:LYS:HE3	1:0:30:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1:MET:HE3	2:1:1:MET:HB2	1.89	0.42
6:B:168:G:C6	6:B:169:C:C4	3.08	0.42
6:B:409:U:H5''	9:E:25:VAL:HG21	2.00	0.42
6:B:1088:G:H4'	26:V:70:LEU:HD13	2.02	0.42
8:D:120:ILE:O	8:D:124:LEU:HG	2.20	0.42
11:G:40:GLU:OE1	11:G:100:SER:HB2	2.20	0.42
27:a:139:U:H5''	27:a:140:C:H5	1.83	0.42
27:a:479:A:H4'	27:a:480:A:OP1	2.20	0.42
27:a:590:A:H2'	27:a:591:U:C6	2.55	0.42
27:a:1726:C:H2'	27:a:1727:C:C6	2.54	0.42
27:a:2295:C:H2'	27:a:2296:U:C6	2.54	0.42
27:a:2644:G:O2'	27:a:2645:G:H5'	2.19	0.42
27:a:2681:C:O2	27:a:2683:C:N4	2.44	0.42
27:a:2783:U:H2'	27:a:2784:U:C6	2.53	0.42
30:d:24:VAL:HG12	30:d:178:VAL:HG21	2.01	0.42
6:B:123:U:O5'	6:B:123:U:H6	2.03	0.42
6:B:472:U:H5''	6:B:472:U:H6	1.85	0.42
7:C:71:GLY:HA3	7:C:80:VAL:HG21	2.00	0.42
8:D:20:SER:HA	8:D:57:ILE:O	2.20	0.42
10:F:75:ALA:HB1	10:F:149:SER:HB3	2.01	0.42
13:I:45:PHE:HE2	13:I:101:ILE:HG12	1.83	0.42
27:a:281:C:H5''	27:a:281:C:C6	2.52	0.42
27:a:662:G:H5'	37:k:14:LYS:O	2.20	0.42
27:a:1504:A:H8	27:a:1504:A:H5''	1.83	0.42
27:a:2578:G:OP2	27:a:2578:G:H4'	2.19	0.42
28:b:39:A:H2'	28:b:40:U:C6	2.54	0.42
36:j:64:ARG:HD3	36:j:102:PRO:O	2.20	0.42
38:l:54:THR:HG22	38:l:59:ARG:HG2	2.02	0.42
3:2:39:LYS:NZ	27:a:2365:G:N7	2.59	0.42
6:B:37:U:H5''	6:B:37:U:H6	1.85	0.42
6:B:419:C:OP1	6:B:513:C:O2'	2.37	0.42
6:B:443:C:H2'	6:B:444:G:O4'	2.19	0.42
6:B:476:U:H2'	6:B:477:C:C6	2.55	0.42
6:B:1023:U:H2'	6:B:1024:G:C8	2.54	0.42
6:B:1390:U:H2'	6:B:1391:U:C6	2.55	0.42
24:T:80:TYR:CZ	24:T:82:GLY:HA2	2.53	0.42
27:a:839:U:H2'	27:a:840:C:C6	2.55	0.42
27:a:2241:A:H2'	27:a:2242:G:C8	2.54	0.42
27:a:2662:A:H2'	27:a:2663:G:O4'	2.19	0.42
27:a:2680:U:OP1	30:d:114:LYS:HG3	2.19	0.42
27:a:2755:C:O2'	27:a:2756:U:H2'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:30:GLU:CD	30:d:30:GLU:H	2.26	0.42
30:d:85:ALA:HB3	30:d:88:GLU:HG3	2.01	0.42
32:f:28:VAL:O	32:f:30:ARG:HD3	2.19	0.42
6:B:1236:A:H2'	6:B:1237:C:C6	2.54	0.42
10:F:38:VAL:HG11	10:F:114:VAL:HG22	2.02	0.42
12:H:132:GLY:O	12:H:135:VAL:HG22	2.19	0.42
25:U:55:GLN:HB3	25:U:56:PRO:HD3	2.01	0.42
27:a:1109:C:O2	27:a:1109:C:C2'	2.67	0.42
27:a:1548:A:H2'	27:a:1549:A:C8	2.54	0.42
27:a:2229:U:O2	49:w:34:HIS:HE1	2.02	0.42
27:a:2751:G:H2'	27:a:2751:G:N3	2.34	0.42
37:k:121:THR:HA	37:k:141:LYS:O	2.19	0.42
45:s:69:ARG:CZ	45:s:74:ILE:HB	2.50	0.42
46:t:95:PHE:CD1	46:t:95:PHE:C	2.97	0.42
4:3:15:LYS:NZ	27:a:2753:A:N3	2.65	0.42
6:B:2:A:C6	6:B:3:A:N1	2.88	0.42
6:B:1306:A:N3	6:B:1306:A:H2'	2.35	0.42
6:B:1477:U:H2'	6:B:1478:U:C6	2.54	0.42
22:R:65:ARG:HB2	22:R:66:PRO:HD2	2.02	0.42
27:a:476:G:H4'	27:a:502:A:N1	2.35	0.42
27:a:548:G:H2'	27:a:549:G:C4	2.55	0.42
27:a:687:C:H2'	27:a:688:U:O4'	2.20	0.42
27:a:1663:G:H5''	27:a:1663:G:H8	1.85	0.42
27:a:1710:G:H4'	27:a:2858:C:O2	2.20	0.42
27:a:1736:U:H2'	27:a:1737:G:C8	2.54	0.42
27:a:2469:A:H2'	27:a:2470:G:O4'	2.19	0.42
27:a:2544:G:H2'	27:a:2545:G:O4'	2.19	0.42
27:a:2713:U:O2'	27:a:2715:C:OP2	2.29	0.42
35:i:98:GLU:O	35:i:102:GLU:HG3	2.20	0.42
41:o:88:ARG:NH2	41:o:110:ILE:O	2.51	0.42
54:Y:49:G:H2'	54:Y:49:G:N3	2.35	0.42
54:Y:61:C:H2'	54:Y:62:C:C6	2.55	0.42
6:B:109:A:H2'	6:B:326:G:N2	2.35	0.42
6:B:489:C:H2'	6:B:490:C:C6	2.54	0.42
6:B:613:C:OP1	9:E:81:ARG:HD2	2.20	0.42
6:B:1035:A:O2'	6:B:1036:A:H5''	2.20	0.42
12:H:84:THR:HG22	12:H:85:TYR:N	2.35	0.42
16:L:114:THR:HG21	26:V:32:VAL:HG21	2.02	0.42
19:O:63:ARG:NH1	19:O:68:GLY:O	2.47	0.42
27:a:823:C:H2'	27:a:824:U:C6	2.55	0.42
27:a:1003:G:O2'	27:a:1010:A:N1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:1196:C:O4'	27:a:1226:A:C2	2.72	0.42
27:a:1524:G:O5'	27:a:1524:G:H8	2.03	0.42
27:a:2291:U:OP1	27:a:2380:C:O2'	2.36	0.42
27:a:2497:A:N3	27:a:2498:OMC:N4	2.67	0.42
31:e:4:VAL:HA	31:e:10:SER:O	2.19	0.42
33:g:109:PHE:C	33:g:111:HIS:H	2.27	0.42
34:h:26:ALA:HA	34:h:30:LEU:HB2	2.02	0.42
40:n:90:VAL:HG21	40:n:115:LEU:HD13	2.02	0.42
42:p:76:TYR:CZ	42:p:80:ILE:HG13	2.55	0.42
52:z:40:ARG:O	52:z:41:HIS:HB2	2.18	0.42
6:B:815:A:H4'	6:B:817:C:C4	2.54	0.42
13:I:112:THR:HG23	13:I:115:ALA:H	1.85	0.42
14:J:106:ARG:O	14:J:107:ASP:C	2.62	0.42
17:M:65:SER:OG	17:M:97:THR:HG23	2.20	0.42
27:a:244:A:H2'	27:a:245:G:O4'	2.20	0.42
27:a:394:C:O2'	27:a:395:U:H5'	2.19	0.42
27:a:594:U:H2'	27:a:595:C:C6	2.54	0.42
27:a:2345:G:N3	27:a:2381:A:H2'	2.35	0.42
32:f:158:THR:HG22	32:f:159:THR:N	2.35	0.42
33:g:94:TYR:HA	33:g:106:SER:O	2.20	0.42
50:x:55:THR:O	50:x:59:GLU:HG3	2.20	0.42
54:Y:50:U:H2'	54:Y:51:C:C6	2.55	0.42
54:Y:59:A:O5'	54:Y:59:A:H8	2.03	0.42
55:8:9:G:N3	55:8:9:G:H2'	2.35	0.42
6:B:135:C:H6	6:B:135:C:O5'	2.02	0.42
6:B:488:C:H2'	6:B:489:C:C6	2.55	0.42
6:B:736:C:H2'	6:B:737:C:C6	2.55	0.42
6:B:922:G:N3	6:B:1398:A:H2	2.18	0.42
6:B:1085:U:H4'	6:B:1086:U:OP2	2.20	0.42
6:B:1469:C:H2'	6:B:1470:U:O4'	2.19	0.42
14:J:51:PRO:O	14:J:55:VAL:HG22	2.20	0.42
19:O:34:VAL:HA	19:O:41:ARG:HH21	1.85	0.42
27:a:2448:A:H3'	27:a:2449:H2U:H61	2.02	0.42
27:a:2530:A:OP2	33:g:175:LYS:NZ	2.52	0.42
27:a:2825:G:H5''	27:a:2825:G:N3	2.35	0.42
32:f:143:TYR:O	32:f:146:VAL:HG12	2.20	0.42
42:p:76:TYR:CD1	42:p:76:TYR:C	2.98	0.42
54:Y:2:G:N3	54:Y:2:G:H2'	2.34	0.42
54:Y:58:A:O2'	54:Y:60:U:OP2	2.29	0.42
2:1:39:ARG:NH2	27:a:468:G:N7	2.59	0.41
6:B:67:C:H2'	6:B:68:G:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:231:U:H2'	6:B:232:G:H8	1.85	0.41
6:B:380:G:H1'	6:B:384:G:H22	1.85	0.41
6:B:1457:G:OP1	25:U:34:LYS:NZ	2.43	0.41
8:D:25:ASN:O	8:D:26:THR:C	2.63	0.41
19:O:63:ARG:HB3	19:O:68:GLY:HA2	2.02	0.41
27:a:176:A:O2'	27:a:177:G:H5'	2.20	0.41
27:a:554:U:H2'	27:a:555:G:O4'	2.20	0.41
27:a:838:C:H2'	27:a:839:U:C6	2.55	0.41
27:a:2366:A:H2'	27:a:2367:G:O4'	2.20	0.41
27:a:2402:U:C4	27:a:2405:G:O6	2.73	0.41
27:a:2441:U:OP2	27:a:2586:U:O2'	2.37	0.41
29:c:183:LYS:HG3	29:c:268:VAL:CG2	2.50	0.41
31:e:136:GLN:O	31:e:139:LYS:HG2	2.20	0.41
53:X:20:U:C2'	53:X:21:A:H4'	2.49	0.41
4:3:26:ILE:O	4:3:26:ILE:HG13	2.20	0.41
6:B:68:G:O4'	6:B:171:A:H1'	2.20	0.41
6:B:144:G:H2'	6:B:145:G:O4'	2.20	0.41
6:B:179:A:H2'	6:B:180:U:O4'	2.20	0.41
6:B:478:A:C2	6:B:479:U:H1'	2.55	0.41
6:B:1283:U:H2'	6:B:1284:C:C6	2.54	0.41
27:a:1252:G:O2'	27:a:1253:A:C8	2.72	0.41
27:a:1482:G:H1'	27:a:1509:A:N1	2.35	0.41
27:a:1515:A:H2'	27:a:1516:G:O4'	2.20	0.41
27:a:1641:A:H2'	27:a:1642:G:O4'	2.20	0.41
27:a:1693:U:O4	27:a:1976:U:O2'	2.34	0.41
27:a:1996:C:OP1	36:j:31:ARG:NE	2.44	0.41
27:a:2031:A:C6	27:a:2498:OMC:H1'	2.55	0.41
27:a:2636:C:H2'	27:a:2637:U:C6	2.55	0.41
27:a:2725:A:C4	27:a:2727:A:C8	3.07	0.41
27:a:2772:C:H2'	27:a:2773:C:C6	2.55	0.41
39:m:86:ARG:HH21	39:m:117:ASP:CG	2.28	0.41
50:x:12:GLU:H	50:x:12:GLU:CD	2.28	0.41
54:Y:21:A:O5'	54:Y:21:A:H8	2.03	0.41
55:8:36:A:H8	55:8:36:A:H5''	1.84	0.41
6:B:69:G:H2'	6:B:70:U:C6	2.55	0.41
6:B:179:A:H2'	6:B:180:U:C6	2.55	0.41
6:B:560:A:H4'	6:B:561:U:H5''	2.03	0.41
6:B:686:U:HO2'	6:B:687:A:H8	1.66	0.41
6:B:757:U:H2'	6:B:758:C:O4'	2.19	0.41
6:B:857:C:H2'	6:B:858:G:O4'	2.21	0.41
6:B:1216:A:H5''	19:O:5:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:77:ILE:HA	8:D:84:VAL:HG13	2.02	0.41
8:D:79:LYS:N	8:D:82:GLU:OE1	2.53	0.41
11:G:98:GLU:H	11:G:98:GLU:CD	2.27	0.41
14:J:39:PHE:O	14:J:45:ARG:NE	2.43	0.41
27:a:82:U:H2'	27:a:83:A:C8	2.55	0.41
27:a:548:G:H2'	27:a:549:G:N9	2.36	0.41
27:a:2214:C:H2'	27:a:2215:G:O4'	2.20	0.41
27:a:2469:A:H4'	38:l:55:ARG:HD2	2.02	0.41
27:a:2494:G:O2'	38:l:79:ALA:HA	2.20	0.41
27:a:2578:G:N3	27:a:2578:G:H2'	2.35	0.41
27:a:2766:A:N3	27:a:2766:A:H2'	2.36	0.41
30:d:77:ARG:NE	30:d:200:ASP:OD1	2.53	0.41
35:i:3:THR:HG22	42:p:64:ARG:NH1	2.34	0.41
37:k:77:ILE:CD1	37:k:108:ALA:HB1	2.49	0.41
38:l:36:VAL:HG21	38:l:129:THR:HG23	2.01	0.41
40:n:64:TYR:HB3	40:n:67:ASN:ND2	2.35	0.41
5:4:60:PHE:CD1	5:4:60:PHE:C	2.99	0.41
6:B:218:U:H2'	6:B:219:U:O4'	2.20	0.41
6:B:600:A:OP1	13:I:89:LYS:HG2	2.19	0.41
6:B:676:A:H5''	16:L:115:PRO:CB	2.50	0.41
6:B:1378:C:OP2	6:B:1378:C:H3'	2.20	0.41
9:E:23:SER:O	9:E:161:LEU:HD13	2.21	0.41
9:E:155:VAL:O	9:E:159:LEU:HG	2.21	0.41
13:I:96:MET:SD	13:I:130:ALA:HB1	2.60	0.41
27:a:347:A:H2'	27:a:348:A:C8	2.56	0.41
27:a:482:A:N6	27:a:506:G:O2'	2.54	0.41
27:a:716:A:H2'	27:a:717:C:O4'	2.21	0.41
27:a:897:C:O2	27:a:897:C:H2'	2.19	0.41
27:a:1386:C:H2'	27:a:1387:A:C8	2.55	0.41
27:a:1563:U:H2'	27:a:1564:C:C6	2.56	0.41
27:a:1569:A:H2'	27:a:1570:A:C8	2.55	0.41
27:a:1995:U:OP2	27:a:1996:C:O2'	2.30	0.41
28:b:61:G:H2'	28:b:62:C:C6	2.55	0.41
45:s:26:LYS:O	45:s:26:LYS:HG2	2.21	0.41
6:B:375:U:H4'	21:Q:17:TYR:CE2	2.56	0.41
6:B:392:C:C2	6:B:393:A:C8	3.09	0.41
6:B:401:C:O2'	6:B:621:A:N3	2.45	0.41
6:B:496:A:N3	6:B:496:A:H2'	2.35	0.41
6:B:608:A:H8	6:B:608:A:O5'	2.03	0.41
6:B:846:G:N3	6:B:846:G:H2'	2.35	0.41
6:B:1038:C:O2	6:B:1038:C:H2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1181:G:H4'	6:B:1182:G:OP1	2.20	0.41
9:E:183:LYS:NZ	9:E:183:LYS:HB2	2.36	0.41
12:H:75:VAL:HG22	12:H:86:GLN:HB3	2.03	0.41
13:I:11:LEU:HD22	13:I:75:ILE:HD11	2.02	0.41
22:R:13:VAL:HG21	22:R:43:LYS:HD2	2.02	0.41
27:a:159:G:C2'	27:a:167:A:H61	2.33	0.41
27:a:339:U:O5'	27:a:339:U:H6	2.04	0.41
27:a:883:G:H2'	27:a:884:U:C6	2.55	0.41
27:a:1577:C:H2'	27:a:1578:U:C1'	2.50	0.41
27:a:1908:C:O2'	54:Y:12:G:H5''	2.20	0.41
27:a:1998:A:O3'	27:a:2724:U:H4'	2.21	0.41
27:a:2283:C:C6	27:a:2389:G:H2'	2.55	0.41
27:a:2609[A]:U:H2'	60:A:101:A2G:O7	2.20	0.41
27:a:2765:A:N3	27:a:2765:A:H2'	2.35	0.41
27:a:2825:G:H2'	27:a:2826:A:H5'	2.02	0.41
46:t:86:ARG:NH2	46:t:102:THR:OG1	2.52	0.41
6:B:153:C:N4	6:B:154:U:O4	2.53	0.41
6:B:279:A:H4'	6:B:280:C:H5''	2.03	0.41
6:B:448:A:N3	6:B:448:A:H2'	2.33	0.41
8:D:6:HIS:CG	19:O:89:MET:HB3	2.55	0.41
8:D:58:GLU:O	8:D:60:PRO:HD3	2.20	0.41
10:F:85:VAL:HG11	10:F:147:MET:HB2	2.03	0.41
11:G:74:LEU:HD22	11:G:78:PHE:CE1	2.56	0.41
20:P:29:VAL:HG11	20:P:67:LEU:HD21	2.03	0.41
27:a:413:C:H6	27:a:413:C:O5'	2.02	0.41
27:a:417:C:H2'	27:a:418:C:C6	2.56	0.41
27:a:578:G:H21	27:a:1252:G:N2	2.18	0.41
27:a:964:C:O2'	27:a:2273:A:N3	2.44	0.41
27:a:1339:G:OP2	45:s:15:HIS:NE2	2.50	0.41
27:a:1384:A:H1'	27:a:1405:U:H1'	2.02	0.41
27:a:1424:G:H2'	27:a:1425:G:C8	2.55	0.41
27:a:2771:C:H2'	27:a:2772:C:C6	2.55	0.41
6:B:38:G:N2	6:B:397:A:H5'	2.36	0.41
6:B:150:U:C4	6:B:170:U:C4	3.08	0.41
6:B:575:G:O2'	6:B:821:G:H5'	2.21	0.41
6:B:908:A:H2'	6:B:909:A:C8	2.56	0.41
13:I:7:ILE:O	13:I:11:LEU:HG	2.21	0.41
16:L:109:ASN:HB2	26:V:4:ILE:O	2.20	0.41
17:M:87:VAL:HG23	17:M:90:LEU:HB2	2.03	0.41
27:a:6:A:H4'	35:i:131:ASN:O	2.20	0.41
27:a:542:C:H2'	27:a:543:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:749:A:H4'	27:a:1271:G:N3	2.35	0.41
27:a:851:C:O4'	51:y:47:MET:HG3	2.21	0.41
27:a:1608:A:H1'	27:a:1610:A:OP2	2.21	0.41
27:a:1676:A:H2'	27:a:1677:A:O4'	2.21	0.41
27:a:1758:U:H2'	27:a:1758:U:O2	2.19	0.41
36:j:66:LYS:HE2	36:j:66:LYS:HB3	1.94	0.41
43:q:28:ALA:HB3	43:q:31:GLU:HG3	2.01	0.41
49:w:40:VAL:HG22	49:w:43:GLU:H	1.86	0.41
6:B:6:G:O2'	6:B:7:A:H8	2.03	0.41
6:B:79:G:H2'	6:B:80:A:O4'	2.21	0.41
6:B:1130:A:H2'	6:B:1131:G:C8	2.56	0.41
6:B:1179:A:H5''	14:J:104:VAL:HG12	2.03	0.41
6:B:1330:U:O4	6:B:1331:G:C6	2.74	0.41
7:C:143:LYS:HE3	7:C:143:LYS:HB2	1.96	0.41
7:C:214:LEU:HA	7:C:217:VAL:HG22	2.03	0.41
15:K:83:THR:O	15:K:87:LEU:HG	2.21	0.41
17:M:18:LYS:NZ	17:M:19:SER:O	2.50	0.41
18:N:95:LEU:O	18:N:96:PRO:C	2.62	0.41
27:a:102:U:H6	27:a:102:U:H5''	1.85	0.41
27:a:181:A:H2'	27:a:182:A:O4'	2.21	0.41
27:a:766:U:H2'	27:a:767:U:C6	2.56	0.41
27:a:999:U:O2'	27:a:1000:A:H5'	2.21	0.41
27:a:1025:G:H1'	27:a:1135:C:O5'	2.21	0.41
27:a:2011:U:H2'	27:a:2012:G:O4'	2.21	0.41
27:a:2011:U:OP1	44:r:42:LYS:NZ	2.38	0.41
27:a:2250:G:O2'	27:a:2496:C:OP1	2.35	0.41
27:a:2328:A:H8	27:a:2328:A:O5'	2.04	0.41
27:a:2811:G:H2'	27:a:2812:G:O4'	2.21	0.41
27:a:2898:U:H2'	27:a:2899:A:C8	2.55	0.41
46:t:96:PHE:O	46:t:100:SER:HA	2.21	0.41
5:4:16:CYS:SG	5:4:17:SER:N	2.93	0.41
5:4:23:LYS:NZ	5:4:23:LYS:HB3	2.35	0.41
5:4:42:PRO:HA	5:4:45:THR:OG1	2.20	0.41
6:B:553:A:H5''	17:M:21:VAL:HG21	2.03	0.41
6:B:969:A:H5'	6:B:969:A:H8	1.86	0.41
6:B:1030:U:O5'	6:B:1030:U:H6	2.03	0.41
6:B:1046:A:H2'	6:B:1047:G:H5'	2.03	0.41
6:B:1120:C:H2'	6:B:1121:U:C6	2.56	0.41
6:B:1255:G:O2'	6:B:1258:G:N3	2.43	0.41
8:D:14:ILE:HD12	8:D:14:ILE:N	2.36	0.41
9:E:91:LEU:HD11	9:E:197:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:81:LEU:HB3	10:F:147:MET:SD	2.61	0.41
12:H:113:ASP:HB2	12:H:119:ARG:CG	2.51	0.41
13:I:66:PHE:CD2	13:I:67:GLN:HG2	2.56	0.41
14:J:118:LEU:CD2	14:J:124:ARG:HG3	2.51	0.41
16:L:16:VAL:HG12	16:L:77:TYR:HB3	2.03	0.41
18:N:51:GLY:O	18:N:55:THR:HG23	2.21	0.41
24:T:14:HIS:ND1	24:T:15:LEU:N	2.68	0.41
27:a:33:C:C6	27:a:446:G:N2	2.89	0.41
27:a:85:G:H8	27:a:85:G:H5''	1.86	0.41
27:a:184:C:H2'	27:a:185:G:H8	1.86	0.41
27:a:196:A:H2'	27:a:196:A:N3	2.35	0.41
27:a:405:U:H3'	27:a:406:G:H8	1.84	0.41
27:a:414:C:H2'	27:a:415:A:C8	2.55	0.41
27:a:532:A:H3'	42:p:28:ARG:NE	2.35	0.41
27:a:813:U:H2'	27:a:814:C:C6	2.56	0.41
27:a:1151:A:H2'	27:a:1152:C:O4'	2.20	0.41
27:a:1383:A:H4'	27:a:1383:A:OP1	2.20	0.41
27:a:1526:C:H6	27:a:1526:C:H5''	1.85	0.41
27:a:1703:G:H2'	27:a:1704:C:C6	2.56	0.41
27:a:1744:A:H3'	27:a:1745:A:C8	2.56	0.41
27:a:1809:A:H2'	27:a:1810:A:C8	2.56	0.41
27:a:1883:U:O2'	27:a:1884:G:H5'	2.20	0.41
27:a:1913:A:N1	55:8:38:A:O2'	2.52	0.41
27:a:2278:A:OP1	38:l:10:ARG:NH1	2.53	0.41
27:a:2329:U:H2'	27:a:2330:G:C8	2.56	0.41
27:a:2480:C:H2'	27:a:2481:G:O4'	2.20	0.41
27:a:2518:A:N3	27:a:2518:A:H2'	2.36	0.41
27:a:2793:C:H2'	27:a:2794:C:C6	2.55	0.41
35:i:97:PRO:HG2	35:i:126:ALA:HB2	2.02	0.41
36:j:88:ASN:HB3	36:j:91:SER:OG	2.21	0.41
37:k:90:VAL:HG23	37:k:120:VAL:HG11	2.03	0.41
41:o:102:GLU:OE1	41:o:102:GLU:N	2.53	0.41
53:X:18:G:C6	53:X:19:A:H1'	2.56	0.41
1:0:11:LEU:HD23	1:0:51:GLU:HA	2.03	0.41
6:B:503:C:O2'	6:B:510:A:N1	2.49	0.41
6:B:854:U:C6	6:B:871:U:O4	2.74	0.41
9:E:201:VAL:O	9:E:205:SER:N	2.53	0.41
22:R:18:GLU:OE2	22:R:19:LYS:HE3	2.21	0.41
24:T:36:ARG:NH1	24:T:53:ASN:HA	2.36	0.41
27:a:3:U:H2'	27:a:4:U:O4'	2.21	0.41
27:a:362:A:N3	27:a:362:A:H2'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:17:GLU:N	30:d:17:GLU:OE1	2.53	0.41
35:i:98:GLU:H	35:i:98:GLU:CD	2.28	0.41
36:j:15:GLY:HA2	36:j:47:ILE:HG12	2.03	0.41
46:t:10:GLU:OE2	46:t:22:ARG:HB3	2.21	0.41
47:u:2:PHE:HB3	47:u:50:MET:CE	2.51	0.41
6:B:382:A:H2'	6:B:383:A:C8	2.57	0.40
6:B:984:C:H6	6:B:984:C:O5'	2.04	0.40
6:B:1030:U:OP2	6:B:1031:C:H5''	2.21	0.40
7:C:152:LYS:HG3	7:C:153:ASP:OD1	2.22	0.40
9:E:153:SER:O	9:E:156:LYS:HG2	2.21	0.40
11:G:98:GLU:OE1	11:G:98:GLU:N	2.48	0.40
27:a:127:A:H5''	27:a:128:C:O4'	2.21	0.40
27:a:153:U:H2'	27:a:154:U:C6	2.56	0.40
27:a:634:C:H6	27:a:634:C:O5'	2.04	0.40
27:a:1223:G:C6	27:a:1227:G:C6	3.09	0.40
27:a:2529:G:H4'	33:g:175:LYS:HB3	2.03	0.40
31:e:77:ILE:O	31:e:77:ILE:HG22	2.21	0.40
33:g:9:VAL:HG22	33:g:50:LEU:HB2	2.03	0.40
37:k:19:LEU:CD2	37:k:27:LEU:HD13	2.51	0.40
49:w:39:TRP:CH2	49:w:44:LYS:HA	2.56	0.40
54:Y:16:C:H3'	54:Y:17:C:C5	2.55	0.40
54:Y:16:C:H1'	54:Y:59:A:H2	1.85	0.40
55:8:3:C:H2'	55:8:4:G:C8	2.56	0.40
3:2:54:ASP:HB3	37:k:57:LEU:HD22	2.04	0.40
4:3:1:MET:SD	4:3:36:ARG:HB3	2.62	0.40
6:B:310:G:H5''	21:Q:31:ARG:CG	2.51	0.40
9:E:28:ILE:HD12	9:E:34:ILE:HD11	2.03	0.40
26:V:57:ALA:HA	26:V:60:LEU:HD23	2.03	0.40
27:a:5:A:C2	27:a:2899:A:C2	3.09	0.40
27:a:323:C:H6	27:a:1205:A:C2	2.39	0.40
27:a:454:A:H4'	27:a:455:C:OP2	2.21	0.40
27:a:753:A:H2'	27:a:754:U:C6	2.56	0.40
27:a:1542:U:H2'	27:a:1543:G:O4'	2.21	0.40
27:a:1829:A:C8	27:a:1830:C:C5	3.09	0.40
27:a:2492:U:H2'	27:a:2493:U:C6	2.56	0.40
27:a:2545:G:H2'	27:a:2546:U:O4'	2.21	0.40
27:a:2615:U:O2	27:a:2615:U:H2'	2.21	0.40
27:a:2887:A:N3	52:z:27:SER:OG	2.46	0.40
34:h:41:LYS:HE2	34:h:41:LYS:HA	2.03	0.40
36:j:16:ALA:HB2	36:j:52:VAL:HG21	2.02	0.40
40:n:35:ILE:HG23	40:n:74:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:y:7:ILE:O	51:y:35:THR:HA	2.21	0.40
6:B:536:C:O2	6:B:536:C:H2'	2.21	0.40
6:B:751:U:H5''	20:P:17:ARG:HH12	1.86	0.40
6:B:1258:G:H2'	6:B:1259:C:C6	2.57	0.40
6:B:1397:C:H4'	6:B:1398:A:OP2	2.22	0.40
6:B:1504:G:H4'	6:B:1505:G:C4	2.56	0.40
9:E:13:ARG:HD2	9:E:33:LYS:O	2.21	0.40
9:E:28:ILE:HG23	9:E:34:ILE:HD11	2.04	0.40
16:L:118:HIS:O	16:L:119:ASN:HB2	2.21	0.40
22:R:59:VAL:HG12	22:R:78:VAL:HA	2.02	0.40
26:V:40:LYS:HD2	26:V:42:THR:HG22	2.03	0.40
27:a:167:A:H2'	27:a:168:G:O4'	2.21	0.40
27:a:248:G:O2'	27:a:2432:A:OP1	2.24	0.40
27:a:743:A:O2'	27:a:1659:G:OP1	2.35	0.40
27:a:756:A:H2'	27:a:757:G:O4'	2.22	0.40
27:a:1759:A:HO2'	27:a:2714:G:HO2'	1.56	0.40
27:a:2030:A:C2	27:a:2499:C:H5''	2.56	0.40
27:a:2205:A:H61	27:a:2219:U:H3	1.69	0.40
27:a:2760:C:O2'	27:a:2761:A:H5'	2.22	0.40
29:c:182:ARG:HG2	29:c:183:LYS:N	2.36	0.40
36:j:58:LEU:HA	36:j:89:ASN:ND2	2.36	0.40
40:n:17:LYS:O	40:n:20:GLU:HG2	2.20	0.40
43:q:37:GLU:HB3	43:q:53:PHE:CD1	2.56	0.40
54:Y:15:G:O2'	54:Y:20:U:O4	2.38	0.40
6:B:97:G:N9	6:B:98:A:H1'	2.37	0.40
6:B:215:C:O2'	6:B:216:U:O5'	2.39	0.40
6:B:260:G:H2'	6:B:261:U:C6	2.56	0.40
6:B:918:A:H2'	6:B:919:A:C8	2.57	0.40
6:B:1074:G:O2'	6:B:1101:A:N1	2.51	0.40
15:K:25:ILE:O	15:K:28:THR:HG22	2.21	0.40
20:P:76:ALA:O	20:P:80:GLN:HG3	2.22	0.40
22:R:11:ARG:HD3	22:R:56:GLY:HA2	2.04	0.40
25:U:44:LYS:C	25:U:44:LYS:HD3	2.46	0.40
27:a:207:A:H2'	27:a:208:C:O4'	2.21	0.40
27:a:465:G:H2'	27:a:466:A:C8	2.57	0.40
27:a:723:C:H2'	27:a:724:U:O4'	2.20	0.40
27:a:987:C:H2'	27:a:988:A:O4'	2.22	0.40
27:a:1964:G:H4'	27:a:1965:C:OP2	2.21	0.40
27:a:2790:U:H5'	27:a:2893:A:H62	1.86	0.40
27:a:2800:A:C2	27:a:2895:G:H1'	2.56	0.40
36:j:39:ILE:HG13	36:j:41:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:110:GLU:O	38:l:114:ARG:HG3	2.21	0.40
47:u:72:VAL:HG12	47:u:93:ARG:HA	2.04	0.40
55:8:85:A:H5''	55:8:85:A:H8	1.85	0.40
6:B:6:G:N3	6:B:6:G:H3'	2.37	0.40
6:B:146:G:C2'	6:B:147:G:H5'	2.51	0.40
6:B:173:U:O4'	6:B:197:A:C4	2.74	0.40
6:B:237:G:OP1	22:R:42:THR:HB	2.22	0.40
6:B:528:C:H5'	6:B:535:A:C6	2.57	0.40
6:B:945:G:C2	6:B:946:A:C8	3.09	0.40
24:T:27:ASP:OD1	24:T:27:ASP:N	2.55	0.40
27:a:123:G:O3'	27:a:1376:C:H4'	2.20	0.40
27:a:157:C:H2'	27:a:158:U:O4'	2.22	0.40
27:a:249:C:OP2	27:a:2394:C:O2'	2.37	0.40
27:a:301:G:H4'	27:a:301:G:OP1	2.21	0.40
27:a:490:C:H6	27:a:490:C:H5'	1.86	0.40
27:a:877:A:O5'	27:a:877:A:H8	2.05	0.40
27:a:1538:G:H4'	27:a:1538:G:OP1	2.22	0.40
27:a:1854:A:O4'	27:a:2233:U:H4'	2.21	0.40
27:a:2261:C:C6	48:v:16:SER:HB3	2.57	0.40
27:a:2625:G:H2'	27:a:2626:C:O4'	2.22	0.40
27:a:2774:C:H2'	27:a:2775:G:O4'	2.22	0.40
30:d:116:LYS:HD2	39:m:1:MET:HE3	2.03	0.40
31:e:149:ILE:HG22	31:e:192:ALA:HB1	2.03	0.40
33:g:157:TYR:CE1	33:g:172:LYS:HG3	2.57	0.40
43:q:40:MET:HA	43:q:48:LYS:O	2.20	0.40
45:s:72:GLN:O	45:s:72:GLN:HG3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
7	C	222/241 (92%)	212 (96%)	10 (4%)	0	100	100
8	D	204/233 (88%)	194 (95%)	9 (4%)	1 (0%)	24	55
9	E	203/206 (98%)	195 (96%)	7 (3%)	1 (0%)	24	55
10	F	154/167 (92%)	144 (94%)	9 (6%)	1 (1%)	21	51
11	G	101/135 (75%)	98 (97%)	2 (2%)	1 (1%)	12	38
12	H	151/179 (84%)	142 (94%)	8 (5%)	1 (1%)	18	47
13	I	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	16	44
14	J	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
15	K	96/103 (93%)	89 (93%)	6 (6%)	1 (1%)	12	38
16	L	115/129 (89%)	111 (96%)	3 (3%)	1 (1%)	14	41
17	M	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
18	N	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
19	O	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
20	P	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	Q	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
22	R	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
23	S	64/75 (85%)	64 (100%)	0	0	100	100
24	T	82/92 (89%)	80 (98%)	2 (2%)	0	100	100
25	U	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	V	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
29	c	269/273 (98%)	253 (94%)	16 (6%)	0	100	100
30	d	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
31	e	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	24	55
32	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
33	g	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	21	51
34	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
35	i	140/142 (99%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	j	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
37	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
38	l	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
39	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
40	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
41	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
42	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
43	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
44	r	108/110 (98%)	106 (98%)	1 (1%)	1 (1%)	14	41
45	s	91/100 (91%)	85 (93%)	5 (6%)	1 (1%)	11	36
46	t	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
47	u	92/94 (98%)	87 (95%)	4 (4%)	1 (1%)	11	36
48	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
49	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
50	x	60/63 (95%)	58 (97%)	1 (2%)	1 (2%)	7	25
51	y	56/59 (95%)	56 (100%)	0	0	100	100
52	z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
56	A	17/19 (90%)	17 (100%)	0	0	100	100
All	All	5503/5932 (93%)	5279 (96%)	210 (4%)	14 (0%)	37	66

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	109	GLY
11	G	33	GLU
44	r	12	SER
15	K	57	VAL
47	u	67	GLY
9	E	155	VAL
12	H	9	GLN
13	I	108	LYS
16	L	121	CYS
33	g	167	GLU
45	s	27	SER
50	x	37	LEU
8	D	17	PRO

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Mol	Chain	Res	Type
31	e	4	VAL

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	
1	0	46/49 (94%)	45 (98%)	1 (2%)	45	78
2	1	38/38 (100%)	36 (95%)	2 (5%)	20	52
3	2	51/52 (98%)	50 (98%)	1 (2%)	48	80
4	3	34/34 (100%)	32 (94%)	2 (6%)	18	48
5	4	55/62 (89%)	52 (94%)	3 (6%)	19	51
7	C	186/199 (94%)	181 (97%)	5 (3%)	39	74
8	D	170/190 (90%)	159 (94%)	11 (6%)	15	43
9	E	172/173 (99%)	159 (92%)	13 (8%)	12	36
10	F	119/126 (94%)	117 (98%)	2 (2%)	53	83
11	G	90/116 (78%)	84 (93%)	6 (7%)	15	42
12	H	126/147 (86%)	122 (97%)	4 (3%)	34	70
13	I	104/105 (99%)	102 (98%)	2 (2%)	50	81
14	J	105/107 (98%)	103 (98%)	2 (2%)	50	81
15	K	86/90 (96%)	81 (94%)	5 (6%)	18	49
16	L	90/99 (91%)	87 (97%)	3 (3%)	33	69
17	M	103/104 (99%)	96 (93%)	7 (7%)	14	42
18	N	93/96 (97%)	87 (94%)	6 (6%)	15	43
19	O	83/84 (99%)	82 (99%)	1 (1%)	63	87
20	P	76/77 (99%)	75 (99%)	1 (1%)	61	86
21	Q	65/65 (100%)	62 (95%)	3 (5%)	24	58
22	R	73/78 (94%)	69 (94%)	4 (6%)	19	51
23	S	57/65 (88%)	54 (95%)	3 (5%)	20	52
24	T	72/79 (91%)	71 (99%)	1 (1%)	59	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	U	65/66 (98%)	64 (98%)	1 (2%)	57	84
26	V	60/61 (98%)	55 (92%)	5 (8%)	10	32
29	c	216/218 (99%)	213 (99%)	3 (1%)	59	85
30	d	163/163 (100%)	159 (98%)	4 (2%)	42	76
31	e	165/165 (100%)	160 (97%)	5 (3%)	36	72
32	f	148/150 (99%)	144 (97%)	4 (3%)	39	74
33	g	137/138 (99%)	132 (96%)	5 (4%)	31	66
34	h	32/114 (28%)	29 (91%)	3 (9%)	8	27
35	i	116/116 (100%)	111 (96%)	5 (4%)	26	60
36	j	104/104 (100%)	102 (98%)	2 (2%)	50	81
37	k	103/103 (100%)	99 (96%)	4 (4%)	28	64
38	l	109/109 (100%)	107 (98%)	2 (2%)	51	82
39	m	98/103 (95%)	96 (98%)	2 (2%)	48	80
40	n	86/87 (99%)	85 (99%)	1 (1%)	63	87
41	o	99/100 (99%)	96 (97%)	3 (3%)	36	72
42	p	89/90 (99%)	86 (97%)	3 (3%)	32	68
43	q	84/84 (100%)	81 (96%)	3 (4%)	31	66
44	r	93/93 (100%)	90 (97%)	3 (3%)	34	70
45	s	80/84 (95%)	79 (99%)	1 (1%)	61	86
46	t	83/85 (98%)	82 (99%)	1 (1%)	63	87
47	u	78/78 (100%)	72 (92%)	6 (8%)	12	36
48	v	58/63 (92%)	57 (98%)	1 (2%)	53	83
49	w	67/68 (98%)	65 (97%)	2 (3%)	36	72
50	x	54/55 (98%)	53 (98%)	1 (2%)	50	81
51	y	48/49 (98%)	46 (96%)	2 (4%)	26	61
52	z	47/48 (98%)	45 (96%)	2 (4%)	26	60
56	A	18/18 (100%)	17 (94%)	1 (6%)	19	50
All	All	4594/4847 (95%)	4431 (96%)	163 (4%)	32	67

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	54	ILE

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Mol	Chain	Res	Type
2	1	1	MET
2	1	42	LEU
3	2	7	VAL
4	3	2	LYS
4	3	36	ARG
5	4	22	MET
5	4	33	ASN
5	4	34	LEU
7	C	6	MET
7	C	8	ASP
7	C	80	VAL
7	C	127	ASP
7	C	184	PHE
8	D	46	GLU
8	D	62	LYS
8	D	70	THR
8	D	80	LYS
8	D	84	VAL
8	D	86	LYS
8	D	132	ARG
8	D	144	LEU
8	D	178	LEU
8	D	195	VAL
8	D	201	TRP
9	E	8	LYS
9	E	10	LYS
9	E	28	ILE
9	E	57	GLU
9	E	60	LYS
9	E	68	LEU
9	E	82	LEU
9	E	117	LEU
9	E	124	MET
9	E	171	LEU
9	E	177	LYS
9	E	183	LYS
9	E	188	ARG
10	F	26	LYS
10	F	116	GLU
11	G	17	GLN
11	G	21	MET
11	G	74	LEU

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Mol	Chain	Res	Type
11	G	90	MET
11	G	91	ARG
11	G	102	MET
12	H	5	ARG
12	H	15	ASP
12	H	25	LYS
12	H	67	GLU
13	I	56	LYS
13	I	89	LYS
14	J	58	VAL
14	J	85	ARG
15	K	17	LEU
15	K	18	ILE
15	K	28	THR
15	K	30	LYS
15	K	35	GLN
16	L	16	VAL
16	L	72	ASP
16	L	79	ILE
17	M	15	LYS
17	M	50	ARG
17	M	54	ARG
17	M	62	GLU
17	M	74	LEU
17	M	114	ARG
17	M	121	ARG
18	N	16	VAL
18	N	27	LYS
18	N	54	ASP
18	N	58	ASP
18	N	68	ASP
18	N	83	LEU
19	O	47	LYS
20	P	54	ARG
21	Q	19	VAL
21	Q	23	ASP
21	Q	80	LYS
22	R	27	ARG
22	R	62	ARG
22	R	67	LEU
22	R	78	VAL
23	S	16	GLU

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Mol	Chain	Res	Type
23	S	18	VAL
23	S	19	GLN
24	T	27	ASP
25	U	27	MET
26	V	2	PRO
26	V	3	VAL
26	V	39	GLU
26	V	63	GLU
26	V	67	ARG
29	c	4	VAL
29	c	132	MET
29	c	147	LYS
30	d	1	MET
30	d	30	GLU
30	d	52	THR
30	d	100	LEU
31	e	4	VAL
31	e	143	LEU
31	e	150	THR
31	e	176	ASP
31	e	191	ASP
32	f	50	LEU
32	f	51	ASP
32	f	120	LYS
32	f	130	MET
33	g	29	LYS
33	g	48	ASN
33	g	52	PHE
33	g	141	ILE
33	g	155	GLU
34	h	9	VAL
34	h	12	LEU
34	h	17	ASP
35	i	1	MET
35	i	4	PHE
35	i	39	LYS
35	i	64	VAL
35	i	131	ASN
36	j	58	LEU
36	j	107	LEU
37	k	70	LYS
37	k	112	LEU

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Mol	Chain	Res	Type
37	k	116	VAL
37	k	129	LYS
38	l	82	MET
38	l	135	VAL
39	m	51	LEU
39	m	96	ARG
40	n	49	VAL
41	o	53	ARG
41	o	68	GLU
41	o	115	ASN
42	p	11	ARG
42	p	71	GLN
42	p	112	LYS
43	q	1	MET
43	q	34	GLU
43	q	40	MET
44	r	66	ILE
44	r	67	ASP
44	r	109	ASP
45	s	1	MET
46	t	52	LEU
47	u	20	LEU
47	u	55	GLU
47	u	61	LEU
47	u	62	THR
47	u	65	VAL
47	u	77	VAL
48	v	85	GLU
49	w	17	ASN
49	w	40	VAL
50	x	14	LEU
51	y	24	LEU
51	y	54	MET
52	z	12	LYS
52	z	32	LYS
56	A	19	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
7	C	18	HIS
7	C	51	ASN

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Mol	Chain	Res	Type
8	D	25	ASN
9	E	131	ASN
11	G	68	GLN
11	G	94	HIS
12	H	97	ASN
13	I	21	ASN
14	J	32	GLN
14	J	75	GLN
16	L	15	GLN
16	L	38	GLN
16	L	119	ASN
19	O	60	GLN
20	P	50	HIS
29	c	46	ASN
30	d	140	HIS
31	e	90	GLN
32	f	5	HIS
33	g	73	ASN
33	g	139	GLN
35	i	86	GLN
35	i	136	GLN
36	j	5	GLN
38	l	60	GLN
39	m	18	GLN
41	o	3	ASN
41	o	41	GLN
41	o	66	ASN
41	o	75	GLN
41	o	115	ASN
42	p	81	ASN
43	q	86	GLN
44	r	61	ASN
50	x	31	GLN
50	x	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	a	2748/2903 (94%)	388 (14%)	0
28	b	118/120 (98%)	21 (17%)	0
53	X	11/12 (91%)	4 (36%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	Y	75/76 (98%)	14 (18%)	4 (5%)
55	8	73/85 (85%)	18 (24%)	2 (2%)
6	B	1516/1534 (98%)	252 (16%)	38 (2%)
All	All	4541/4730 (96%)	697 (15%)	44 (0%)

All (697) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B	4	U
6	B	5	U
6	B	6	G
6	B	8	A
6	B	9	G
6	B	23	C
6	B	31	G
6	B	39	G
6	B	47	C
6	B	48	C
6	B	51	A
6	B	54	C
6	B	58	C
6	B	64	G
6	B	65	A
6	B	66	A
6	B	70	U
6	B	72	A
6	B	75	G
6	B	83	C
6	B	85	U
6	B	86	G
6	B	87	C
6	B	93	U
6	B	94	G
6	B	95	C
6	B	96	U
6	B	98	A
6	B	99	C
6	B	102	G
6	B	116	A
6	B	119	A
6	B	120	A
6	B	121	U

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Mol	Chain	Res	Type
6	B	122	G
6	B	131	A
6	B	144	G
6	B	174	A
6	B	182	A
6	B	197	A
6	B	198	G
6	B	199	A
6	B	200	G
6	B	202	G
6	B	204	G
6	B	215	C
6	B	216	U
6	B	226	G
6	B	240	G
6	B	245	U
6	B	247	G
6	B	251	G
6	B	266	G
6	B	267	C
6	B	289	G
6	B	315	A
6	B	316	C
6	B	328	C
6	B	329	A
6	B	330	C
6	B	351	G
6	B	352	C
6	B	354	G
6	B	367	U
6	B	369	G
6	B	372	C
6	B	373	A
6	B	382	A
6	B	384	G
6	B	397	A
6	B	398	U
6	B	406	G
6	B	411	A
6	B	412	A
6	B	413	G
6	B	414	A

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Mol	Chain	Res	Type
6	B	421	U
6	B	422	C
6	B	423	G
6	B	429	U
6	B	435	A
6	B	439	U
6	B	446	G
6	B	447	G
6	B	451	A
6	B	453	G
6	B	454	G
6	B	456	A
6	B	457	G
6	B	462	G
6	B	463	U
6	B	467	U
6	B	468	A
6	B	469	C
6	B	479	U
6	B	484	G
6	B	486	U
6	B	491	G
6	B	495	A
6	B	496	A
6	B	497	G
6	B	499	A
6	B	500	G
6	B	505	G
6	B	511	C
6	B	518	C
6	B	521	G
6	B	524	G
6	B	531	U
6	B	532	A
6	B	536	C
6	B	547	A
6	B	562	U
6	B	564	C
6	B	572	A
6	B	573	A
6	B	574	A
6	B	576	C

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Mol	Chain	Res	Type
6	B	577	G
6	B	596	A
6	B	617	G
6	B	619	U
6	B	620	C
6	B	633	G
6	B	650	G
6	B	653	U
6	B	665	A
6	B	687	A
6	B	688	G
6	B	695	A
6	B	703	G
6	B	721	G
6	B	722	G
6	B	723	U
6	B	724	G
6	B	734	G
6	B	748	G
6	B	755	G
6	B	777	A
6	B	782	A
6	B	793	U
6	B	794	A
6	B	815	A
6	B	817	C
6	B	832	G
6	B	849	G
6	B	851	G
6	B	885	G
6	B	890	G
6	B	902	G
6	B	914	A
6	B	926	G
6	B	934	C
6	B	935	A
6	B	960	U
6	B	963	G
6	B	966	2MG
6	B	969	A
6	B	975	A
6	B	976	G

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Mol	Chain	Res	Type
6	B	977	A
6	B	993	G
6	B	996	A
6	B	1003	G
6	B	1004	A
6	B	1005	A
6	B	1006	G
6	B	1007	U
6	B	1008	U
6	B	1024	G
6	B	1025	U
6	B	1026	G
6	B	1030	U
6	B	1031	C
6	B	1032	G
6	B	1033	G
6	B	1034	G
6	B	1036	A
6	B	1039	G
6	B	1040	U
6	B	1042	A
6	B	1044	A
6	B	1065	U
6	B	1085	U
6	B	1094	G
6	B	1095	U
6	B	1101	A
6	B	1124	G
6	B	1125	U
6	B	1129	C
6	B	1132	C
6	B	1137	C
6	B	1139	G
6	B	1140	C
6	B	1159	U
6	B	1160	G
6	B	1182	G
6	B	1184	G
6	B	1193	G
6	B	1196	A
6	B	1197	A
6	B	1202	U

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Mol	Chain	Res	Type
6	B	1213	A
6	B	1214	C
6	B	1215	G
6	B	1226	C
6	B	1227	A
6	B	1238	A
6	B	1248	A
6	B	1256	A
6	B	1257	A
6	B	1258	G
6	B	1260	G
6	B	1275	A
6	B	1280	A
6	B	1287	A
6	B	1300	G
6	B	1302	C
6	B	1312	G
6	B	1317	C
6	B	1319	A
6	B	1320	C
6	B	1336	C
6	B	1337	G
6	B	1338	G
6	B	1346	A
6	B	1353	G
6	B	1363	A
6	B	1364	U
6	B	1370	G
6	B	1378	C
6	B	1379	G
6	B	1381	U
6	B	1397	C
6	B	1398	A
6	B	1419	G
6	B	1432	G
6	B	1441	A
6	B	1442	G
6	B	1446	A
6	B	1451	U
6	B	1452	C
6	B	1453	G
6	B	1492	A

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Mol	Chain	Res	Type
6	B	1497	G
6	B	1506	U
6	B	1517	G
6	B	1519	MA6
6	B	1520	C
6	B	1529	G
6	B	1530	G
6	B	1534	A
27	a	10	A
27	a	27	G
27	a	34	U
27	a	42	A
27	a	61	C
27	a	71	A
27	a	74	A
27	a	75	G
27	a	91	A
27	a	101	A
27	a	102	U
27	a	119	A
27	a	120	U
27	a	125	A
27	a	126	A
27	a	135	U
27	a	136	G
27	a	139	U
27	a	140	C
27	a	142	A
27	a	163	C
27	a	181	A
27	a	196	A
27	a	199	A
27	a	200	U
27	a	215	G
27	a	216	A
27	a	221	A
27	a	222	A
27	a	223	A
27	a	228	C
27	a	229	C
27	a	233	A
27	a	248	G

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Mol	Chain	Res	Type
27	a	272	A
27	a	276	U
27	a	279	A
27	a	281	C
27	a	282	A
27	a	285	G
27	a	289	G
27	a	291	G
27	a	311	A
27	a	329	G
27	a	330	A
27	a	332	A
27	a	361	G
27	a	362	A
27	a	363	G
27	a	367	G
27	a	386	G
27	a	396	G
27	a	404	A
27	a	405	U
27	a	406	G
27	a	411	G
27	a	412	A
27	a	480	A
27	a	481	G
27	a	490	C
27	a	491	G
27	a	504	A
27	a	505	A
27	a	509	C
27	a	513	A
27	a	530	G
27	a	531	C
27	a	532	A
27	a	545	U
27	a	546	U
27	a	547	A
27	a	548	G
27	a	549	G
27	a	555	G
27	a	556	A
27	a	563	A

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Mol	Chain	Res	Type
27	a	568	U
27	a	573	U
27	a	575	A
27	a	586	A
27	a	588	U
27	a	603	A
27	a	613	A
27	a	614	A
27	a	615	U
27	a	616	A
27	a	620	G
27	a	621	A
27	a	627	A
27	a	637	A
27	a	645	C
27	a	651	G
27	a	654	A
27	a	655	A
27	a	656	G
27	a	686	U
27	a	717	C
27	a	730	A
27	a	738	G
27	a	747	5MU
27	a	764	A
27	a	765	C
27	a	775	G
27	a	776	G
27	a	782	A
27	a	784	G
27	a	785	G
27	a	792	A
27	a	805	G
27	a	812	C
27	a	827	U
27	a	828	U
27	a	845	A
27	a	846	U
27	a	847	U
27	a	856	G
27	a	858	G
27	a	859	G

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Mol	Chain	Res	Type
27	a	866	A
27	a	869	G
27	a	879	G
27	a	881	G
27	a	883	G
27	a	884	U
27	a	890	C
27	a	891	G
27	a	894	U
27	a	895	U
27	a	896	A
27	a	897	C
27	a	910	A
27	a	915	C
27	a	931	U
27	a	941	A
27	a	946	C
27	a	961	C
27	a	962	G
27	a	974	G
27	a	983	A
27	a	996	A
27	a	999	U
27	a	1005	C
27	a	1012	U
27	a	1013	C
27	a	1022	G
27	a	1025	G
27	a	1026	G
27	a	1033	U
27	a	1047	G
27	a	1048	A
27	a	1108	U
27	a	1109	C
27	a	1110	G
27	a	1111	A
27	a	1112	G
27	a	1115	G
27	a	1116	G
27	a	1130	U
27	a	1132	U
27	a	1133	A

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Mol	Chain	Res	Type
27	a	1134	A
27	a	1135	C
27	a	1136	G
27	a	1141	U
27	a	1142	A
27	a	1143	A
27	a	1169	A
27	a	1171	G
27	a	1187	G
27	a	1188	U
27	a	1205	A
27	a	1250	G
27	a	1253	A
27	a	1256	G
27	a	1271	G
27	a	1272	A
27	a	1276	A
27	a	1300	G
27	a	1301	A
27	a	1302	A
27	a	1321	A
27	a	1329	U
27	a	1345	C
27	a	1352	U
27	a	1359	A
27	a	1365	A
27	a	1376	C
27	a	1378	A
27	a	1379	U
27	a	1383	A
27	a	1395	A
27	a	1416	G
27	a	1420	A
27	a	1427	A
27	a	1428	C
27	a	1452	G
27	a	1460	U
27	a	1482	G
27	a	1490	A
27	a	1497	U
27	a	1498	C
27	a	1508	A

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Mol	Chain	Res	Type
27	a	1515	A
27	a	1529	G
27	a	1530	G
27	a	1534	U
27	a	1535	A
27	a	1536	C
27	a	1537	G
27	a	1538	G
27	a	1553	A
27	a	1554	U
27	a	1558	C
27	a	1560	G
27	a	1566	A
27	a	1569	A
27	a	1578	U
27	a	1583	A
27	a	1585	C
27	a	1587	G
27	a	1608	A
27	a	1610	A
27	a	1618	6MZ
27	a	1634	A
27	a	1635	A
27	a	1647	U
27	a	1648	U
27	a	1663	G
27	a	1674	G
27	a	1675	C
27	a	1696	G
27	a	1700	A
27	a	1701	A
27	a	1713	A
27	a	1715	G
27	a	1716	U
27	a	1729	U
27	a	1730	C
27	a	1732	C
27	a	1733	G
27	a	1738	G
27	a	1739	A
27	a	1758	U
27	a	1764	C

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Mol	Chain	Res	Type
27	a	1773	A
27	a	1791	A
27	a	1800	C
27	a	1801	A
27	a	1802	A
27	a	1808	A
27	a	1811	G
27	a	1816	C
27	a	1829	A
27	a	1847	A
27	a	1848	A
27	a	1858	A
27	a	1871	A
27	a	1872	A
27	a	1873	G
27	a	1874	C
27	a	1906	G
27	a	1907	G
27	a	1913	A
27	a	1929	G
27	a	1930	G
27	a	1936	A
27	a	1937	A
27	a	1938	A
27	a	1939	5MU
27	a	1955	U
27	a	1967	C
27	a	1970	A
27	a	1971	U
27	a	1972	G
27	a	1991	U
27	a	1993	U
27	a	1996	C
27	a	2020	A
27	a	2022	U
27	a	2023	C
27	a	2029	G
27	a	2030	A
27	a	2031	A
27	a	2033	A
27	a	2043	C
27	a	2055	C

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Mol	Chain	Res	Type
27	a	2056	G
27	a	2060	A
27	a	2061	G
27	a	2062	A
27	a	2069	G7M
27	a	2192	U
27	a	2193	G
27	a	2198	A
27	a	2203	U
27	a	2204	G
27	a	2211	A
27	a	2223	G
27	a	2225	A
27	a	2238	G
27	a	2239	G
27	a	2268	A
27	a	2278	A
27	a	2282	G
27	a	2283	C
27	a	2287	A
27	a	2305	U
27	a	2308	G
27	a	2311	A
27	a	2322	A
27	a	2325	G
27	a	2333	A
27	a	2335	A
27	a	2336	A
27	a	2347	C
27	a	2350	C
27	a	2361	G
27	a	2383	G
27	a	2385	C
27	a	2390	U
27	a	2396	G
27	a	2402	U
27	a	2403	C
27	a	2406	A
27	a	2424	C
27	a	2425	A
27	a	2429	G
27	a	2430	A

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Mol	Chain	Res	Type
27	a	2435	A
27	a	2441	U
27	a	2448	A
27	a	2459	A
27	a	2469	A
27	a	2470	G
27	a	2476	A
27	a	2478	A
27	a	2498	OMC
27	a	2502	G
27	a	2505	G
27	a	2506	U
27	a	2518	A
27	a	2520	C
27	a	2529	G
27	a	2547	A
27	a	2566	A
27	a	2567	G
27	a	2572	A
27	a	2599	G
27	a	2602	A
27	a	2603	G
27	a	2610	C
27	a	2613	U
27	a	2615	U
27	a	2629	U
27	a	2630	G
27	a	2632	A
27	a	2639	A
27	a	2656	U
27	a	2661	G
27	a	2662	A
27	a	2663	G
27	a	2682	A
27	a	2689	U
27	a	2690	U
27	a	2714	G
27	a	2716	C
27	a	2726	A
27	a	2733	A
27	a	2744	G
27	a	2748	A

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Mol	Chain	Res	Type
27	a	2757	A
27	a	2765	A
27	a	2778	A
27	a	2779	U
27	a	2798	U
27	a	2809	A
27	a	2820	A
27	a	2821	A
27	a	2835	A
27	a	2836	U
27	a	2873	A
27	a	2874	C
27	a	2880	C
27	a	2883	A
27	a	2884	U
27	a	2885	G
27	a	2886	A
27	a	2903	U
28	b	9	G
28	b	21	G
28	b	22	U
28	b	25	U
28	b	33	G
28	b	34	A
28	b	35	C
28	b	36	C
28	b	44	G
28	b	45	A
28	b	51	G
28	b	56	G
28	b	57	A
28	b	67	G
28	b	87	U
28	b	89	U
28	b	90	C
28	b	99	A
28	b	105	G
28	b	108	A
28	b	109	A
53	X	12	U
53	X	19	A
53	X	20	U

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Mol	Chain	Res	Type
53	X	21	A
54	Y	7	G
54	Y	9	G
54	Y	17	C
54	Y	17(A)	U
54	Y	18	G
54	Y	20	U
54	Y	21	A
54	Y	22	G
54	Y	23	C
54	Y	46	G
54	Y	47	U
54	Y	48	C
54	Y	55	PSU
54	Y	76	A
55	8	6	A
55	8	7	G
55	8	9	G
55	8	10	G
55	8	14	A
55	8	16	U
55	8	18	G
55	8	20	U
55	8	22	G
55	8	23	A
55	8	24	C
55	8	35	C
55	8	37	A
55	8	43	A
55	8	46	G
55	8	58	G
55	8	83	C
55	8	85	A

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	B	7	A
6	B	21	G
6	B	95	C
6	B	98	A
6	B	119	A

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Mol	Chain	Res	Type
6	B	198	G
6	B	315	A
6	B	351	G
6	B	384	G
6	B	446	G
6	B	453	G
6	B	462	G
6	B	468	A
6	B	491	G
6	B	496	A
6	B	499	A
6	B	573	A
6	B	575	G
6	B	619	U
6	B	686	U
6	B	722	G
6	B	1005	A
6	B	1006	G
6	B	1024	G
6	B	1035	A
6	B	1039	G
6	B	1094	G
6	B	1129	C
6	B	1145	A
6	B	1181	G
6	B	1214	C
6	B	1225	A
6	B	1239	A
6	B	1319	A
6	B	1337	G
6	B	1397	C
6	B	1441	A
6	B	1505	G
54	Y	16	C
54	Y	17	C
54	Y	22	G
54	Y	47	U
55	8	6	A
55	8	23	A

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

38 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$
27	OMG	a	2251	58,27,54	23,26,27	2.44	7 (30%)	33,38,41	2.24	10 (30%)
27	5MU	a	1939	27	19,22,23	7.52	7 (36%)	28,32,35	3.12	9 (32%)
6	4OC	B	1402	6	20,23,24	2.96	8 (40%)	26,32,35	1.02	2 (7%)
6	PSU	B	516	6	18,21,22	1.09	2 (11%)	22,30,33	1.77	4 (18%)
27	6MZ	a	1618	27	22,25,26	3.50	5 (22%)	30,36,39	2.45	12 (40%)
27	PSU	a	2605	27	18,21,22	1.07	2 (11%)	22,30,33	1.83	4 (18%)
6	MA6	B	1519	6	23,26,27	1.46	3 (13%)	34,38,41	2.96	12 (35%)
27	OMC	a	2498	58,27	19,22,23	2.79	8 (42%)	26,31,34	0.76	0
27	PSU	a	2604	27	18,21,22	1.11	2 (11%)	22,30,33	1.96	4 (18%)
54	PSU	Y	55	54	18,21,22	1.17	2 (11%)	22,30,33	1.63	3 (13%)
6	5MC	B	967	6	18,22,23	3.60	7 (38%)	26,32,35	0.95	1 (3%)
6	UR3	B	1498	6	19,22,23	2.88	8 (42%)	26,32,35	1.46	2 (7%)
27	PSU	a	2504	27	18,21,22	1.14	2 (11%)	22,30,33	1.79	3 (13%)
6	5MC	B	1407	6	18,22,23	3.56	7 (38%)	26,32,35	1.03	3 (11%)
6	2MG	B	1207	6	23,26,27	2.82	8 (34%)	32,38,41	2.18	10 (31%)
6	2MG	B	1516	6	23,26,27	2.78	7 (30%)	32,38,41	2.30	12 (37%)
27	H2U	a	2449	27	18,21,22	3.25	6 (33%)	21,30,33	2.23	5 (23%)
27	OMU	a	2552	27	19,22,23	2.92	8 (42%)	26,31,34	1.80	5 (19%)
27	PSU	a	1911	27	18,21,22	1.09	2 (11%)	22,30,33	1.75	3 (13%)
27	5MU	a	747	27	19,22,23	7.49	7 (36%)	28,32,35	3.17	10 (35%)
54	5MU	Y	54	54	19,22,23	7.47	7 (36%)	28,32,35	3.05	9 (32%)
54	4SU	Y	8	54	18,21,22	3.54	8 (44%)	26,30,33	2.06	4 (15%)
54	5MC	Y	32	54	18,22,23	3.59	7 (38%)	26,32,35	0.97	1 (3%)
27	PSU	a	2580	27	18,21,22	1.23	2 (11%)	22,30,33	2.00	6 (27%)
27	PSU	a	955	27	18,21,22	1.05	1 (5%)	22,30,33	1.86	3 (13%)
27	PSU	a	746	58,27	18,21,22	1.14	2 (11%)	22,30,33	1.71	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	2MG	a	2445	27	23,26,27	2.77	8 (34%)	32,38,41	2.26	11 (34%)
6	MA6	B	1518	6	23,26,27	1.50	4 (17%)	34,38,41	2.82	10 (29%)
6	G7M	B	527	6	23,26,27	2.51	9 (39%)	35,39,42	1.92	11 (31%)
27	2MG	a	1835	27	23,26,27	2.73	8 (34%)	32,38,41	2.14	9 (28%)
27	2MA	a	2503	58,27	22,25,26	4.02	9 (40%)	33,37,40	2.25	9 (27%)
30	MEQ	d	150	30	8,9,10	0.93	0	5,10,12	1.28	1 (20%)
6	2MG	B	966	6	23,26,27	2.85	8 (34%)	32,38,41	2.26	9 (28%)
27	PSU	a	2457	27	18,21,22	1.17	1 (5%)	22,30,33	1.81	4 (18%)
27	5MC	a	1962	27	18,22,23	3.59	7 (38%)	26,32,35	1.12	3 (11%)
27	1MG	a	745	27	22,26,27	2.77	7 (31%)	33,39,42	2.11	9 (27%)
27	G7M	a	2069	27	23,26,27	2.44	9 (39%)	35,39,42	1.92	11 (31%)
27	PSU	a	1917	27	18,21,22	1.16	2 (11%)	22,30,33	1.84	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMG	a	2251	58,27,54	-	1/9/27/28	0/3/3/3
27	5MU	a	1939	27	-	0/7/25/26	0/2/2/2
6	4OC	B	1402	6	-	0/9/29/30	0/2/2/2
6	PSU	B	516	6	-	0/7/25/26	0/2/2/2
27	6MZ	a	1618	27	-	3/9/27/28	0/3/3/3
27	PSU	a	2605	27	-	0/7/25/26	0/2/2/2
6	MA6	B	1519	6	-	0/11/29/30	0/3/3/3
27	OMC	a	2498	58,27	-	0/9/27/28	0/2/2/2
27	PSU	a	2604	27	-	0/7/25/26	0/2/2/2
54	PSU	Y	55	54	-	2/7/25/26	0/2/2/2
6	5MC	B	967	6	-	0/7/25/26	0/2/2/2
6	UR3	B	1498	6	-	0/7/25/26	0/2/2/2
27	PSU	a	2504	27	-	0/7/25/26	0/2/2/2
6	5MC	B	1407	6	-	0/7/25/26	0/2/2/2
6	2MG	B	1207	6	-	0/9/27/28	0/3/3/3
6	2MG	B	1516	6	-	0/9/27/28	0/3/3/3
27	H2U	a	2449	27	-	0/7/38/39	0/2/2/2
27	OMU	a	2552	27	-	0/9/27/28	0/2/2/2
27	PSU	a	1911	27	-	0/7/25/26	0/2/2/2
27	5MU	a	747	27	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MU	Y	54	54	-	2/7/25/26	0/2/2/2
54	4SU	Y	8	54	-	0/7/25/26	0/2/2/2
54	5MC	Y	32	54	-	0/7/25/26	0/2/2/2
27	PSU	a	2580	27	-	0/7/25/26	0/2/2/2
27	PSU	a	955	27	-	0/7/25/26	0/2/2/2
27	PSU	a	746	58,27	-	3/7/25/26	0/2/2/2
27	2MG	a	2445	27	-	0/9/27/28	0/3/3/3
6	MA6	B	1518	6	-	0/11/29/30	0/3/3/3
6	G7M	B	527	6	-	1/7/25/26	0/3/3/3
27	2MG	a	1835	27	-	0/9/27/28	0/3/3/3
27	2MA	a	2503	58,27	-	2/7/25/26	0/3/3/3
30	MEQ	d	150	30	-	2/8/9/11	-
6	2MG	B	966	6	-	2/9/27/28	0/3/3/3
27	PSU	a	2457	27	-	0/7/25/26	0/2/2/2
27	5MC	a	1962	27	-	4/7/25/26	0/2/2/2
27	1MG	a	745	27	-	0/7/25/26	0/3/3/3
27	G7M	a	2069	27	-	1/7/25/26	0/3/3/3
27	PSU	a	1917	27	-	0/7/25/26	0/2/2/2

All (207) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	747	5MU	C4-C5	21.48	1.80	1.44
27	a	1939	5MU	C4-C5	21.40	1.80	1.44
54	Y	54	5MU	C4-C5	21.18	1.79	1.44
54	Y	54	5MU	C6-N1	16.00	1.65	1.38
27	a	1939	5MU	C6-N1	15.68	1.64	1.38
27	a	747	5MU	C6-N1	15.54	1.64	1.38
27	a	1618	6MZ	C6-N6	15.01	1.50	1.34
27	a	2503	2MA	C4-N3	13.17	1.51	1.34
27	a	747	5MU	C6-C5	-12.75	1.13	1.34
27	a	1939	5MU	C6-C5	-12.66	1.13	1.34
54	Y	54	5MU	C6-C5	-12.54	1.14	1.34
27	a	1939	5MU	C4-N3	-11.94	1.16	1.38
27	a	747	5MU	C4-N3	-11.87	1.16	1.38
54	Y	54	5MU	C4-N3	-11.67	1.17	1.38
27	a	2449	H2U	C2-N1	9.83	1.49	1.35
6	B	1407	5MC	C6-C5	9.24	1.49	1.34
27	a	1962	5MC	C6-C5	9.14	1.49	1.34
6	B	967	5MC	C6-C5	9.06	1.49	1.34
54	Y	32	5MC	C6-C5	9.04	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	966	2MG	C2-N3	7.83	1.46	1.31
6	B	1498	UR3	C2-N1	7.76	1.49	1.38
6	B	1207	2MG	C2-N3	7.54	1.46	1.31
6	B	1516	2MG	C2-N3	7.45	1.46	1.31
27	a	2445	2MG	C2-N3	7.34	1.46	1.31
54	Y	8	4SU	C4-N3	7.21	1.45	1.37
54	Y	32	5MC	C4-N3	7.19	1.46	1.34
27	a	1835	2MG	C2-N3	7.06	1.45	1.31
6	B	967	5MC	C4-N3	7.03	1.46	1.34
27	a	1962	5MC	C4-N3	6.85	1.45	1.34
27	a	2251	OMG	C4-N3	6.82	1.50	1.34
27	a	745	1MG	C2-N3	6.67	1.46	1.34
6	B	1407	5MC	C4-N3	6.65	1.45	1.34
27	a	2503	2MA	C2-N1	6.63	1.45	1.34
27	a	2503	2MA	C2-N3	6.63	1.45	1.34
27	a	2552	OMU	C2-N1	6.59	1.49	1.38
6	B	1402	4OC	C4-N3	6.57	1.44	1.32
54	Y	8	4SU	C2-N3	6.53	1.49	1.38
54	Y	8	4SU	C2-N1	6.50	1.48	1.38
6	B	966	2MG	C4-N3	6.41	1.49	1.34
27	a	2552	OMU	C2-N3	6.34	1.49	1.38
27	a	2449	H2U	C2-N3	6.29	1.49	1.38
6	B	1516	2MG	C4-N3	6.28	1.49	1.34
6	B	1207	2MG	C4-N3	6.26	1.49	1.34
27	a	1939	5MU	O2-C2	-6.23	1.11	1.23
27	a	1835	2MG	C4-N3	6.12	1.48	1.34
27	a	2069	G7M	C4-N3	6.06	1.48	1.34
6	B	1402	4OC	C6-C5	6.05	1.49	1.35
6	B	527	G7M	C4-N3	6.03	1.48	1.34
27	a	747	5MU	O2-C2	-5.97	1.12	1.23
27	a	2445	2MG	C4-N3	5.93	1.48	1.34
27	a	2498	OMC	C2-N3	5.91	1.48	1.36
27	a	2251	OMG	C2-N3	5.87	1.47	1.33
6	B	1498	UR3	C6-C5	5.77	1.48	1.35
27	a	2498	OMC	C6-C5	5.74	1.48	1.35
27	a	745	1MG	C4-N3	5.70	1.47	1.34
54	Y	54	5MU	O2-C2	-5.58	1.12	1.23
6	B	967	5MC	C2-N3	5.57	1.47	1.36
27	a	2552	OMU	C6-C5	5.57	1.48	1.35
54	Y	8	4SU	C6-C5	5.55	1.48	1.35
27	a	745	1MG	C2-N2	5.53	1.44	1.34
6	B	966	2MG	C2-N2	5.46	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Y	32	5MC	C2-N3	5.43	1.47	1.36
6	B	1207	2MG	C2-N2	5.42	1.45	1.33
27	a	1962	5MC	C2-N3	5.34	1.47	1.36
6	B	1407	5MC	C2-N3	5.34	1.47	1.36
6	B	527	G7M	C2-N3	5.32	1.46	1.33
27	a	1835	2MG	C2-N2	5.26	1.45	1.33
6	B	1498	UR3	C2-N3	5.24	1.49	1.39
27	a	1962	5MC	C6-N1	5.23	1.47	1.38
6	B	1402	4OC	C2-N3	5.20	1.46	1.36
6	B	967	5MC	C6-N1	5.20	1.46	1.38
6	B	1516	2MG	C2-N2	5.18	1.44	1.33
27	a	2069	G7M	C2-N3	5.13	1.45	1.33
27	a	2445	2MG	C2-N2	5.12	1.44	1.33
27	a	2503	2MA	C6-N1	5.11	1.42	1.35
6	B	1407	5MC	C6-N1	5.03	1.46	1.38
27	a	1962	5MC	C2-N1	5.02	1.50	1.40
27	a	2449	H2U	C4-N3	4.87	1.45	1.37
54	Y	32	5MC	C6-N1	4.82	1.46	1.38
6	B	1407	5MC	C2-N1	4.77	1.50	1.40
54	Y	32	5MC	C2-N1	4.77	1.50	1.40
6	B	967	5MC	C2-N1	4.74	1.50	1.40
6	B	527	G7M	C2-N2	4.70	1.45	1.34
27	a	2251	OMG	C2-N2	4.66	1.45	1.34
54	Y	8	4SU	C5-C4	4.66	1.48	1.42
27	a	2503	2MA	C5-N7	-4.59	1.30	1.39
27	a	2498	OMC	C4-N3	4.56	1.43	1.34
27	a	2503	2MA	C5-C6	4.53	1.53	1.41
27	a	2069	G7M	C2-N2	4.51	1.44	1.34
6	B	1207	2MG	C2-N1	4.49	1.43	1.36
27	a	2498	OMC	C4-N4	4.47	1.44	1.33
54	Y	8	4SU	C4-S4	-4.46	1.59	1.68
6	B	966	2MG	C2-N1	4.37	1.43	1.36
6	B	1402	4OC	C4-N4	4.36	1.44	1.35
27	a	1835	2MG	C2-N1	4.31	1.43	1.36
6	B	1516	2MG	C2-N1	4.28	1.43	1.36
27	a	745	1MG	O6-C6	-4.26	1.14	1.23
6	B	527	G7M	C5-N7	-4.16	1.34	1.39
27	a	2445	2MG	C2-N1	4.11	1.43	1.36
27	a	745	1MG	C5-C6	3.90	1.55	1.45
27	a	2069	G7M	C5-N7	-3.87	1.34	1.39
6	B	1402	4OC	C5-C4	3.85	1.49	1.40
6	B	1402	4OC	C2-N1	3.82	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	2498	OMC	C2-N1	3.81	1.48	1.40
54	Y	54	5MU	C2-N1	3.71	1.44	1.38
27	a	2445	2MG	C5-N7	-3.58	1.32	1.39
27	a	2552	OMU	O4-C4	-3.57	1.17	1.24
27	a	2457	PSU	C6-C5	3.57	1.39	1.35
6	B	1518	MA6	C6-N6	3.49	1.47	1.36
6	B	1519	MA6	C6-N6	3.46	1.47	1.36
27	a	745	1MG	C5-N7	-3.45	1.32	1.39
27	a	2580	PSU	C6-C5	3.44	1.39	1.35
27	a	1835	2MG	C5-N7	-3.44	1.32	1.39
6	B	966	2MG	C5-N7	-3.43	1.32	1.39
27	a	2449	H2U	O2-C2	-3.40	1.16	1.23
27	a	2552	OMU	C4-N3	3.37	1.44	1.38
54	Y	55	PSU	C6-C5	3.37	1.39	1.35
54	Y	54	5MU	C2-N3	3.32	1.43	1.38
6	B	527	G7M	C5-C6	3.31	1.52	1.43
27	a	1618	6MZ	C5-N7	-3.31	1.32	1.39
27	a	1917	PSU	C6-C5	3.30	1.39	1.35
27	a	746	PSU	C6-C5	3.30	1.39	1.35
27	a	1939	5MU	C2-N3	3.25	1.43	1.38
27	a	747	5MU	C2-N3	3.25	1.43	1.38
27	a	2445	2MG	O6-C6	-3.24	1.17	1.23
27	a	1939	5MU	C2-N1	3.24	1.43	1.38
6	B	1516	2MG	C5-N7	-3.21	1.32	1.39
6	B	967	5MC	C4-N4	3.21	1.42	1.34
6	B	1207	2MG	C5-N7	-3.16	1.32	1.39
27	a	2503	2MA	C6-N6	-3.16	1.26	1.34
27	a	2069	G7M	C5-C6	3.15	1.52	1.43
6	B	1407	5MC	C4-N4	3.14	1.42	1.34
27	a	1962	5MC	O2-C2	-3.14	1.17	1.23
27	a	2504	PSU	C6-C5	3.13	1.39	1.35
27	a	1618	6MZ	C5-C4	-3.12	1.33	1.39
54	Y	32	5MC	C4-N4	3.11	1.42	1.34
54	Y	32	5MC	O2-C2	-3.10	1.18	1.23
6	B	1518	MA6	C5-N7	-3.09	1.33	1.39
6	B	1519	MA6	C5-N7	-3.09	1.33	1.39
6	B	1402	4OC	O2-C2	-3.07	1.18	1.23
27	a	2604	PSU	C6-C5	3.06	1.38	1.35
6	B	1402	4OC	C6-N1	3.06	1.45	1.38
6	B	1519	MA6	C5-C4	-3.05	1.33	1.39
6	B	516	PSU	C6-C5	3.04	1.38	1.35
27	a	2498	OMC	O2-C2	-2.99	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1498	UR3	O2-C2	-2.97	1.17	1.22
27	a	1962	5MC	C4-N4	2.97	1.41	1.34
6	B	1407	5MC	O2-C2	-2.96	1.18	1.23
6	B	1518	MA6	C5-C4	-2.94	1.33	1.39
27	a	1835	2MG	O6-C6	-2.91	1.18	1.23
27	a	2552	OMU	C6-N1	2.91	1.45	1.38
6	B	1516	2MG	O6-C6	-2.88	1.18	1.23
27	a	2498	OMC	C6-N1	2.88	1.45	1.38
6	B	967	5MC	O2-C2	-2.88	1.18	1.23
27	a	2605	PSU	C6-C5	2.88	1.38	1.35
27	a	1911	PSU	C6-C5	2.85	1.38	1.35
6	B	527	G7M	O6-C6	-2.84	1.18	1.23
27	a	2449	H2U	O4-C4	-2.82	1.17	1.23
27	a	2251	OMG	C5-N7	-2.81	1.33	1.39
27	a	2552	OMU	O2-C2	-2.80	1.17	1.23
54	Y	8	4SU	C6-N1	2.80	1.44	1.38
27	a	747	5MU	C2-N1	2.80	1.42	1.38
6	B	1498	UR3	C6-N1	2.79	1.44	1.38
6	B	527	G7M	C6-N1	2.78	1.44	1.38
27	a	2069	G7M	O6-C6	-2.73	1.18	1.23
6	B	1498	UR3	O4-C4	-2.73	1.17	1.23
27	a	955	PSU	C6-C5	2.73	1.38	1.35
27	a	1618	6MZ	C8-N9	-2.71	1.32	1.37
6	B	966	2MG	O6-C6	-2.69	1.18	1.23
6	B	1207	2MG	C5-C6	2.67	1.54	1.44
27	a	2580	PSU	O4'-C1'	-2.66	1.40	1.43
27	a	2251	OMG	C5-C6	2.64	1.54	1.44
6	B	1207	2MG	O6-C6	-2.61	1.18	1.23
27	a	745	1MG	C8-N9	-2.59	1.31	1.37
6	B	1516	2MG	C5-C6	2.52	1.53	1.44
27	a	2069	G7M	C4-N9	-2.50	1.31	1.38
27	a	2069	G7M	C6-N1	2.48	1.43	1.38
54	Y	8	4SU	O2-C2	-2.48	1.18	1.23
6	B	966	2MG	C5-C6	2.46	1.53	1.44
6	B	1498	UR3	C5-C4	2.35	1.49	1.43
6	B	1518	MA6	C4-N9	-2.35	1.32	1.37
27	a	2445	2MG	C5-C6	2.32	1.53	1.44
6	B	527	G7M	C2-N1	2.29	1.43	1.37
6	B	527	G7M	C4-N9	-2.29	1.32	1.38
54	Y	55	PSU	O4'-C1'	-2.29	1.40	1.43
27	a	2251	OMG	C2-N1	2.28	1.43	1.37
27	a	2552	OMU	C5-C4	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	1835	2MG	C5-C6	2.27	1.52	1.44
27	a	2503	2MA	C4-N9	-2.26	1.32	1.37
27	a	2503	2MA	C8-N9	-2.18	1.33	1.37
27	a	2251	OMG	C6-N1	2.17	1.42	1.38
27	a	2069	G7M	C2-N1	2.13	1.42	1.37
6	B	516	PSU	O4'-C1'	-2.12	1.40	1.43
6	B	1207	2MG	C6-N1	2.10	1.42	1.38
27	a	2445	2MG	C4-N9	-2.09	1.32	1.38
6	B	1498	UR3	C4-N3	2.07	1.45	1.40
27	a	1618	6MZ	C6-N1	-2.07	1.31	1.35
27	a	2604	PSU	C4-C5	-2.07	1.38	1.44
6	B	966	2MG	C6-N1	2.07	1.42	1.38
27	a	2449	H2U	C6-C5	-2.06	1.46	1.52
27	a	2504	PSU	C4-C5	-2.06	1.38	1.44
27	a	1911	PSU	C4-C5	-2.05	1.38	1.44
27	a	2498	OMC	C5-C4	2.05	1.47	1.42
27	a	1835	2MG	C6-N1	2.03	1.42	1.38
27	a	746	PSU	O4'-C1'	-2.03	1.41	1.43
27	a	1917	PSU	C4-C5	-2.02	1.38	1.44
27	a	2605	PSU	C4-C5	-2.01	1.38	1.44

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1519	MA6	N1-C6-N6	-10.60	105.49	117.08
6	B	1518	MA6	N1-C6-N6	-10.04	106.11	117.08
54	Y	54	5MU	C5-C4-N3	9.89	123.75	115.31
27	a	1939	5MU	C5-C4-N3	9.82	123.69	115.31
27	a	747	5MU	C5-C4-N3	9.48	123.40	115.31
27	a	747	5MU	C5-C6-N1	-7.92	115.19	123.34
27	a	2503	2MA	C5-C4-N3	-7.49	118.76	127.19
54	Y	54	5MU	C5-C6-N1	-7.37	115.75	123.34
27	a	1939	5MU	C5-C6-N1	-7.31	115.82	123.34
54	Y	8	4SU	C4-N3-C2	-7.17	120.37	127.34
6	B	966	2MG	C2-N3-C4	6.91	120.60	112.04
27	a	2445	2MG	C2-N3-C4	6.66	120.30	112.04
6	B	1516	2MG	C2-N3-C4	6.57	120.19	112.04
27	a	2449	H2U	C4-N3-C2	-6.56	120.35	125.79
27	a	1835	2MG	C2-N3-C4	6.55	120.16	112.04
6	B	1207	2MG	C2-N3-C4	6.52	120.12	112.04
27	a	747	5MU	C4-N3-C2	-6.30	119.20	127.35
27	a	1939	5MU	C4-N3-C2	-6.10	119.45	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Y	54	5MU	C4-N3-C2	-6.02	119.55	127.35
27	a	2251	OMG	C5-C4-N3	-6.00	118.73	128.46
6	B	1519	MA6	C5-C4-N3	-5.92	119.03	126.75
6	B	966	2MG	C5-C4-N3	-5.89	118.91	128.46
27	a	1618	6MZ	C5-C4-N3	-5.76	119.23	126.75
6	B	1518	MA6	N1-C2-N3	-5.71	119.68	128.60
27	a	745	1MG	C5-C4-N3	-5.70	119.21	128.46
27	a	1618	6MZ	N1-C2-N3	-5.51	119.98	128.60
27	a	2552	OMU	C4-N3-C2	-5.49	119.34	126.58
27	a	2445	2MG	C5-C4-N3	-5.44	119.63	128.46
27	a	1835	2MG	C5-C4-N3	-5.37	119.75	128.46
6	B	1518	MA6	C5-C6-N6	5.31	134.55	125.30
27	a	2449	H2U	N3-C2-N1	5.28	122.24	116.65
27	a	2604	PSU	C4-N3-C2	-5.26	118.76	126.34
6	B	1519	MA6	N1-C2-N3	-5.23	120.42	128.60
6	B	1519	MA6	C5-C6-N6	5.20	134.37	125.30
6	B	1516	2MG	C5-C4-N3	-5.18	120.06	128.46
6	B	1207	2MG	C5-C4-N3	-5.16	120.09	128.46
54	Y	8	4SU	C5-C4-N3	5.15	119.46	114.69
27	a	955	PSU	C4-N3-C2	-5.05	119.06	126.34
27	a	2580	PSU	N1-C2-N3	4.97	120.76	115.13
27	a	2457	PSU	N1-C2-N3	4.96	120.75	115.13
27	a	2503	2MA	N3-C4-N9	4.95	133.86	126.99
27	a	1917	PSU	C4-N3-C2	-4.94	119.23	126.34
27	a	2445	2MG	C2-N1-C6	-4.92	118.82	124.48
6	B	1498	UR3	C4-N3-C2	-4.90	119.95	124.56
27	a	2604	PSU	N1-C2-N3	4.90	120.68	115.13
27	a	2605	PSU	C4-N3-C2	-4.89	119.29	126.34
27	a	955	PSU	N1-C2-N3	4.84	120.61	115.13
6	B	1518	MA6	C5-C4-N3	-4.83	120.45	126.75
27	a	2504	PSU	C4-N3-C2	-4.83	119.38	126.34
27	a	2251	OMG	C1'-N9-C4	-4.75	112.41	126.50
6	B	516	PSU	C4-N3-C2	-4.72	119.54	126.34
54	Y	55	PSU	C4-N3-C2	-4.71	119.56	126.34
27	a	2605	PSU	N1-C2-N3	4.69	120.45	115.13
27	a	746	PSU	C4-N3-C2	-4.64	119.66	126.34
27	a	1911	PSU	C4-N3-C2	-4.63	119.66	126.34
27	a	1917	PSU	N1-C2-N3	4.62	120.37	115.13
6	B	966	2MG	C2-N1-C6	-4.60	119.19	124.48
27	a	745	1MG	C1'-N9-C4	-4.60	112.84	126.50
27	a	2504	PSU	N1-C2-N3	4.55	120.28	115.13
6	B	1516	2MG	C2-N1-C6	-4.52	119.28	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	2251	OMG	C1'-N9-C8	4.52	139.56	126.70
27	a	2580	PSU	C4-N3-C2	-4.50	119.86	126.34
27	a	1618	6MZ	C4-C5-C6	4.49	120.29	116.81
27	a	747	5MU	N3-C2-N1	4.49	120.85	114.89
27	a	2069	G7M	C2-N3-C4	4.45	120.24	112.30
6	B	527	G7M	C2-N3-C4	4.45	120.23	112.30
27	a	2457	PSU	C4-N3-C2	-4.45	119.93	126.34
6	B	516	PSU	N1-C2-N3	4.45	120.17	115.13
27	a	2251	OMG	C2-N3-C4	4.43	120.19	112.30
27	a	1618	6MZ	N9-C8-N7	-4.42	107.86	113.91
27	a	745	1MG	C1'-N9-C8	4.42	139.27	126.70
27	a	1939	5MU	C5M-C5-C6	-4.42	116.95	122.85
27	a	1911	PSU	N1-C2-N3	4.40	120.12	115.13
27	a	746	PSU	N1-C2-N3	4.39	120.11	115.13
27	a	1939	5MU	N3-C2-N1	4.32	120.63	114.89
27	a	2552	OMU	N3-C2-N1	4.30	120.60	114.89
27	a	2503	2MA	N9-C8-N7	-4.29	108.04	113.91
27	a	747	5MU	C5M-C5-C6	-4.24	117.18	122.85
54	Y	54	5MU	N3-C2-N1	4.18	120.44	114.89
27	a	1835	2MG	C2-N1-C6	-4.18	119.67	124.48
6	B	1519	MA6	C4-C5-C6	4.15	120.53	115.88
27	a	1939	5MU	C5M-C5-C4	4.12	123.30	118.77
54	Y	55	PSU	N1-C2-N3	4.10	119.78	115.13
54	Y	54	5MU	O4-C4-C5	-4.08	120.17	124.90
6	B	1207	2MG	C2-N1-C6	-4.05	119.82	124.48
27	a	2251	OMG	N9-C4-N3	4.05	134.07	125.94
27	a	2069	G7M	C5-C6-N1	4.05	120.25	111.79
27	a	745	1MG	C2-N3-C4	4.03	121.03	111.98
27	a	2449	H2U	O2-C2-N1	-4.01	118.07	123.11
6	B	527	G7M	C5-C6-N1	3.95	120.03	111.79
6	B	1519	MA6	N9-C8-N7	-3.90	108.58	113.91
6	B	966	2MG	N9-C4-N3	3.86	133.68	125.94
6	B	527	G7M	C5-C4-N3	-3.83	120.81	128.15
6	B	1518	MA6	C2-N1-C6	3.82	120.77	111.75
27	a	1618	6MZ	C2-N3-C4	3.79	120.71	111.75
6	B	1518	MA6	C4-C5-C6	3.75	120.08	115.88
6	B	1519	MA6	C2-N3-C4	3.70	120.48	111.75
27	a	2069	G7M	C5-C4-N3	-3.65	121.14	128.15
27	a	1618	6MZ	N3-C4-N9	3.65	133.10	127.08
6	B	1518	MA6	N9-C8-N7	-3.61	108.98	113.91
27	a	2552	OMU	C5-C4-N3	3.60	120.23	114.84
27	a	2069	G7M	O6-C6-C5	-3.55	120.04	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	747	5MU	O4-C4-C5	-3.52	120.82	124.90
54	Y	8	4SU	N3-C2-N1	3.51	119.55	114.89
27	a	2503	2MA	C5-N7-C8	3.46	108.42	103.51
27	a	1835	2MG	N9-C4-N3	3.45	132.86	125.94
27	a	745	1MG	N9-C4-N3	3.45	132.86	125.94
27	a	747	5MU	C5M-C5-C4	3.41	122.52	118.77
27	a	1618	6MZ	C5-N7-C8	3.38	108.31	103.51
6	B	1498	UR3	C1'-N1-C2	3.37	122.67	116.99
6	B	1518	MA6	C2-N3-C4	3.36	119.69	111.75
6	B	527	G7M	O6-C6-C5	-3.35	120.51	128.06
6	B	1519	MA6	N3-C4-N9	3.34	132.58	127.08
6	B	967	5MC	C5-C6-N1	-3.33	119.91	123.34
27	a	2069	G7M	CN7-N7-C5	3.33	130.91	126.77
27	a	2069	G7M	N9-C4-N3	3.32	132.61	125.94
6	B	527	G7M	N9-C4-N3	3.27	132.51	125.94
54	Y	54	5MU	C5M-C5-C6	-3.27	118.48	122.85
6	B	1519	MA6	C2-N1-C6	3.24	119.41	111.75
27	a	2445	2MG	N9-C4-N3	3.22	132.41	125.94
6	B	527	G7M	C1'-N9-C4	-3.22	116.94	126.50
27	a	2503	2MA	C6-C5-C4	3.21	121.50	117.18
6	B	1519	MA6	C5-N7-C8	3.21	108.06	103.51
27	a	745	1MG	C5-C6-N1	3.20	121.10	114.91
54	Y	8	4SU	C5-C4-S4	-3.20	120.34	124.47
6	B	1516	2MG	C1'-N9-C4	-3.17	117.08	126.50
27	a	2251	OMG	C2-N1-C6	-3.08	119.48	125.10
27	a	747	5MU	O2-C2-N1	-3.08	118.70	122.79
27	a	2503	2MA	N3-C2-N1	-3.02	120.16	125.72
6	B	1407	5MC	C5-C6-N1	-3.01	120.24	123.34
27	a	2069	G7M	C1'-N9-C4	-2.94	117.77	126.50
6	B	1518	MA6	N3-C4-N9	2.94	131.92	127.08
6	B	1207	2MG	N9-C4-N3	2.93	131.82	125.94
6	B	1516	2MG	N9-C8-N7	-2.92	107.88	113.39
6	B	1516	2MG	C5-C6-N1	2.92	120.62	113.19
6	B	1516	2MG	C1'-N9-C8	2.90	134.95	126.70
27	a	2445	2MG	C5-C6-N1	2.90	120.55	113.19
27	a	1618	6MZ	C9-N6-C6	-2.89	120.38	122.87
27	a	2580	PSU	O2-C2-N1	-2.88	119.62	122.79
27	a	1939	5MU	O4-C4-N3	-2.88	114.60	120.12
6	B	1516	2MG	N9-C4-N3	2.86	131.69	125.94
54	Y	32	5MC	C5-C6-N1	-2.82	120.44	123.34
27	a	1962	5MC	C5-C6-N1	-2.81	120.44	123.34
6	B	527	G7M	CN7-N7-C5	2.81	130.26	126.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	966	2MG	C5-C6-N1	2.80	120.30	113.19
6	B	527	G7M	C2-N1-C6	-2.80	120.00	125.10
27	a	1939	5MU	O4-C4-C5	-2.75	121.71	124.90
27	a	2445	2MG	N9-C8-N7	-2.75	108.21	113.39
27	a	2251	OMG	N9-C8-N7	-2.72	108.26	113.39
27	a	747	5MU	C6-C5-C4	2.71	120.30	118.03
27	a	2580	PSU	C3'-C2'-C1'	2.70	104.78	101.64
6	B	1207	2MG	C1'-N9-C4	-2.69	118.50	126.50
27	a	745	1MG	N9-C8-N7	-2.69	108.33	113.39
27	a	746	PSU	O2-C2-N1	-2.68	119.84	122.79
27	a	1835	2MG	O6-C6-C5	-2.68	119.50	126.60
27	a	2457	PSU	C6-N1-C2	-2.62	120.00	122.68
27	a	2605	PSU	O2-C2-N1	-2.61	119.91	122.79
6	B	966	2MG	N9-C8-N7	-2.61	108.48	113.39
27	a	2251	OMG	C5-C6-N1	2.60	119.80	113.19
27	a	2069	G7M	C2-N1-C6	-2.60	120.36	125.10
6	B	516	PSU	O2-C2-N1	-2.60	119.93	122.79
27	a	2580	PSU	C6-N1-C2	-2.58	120.04	122.68
27	a	2445	2MG	O6-C6-C5	-2.58	119.77	126.60
30	d	150	MEQ	CG-CD-NE2	2.57	119.86	116.29
6	B	1207	2MG	C5-C6-N1	2.57	119.71	113.19
54	Y	54	5MU	C5M-C5-C4	2.55	121.58	118.77
27	a	1835	2MG	C5-C6-N1	2.55	119.67	113.19
6	B	966	2MG	O6-C6-C5	-2.54	119.85	126.60
6	B	1207	2MG	C1'-N9-C8	2.54	133.92	126.70
27	a	2251	OMG	O6-C6-C5	-2.54	119.87	126.60
6	B	1207	2MG	N9-C8-N7	-2.52	108.64	113.39
27	a	2580	PSU	O4'-C1'-C2'	2.52	108.70	105.14
27	a	2445	2MG	CM2-N2-C2	-2.51	118.31	123.86
27	a	2552	OMU	O4-C4-C5	-2.51	120.75	125.16
27	a	2604	PSU	O2-C2-N1	-2.50	120.04	122.79
6	B	527	G7M	N9-C8-N7	-2.48	106.07	112.21
6	B	527	G7M	CN7-N7-C8	-2.48	121.01	124.84
27	a	745	1MG	CM1-N1-C2	2.48	123.29	120.72
6	B	1516	2MG	O6-C6-C5	-2.47	120.05	126.60
27	a	1835	2MG	N9-C8-N7	-2.47	108.74	113.39
6	B	1207	2MG	N1-C2-N3	-2.47	120.14	123.95
27	a	745	1MG	C2-N1-C6	-2.46	118.95	120.95
6	B	1516	2MG	N1-C2-N3	-2.45	120.16	123.95
27	a	1618	6MZ	O5'-C5'-C4'	2.45	117.32	108.99
27	a	2069	G7M	CN7-N7-C8	-2.44	121.07	124.84
27	a	1962	5MC	O2-C2-N3	-2.43	118.37	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	2604	PSU	C6-C5-C4	2.42	119.89	118.20
6	B	1518	MA6	C5-N7-C8	2.41	106.94	103.51
6	B	966	2MG	N1-C2-N3	-2.41	120.22	123.95
27	a	1835	2MG	N1-C2-N3	-2.41	120.23	123.95
6	B	1207	2MG	O6-C6-C5	-2.38	120.29	126.60
27	a	1962	5MC	CM5-C5-C6	-2.37	119.69	122.85
54	Y	55	PSU	O2-C2-N1	-2.33	120.22	122.79
27	a	2069	G7M	N9-C8-N7	-2.33	106.46	112.21
27	a	2449	H2U	O4-C4-N3	2.30	123.93	120.28
6	B	1516	2MG	CM2-N2-C2	-2.29	118.80	123.86
54	Y	54	5MU	C6-C5-C4	2.29	119.94	118.03
27	a	747	5MU	O4-C4-N3	-2.26	115.78	120.12
27	a	2457	PSU	O2-C2-N1	-2.25	120.31	122.79
27	a	2445	2MG	N1-C2-N3	-2.25	120.48	123.95
6	B	1519	MA6	C5-C4-N9	2.24	108.39	105.78
27	a	2069	G7M	N1-C2-N3	-2.23	119.16	123.32
27	a	2504	PSU	O2-C2-N1	-2.23	120.33	122.79
27	a	2251	OMG	C8-N7-C5	2.23	108.27	104.24
27	a	1618	6MZ	C4-N9-C8	2.21	108.12	105.73
27	a	1835	2MG	CM2-N2-C2	-2.18	119.04	123.86
6	B	1402	4OC	C6-C5-C4	2.18	119.63	116.96
27	a	2449	H2U	C5-C4-N3	-2.17	114.21	116.65
27	a	2552	OMU	O2-C2-N1	-2.16	119.91	122.79
6	B	1516	2MG	C8-N7-C5	2.16	108.15	104.24
6	B	1407	5MC	CM5-C5-C6	-2.16	119.97	122.85
27	a	1911	PSU	O2-C2-N1	-2.13	120.44	122.79
6	B	966	2MG	C8-N7-C5	2.13	108.09	104.24
27	a	1618	6MZ	C4-C5-N7	-2.12	108.03	110.62
6	B	1519	MA6	C4-C5-N7	-2.12	108.04	110.62
27	a	2503	2MA	CM2-C2-N3	2.12	120.45	117.15
27	a	2605	PSU	C6-N1-C2	-2.11	120.53	122.68
54	Y	54	5MU	O4-C4-N3	-2.11	116.08	120.12
27	a	1618	6MZ	C5-C6-N1	2.10	120.44	118.20
6	B	516	PSU	C6-N1-C2	-2.10	120.54	122.68
6	B	1407	5MC	C5-C4-N3	-2.10	119.41	121.67
27	a	2445	2MG	C8-N7-C5	2.09	108.02	104.24
27	a	2503	2MA	N6-C6-N1	2.08	119.98	117.03
27	a	2445	2MG	C1'-N9-C4	-2.08	120.33	126.50
27	a	2503	2MA	C4-N9-C1'	-2.06	121.68	126.59
6	B	1402	4OC	O2-C2-N3	-2.05	118.99	122.33
27	a	1939	5MU	C6-C5-C4	2.05	119.75	118.03
27	a	955	PSU	C6-N1-C2	-2.02	120.62	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	527	G7M	N1-C2-N3	-2.00	119.58	123.32
27	a	1917	PSU	O2-C2-N1	-2.00	120.59	122.79
27	a	1917	PSU	C6-N1-C2	-2.00	120.64	122.68

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	a	746	PSU	C2'-C1'-C5-C4
27	a	746	PSU	O4'-C1'-C5-C6
27	a	1618	6MZ	C4'-C5'-O5'-P
30	d	150	MEQ	NE2-CD-CG-CB
30	d	150	MEQ	OE1-CD-CG-CB
54	Y	54	5MU	O4'-C4'-C5'-O5'
54	Y	54	5MU	C3'-C4'-C5'-O5'
27	a	1962	5MC	C2'-C1'-N1-C6
6	B	527	G7M	C4'-C5'-O5'-P
27	a	2503	2MA	C4'-C5'-O5'-P
6	B	966	2MG	C3'-C4'-C5'-O5'
27	a	1962	5MC	O4'-C1'-N1-C6
27	a	1618	6MZ	C2'-C1'-N9-C8
27	a	2069	G7M	O4'-C4'-C5'-O5'
27	a	746	PSU	O4'-C1'-C5-C4
27	a	1618	6MZ	C2'-C1'-N9-C4
6	B	966	2MG	O4'-C4'-C5'-O5'
27	a	1962	5MC	O4'-C1'-N1-C2
27	a	2251	OMG	C1'-C2'-O2'-CM2
54	Y	55	PSU	C4'-C5'-O5'-P
27	a	2503	2MA	O4'-C4'-C5'-O5'
54	Y	55	PSU	C3'-C4'-C5'-O5'
27	a	1962	5MC	C2'-C1'-N1-C2

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	2251	OMG	1	0
27	a	1939	5MU	1	0
6	B	1519	MA6	1	0
27	a	2498	OMC	2	0
6	B	1207	2MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	2449	H2U	1	0
27	a	747	5MU	1	0
54	Y	54	5MU	1	0
54	Y	8	4SU	1	0
6	B	1518	MA6	2	0
27	a	2503	2MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 297 ligands modelled in this entry, 295 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	A2G	A	101	56	14,14,15	0.47	0	17,19,21	0.58	0
59	SPM	a	3209	-	13,13,13	0.31	0	12,12,12	0.86	0

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
60	A2G	A	101	56	-	0/6/23/26	0/1/1/1
59	SPM	a	3209	-	-	2/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

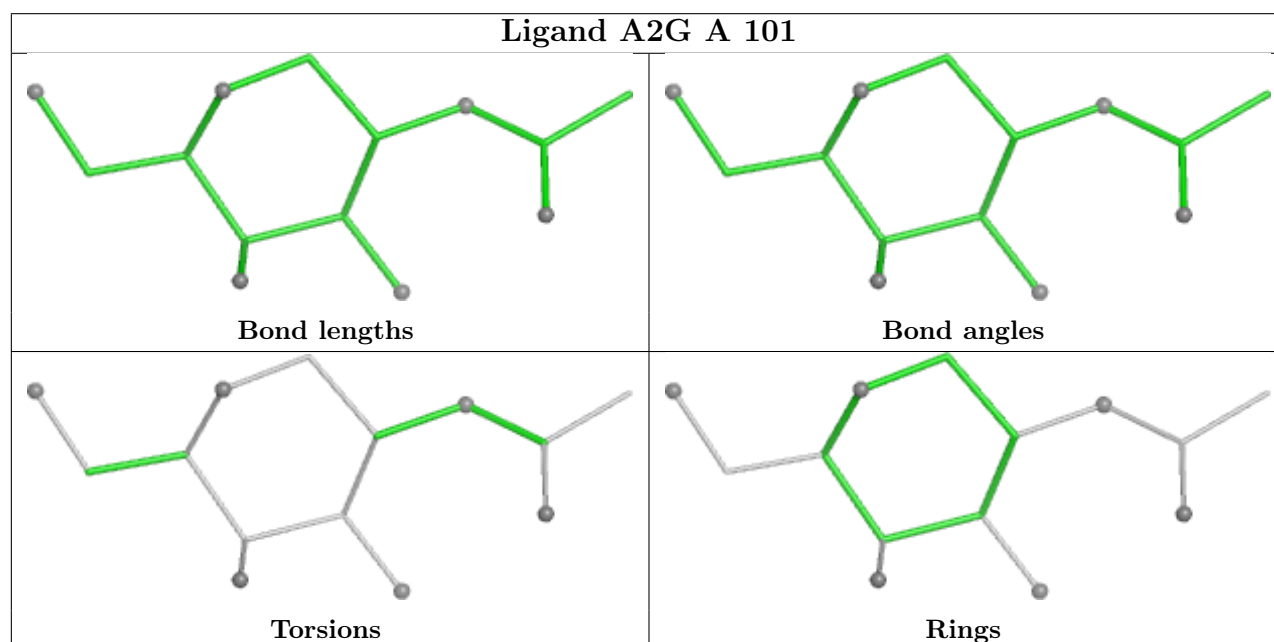
Mol	Chain	Res	Type	Atoms
59	a	3209	SPM	C12-C11-N10-C9
59	a	3209	SPM	C3-C4-N5-C6

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	A	101	A2G	14	0
59	a	3209	SPM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

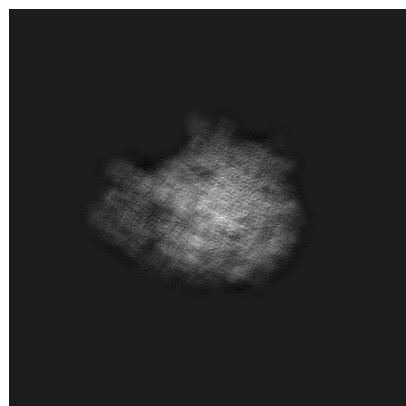
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15523. These allow visual inspection of the internal detail of the map and identification of artifacts.

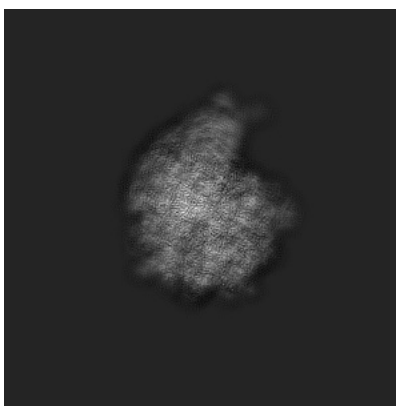
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

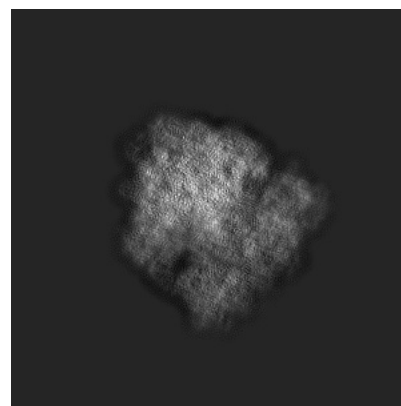
6.1.1 Primary map



X

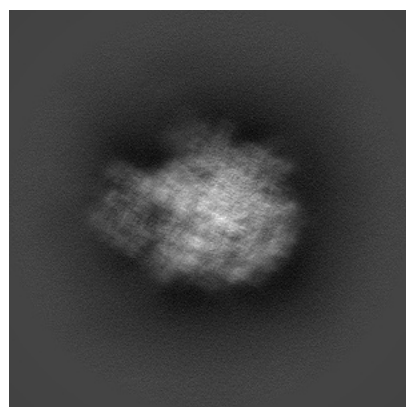


Y

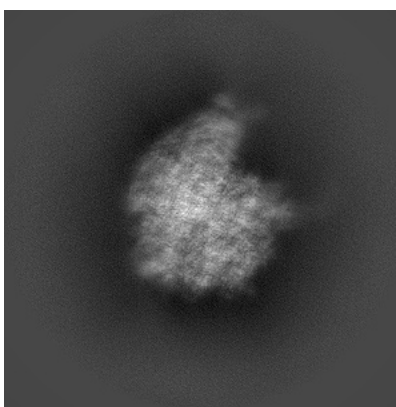


Z

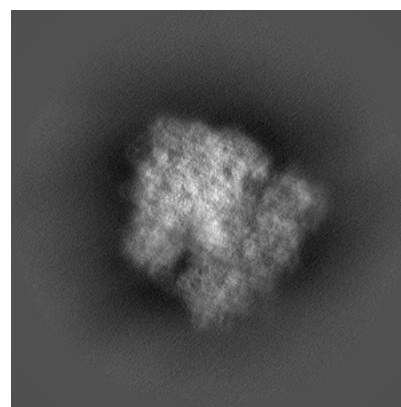
6.1.2 Raw map



X



Y

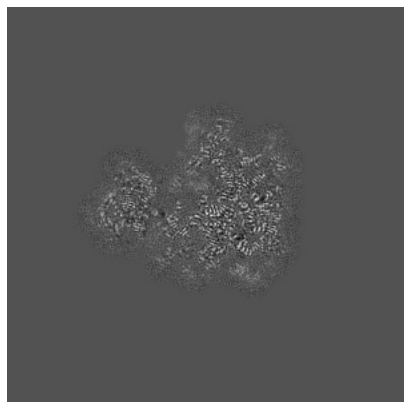


Z

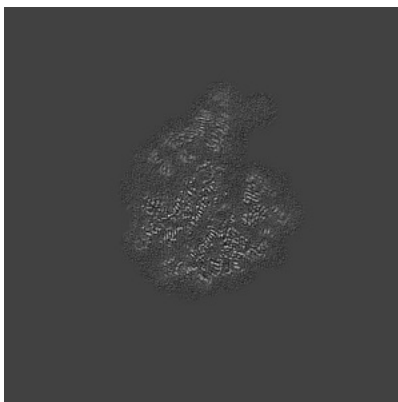
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

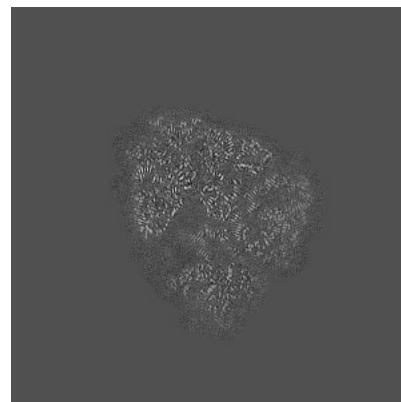
6.2.1 Primary map



X Index: 300

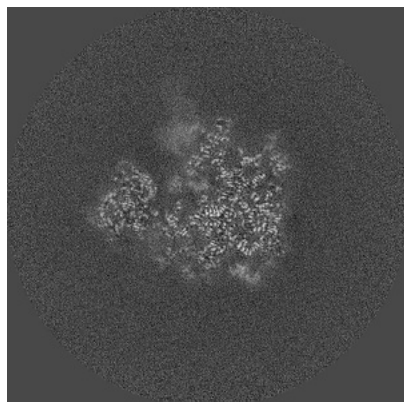


Y Index: 300

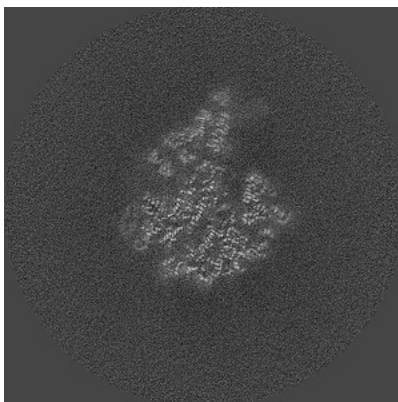


Z Index: 300

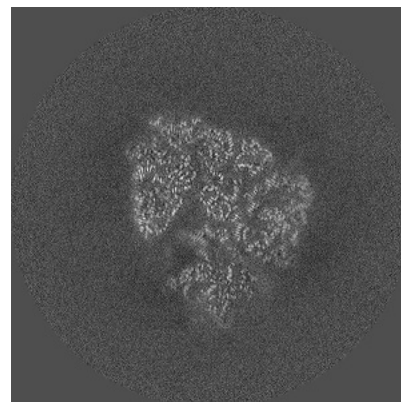
6.2.2 Raw map



X Index: 300



Y Index: 300

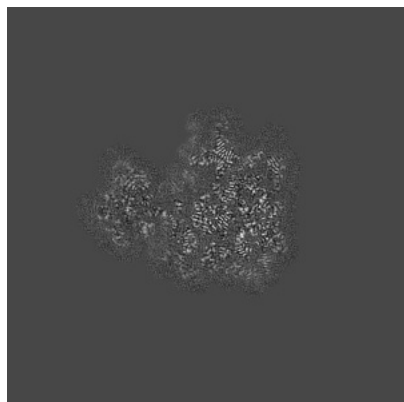


Z Index: 300

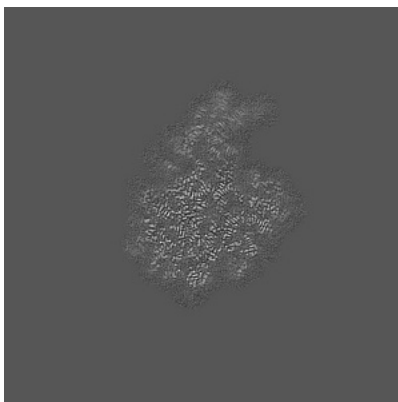
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

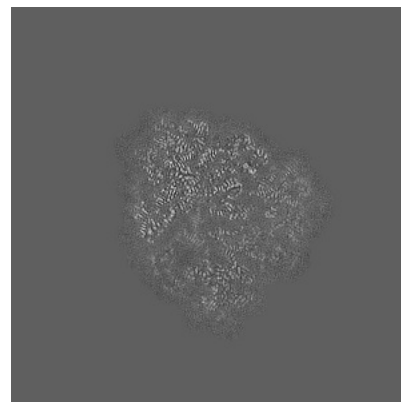
6.3.1 Primary map



X Index: 307

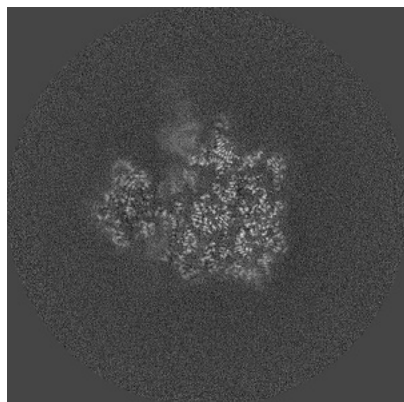


Y Index: 312

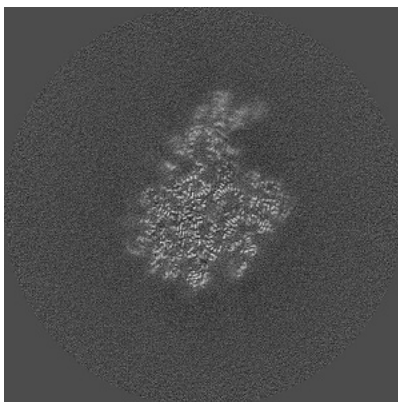


Z Index: 309

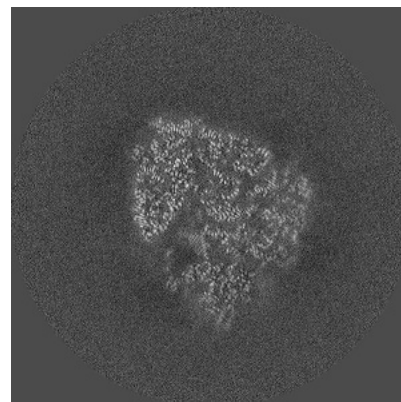
6.3.2 Raw map



X Index: 307



Y Index: 313

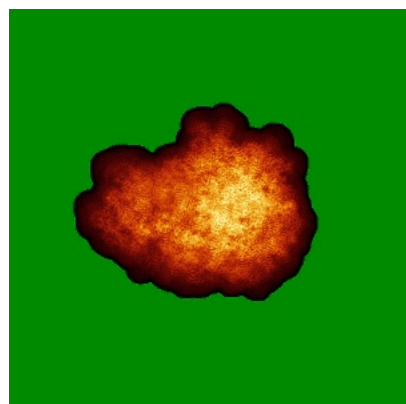


Z Index: 303

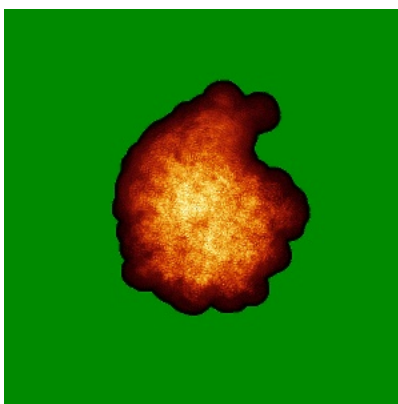
The images above show the largest variance slices of the map in three orthogonal directions.

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

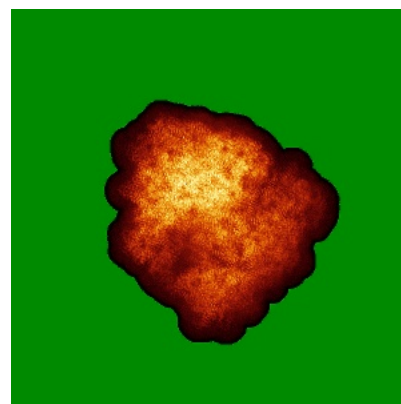
6.4.1 Primary map



X

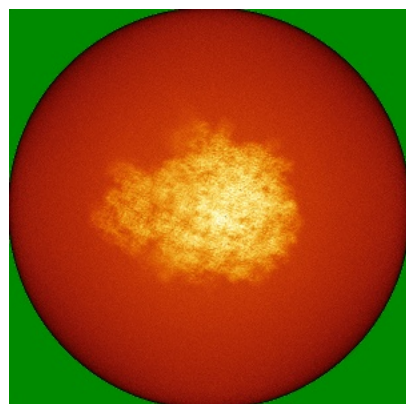


Y

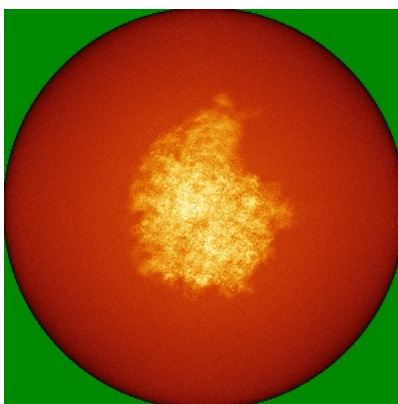


Z

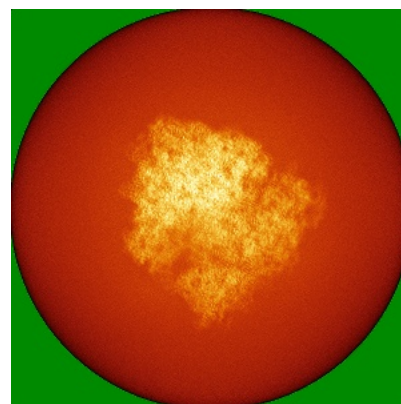
6.4.2 Raw map



X



Y

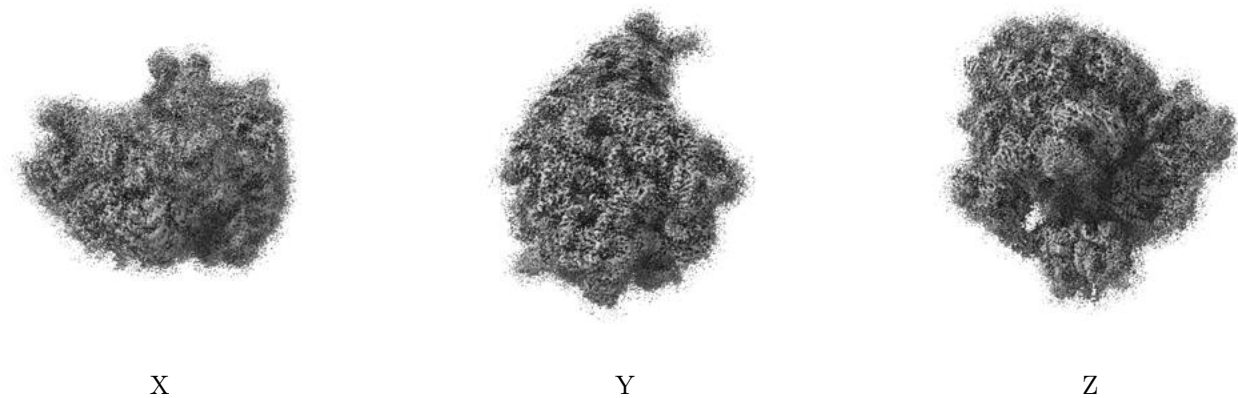


Z

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.

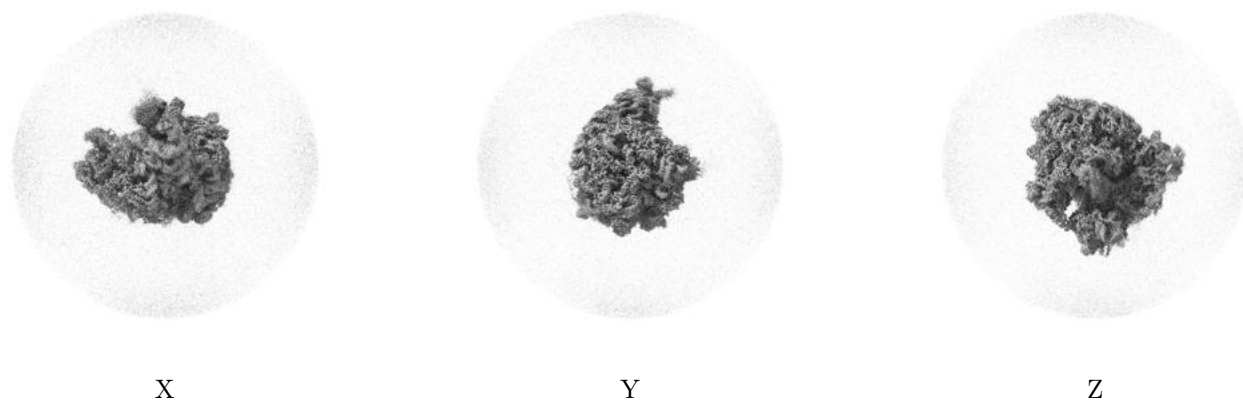
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

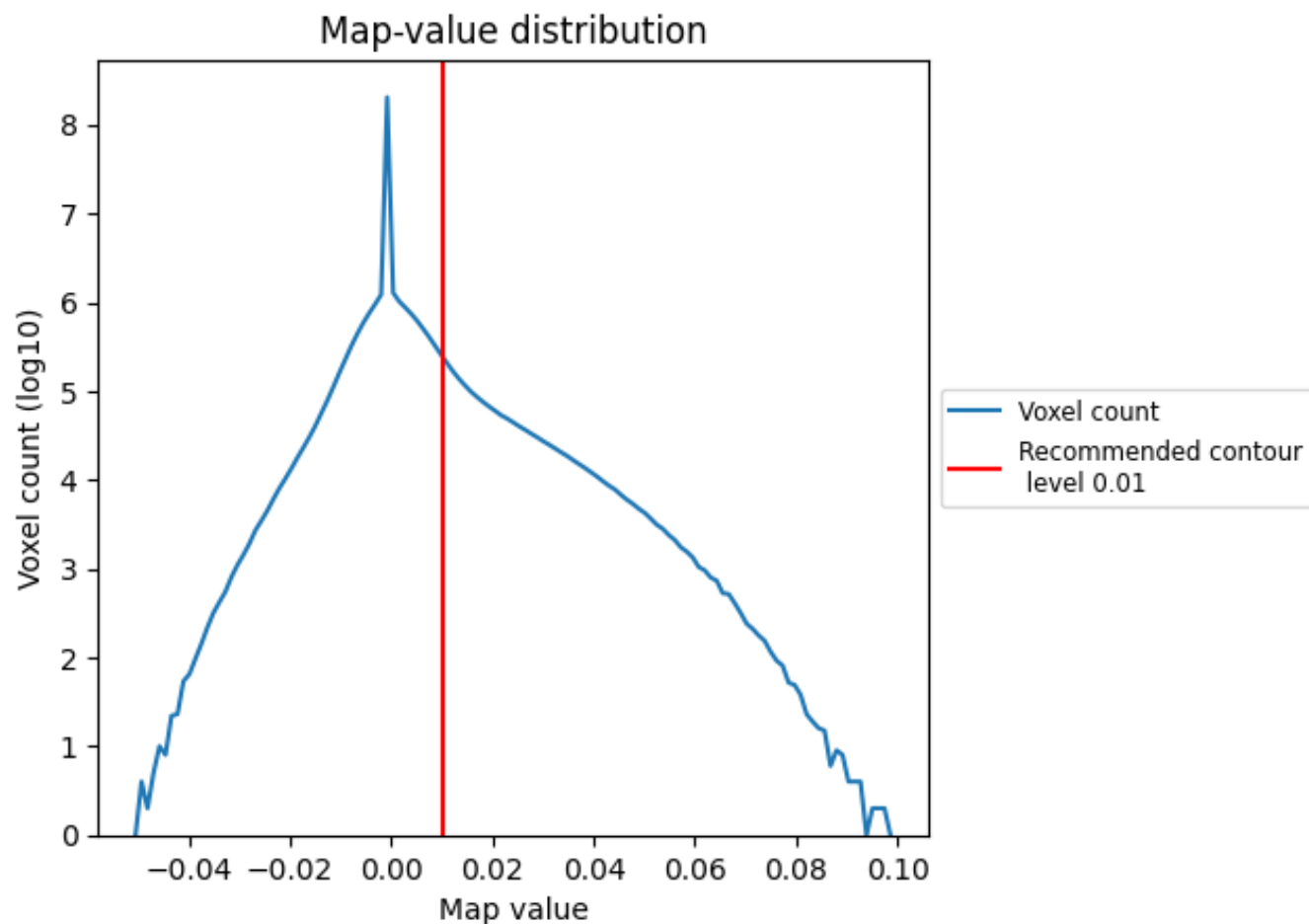
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

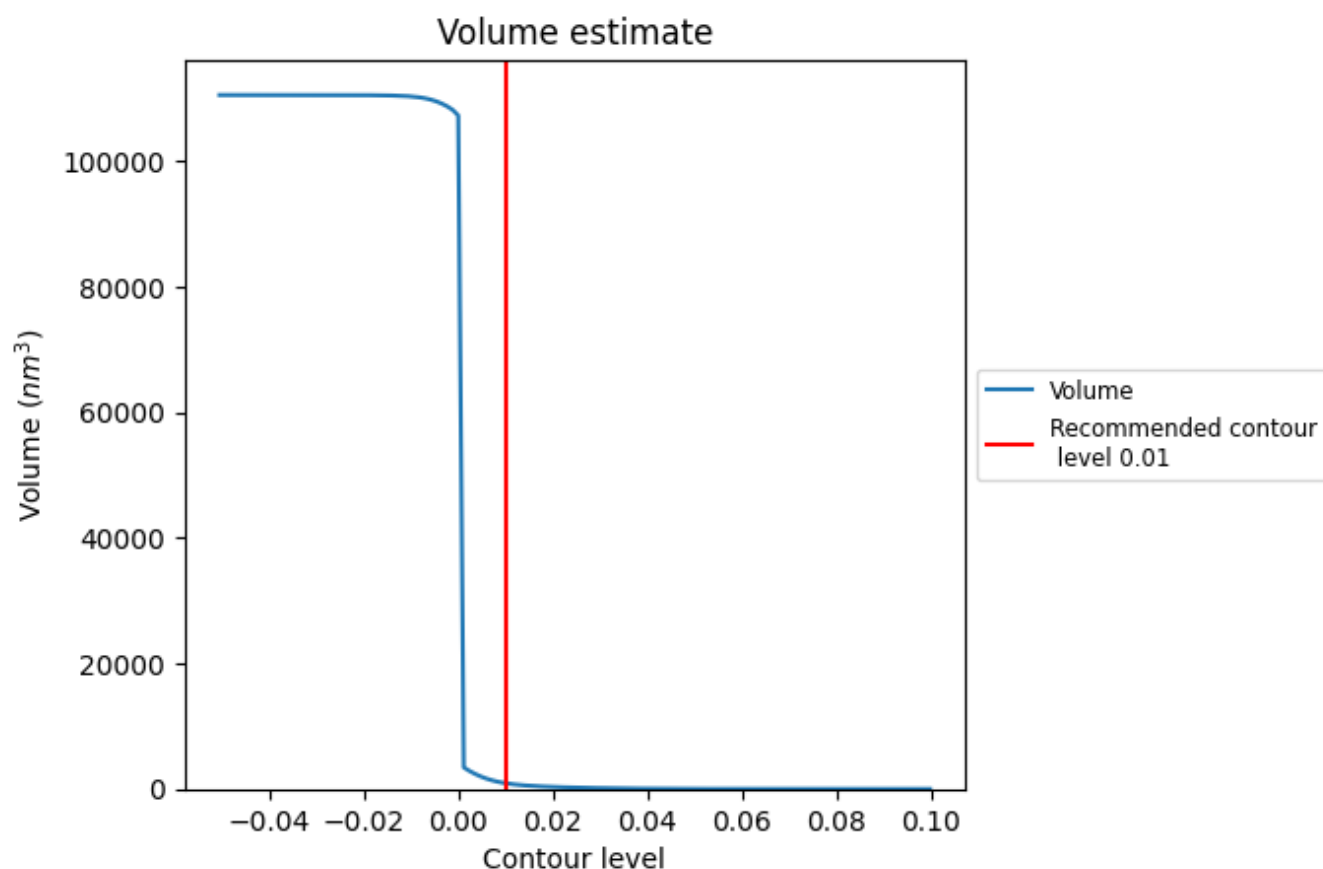
This section contains the results of statistical analysis of the map.

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.

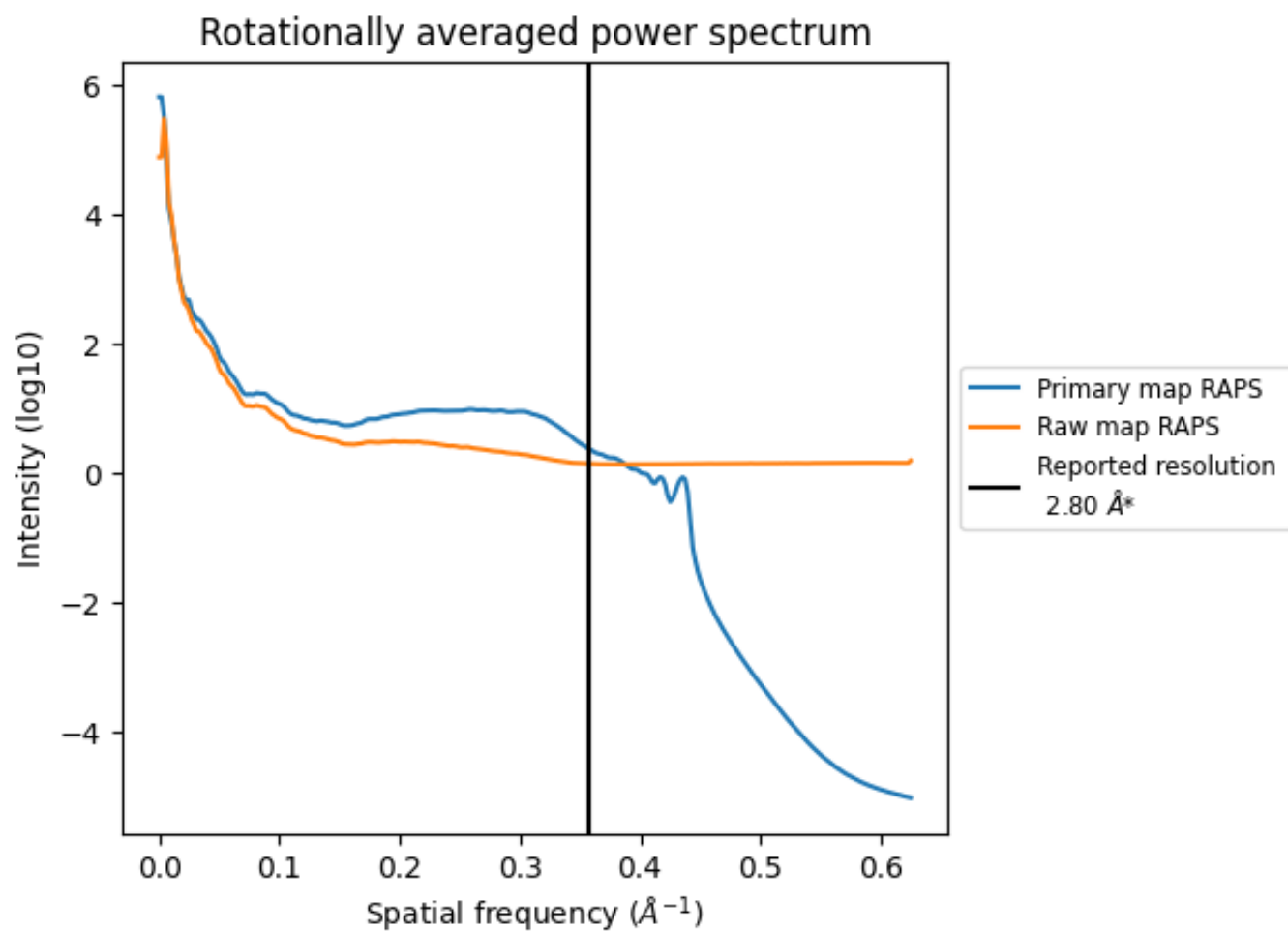
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 915 nm^3 ; this corresponds to an approximate mass of 826 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 ⓘ

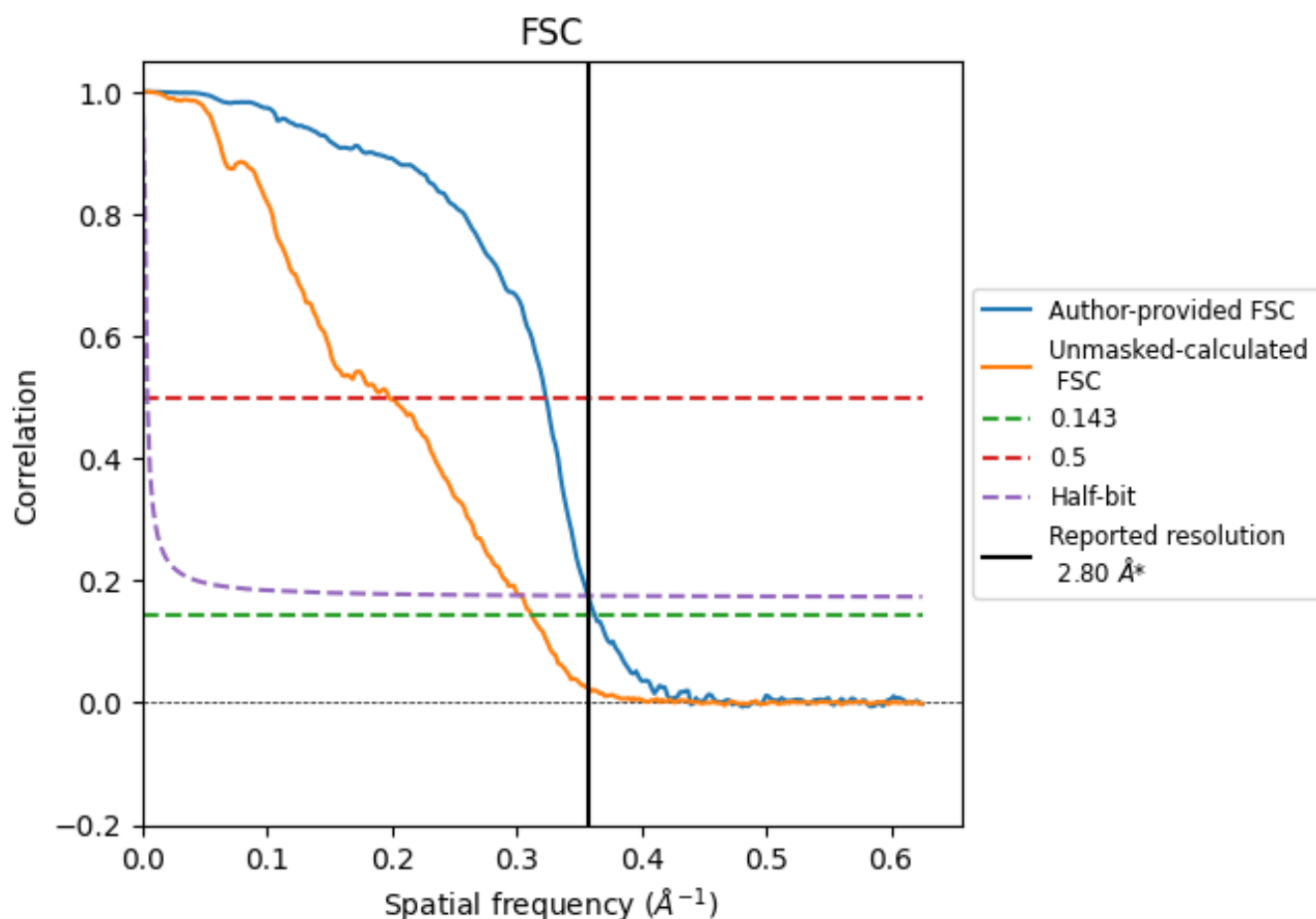


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

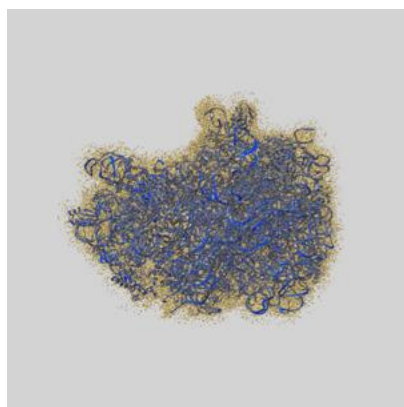
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.09	2.80
Unmasked-calculated*	3.20	5.06	3.29

*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 3.20 differs from the reported value 2.8 by more than 10 %

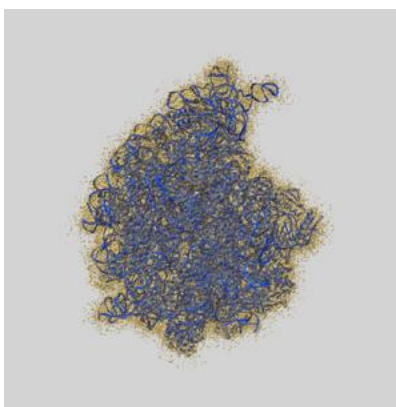
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15523 and PDB model 8AM9. Per-residue inclusion information can be found in section 3 on page 17.

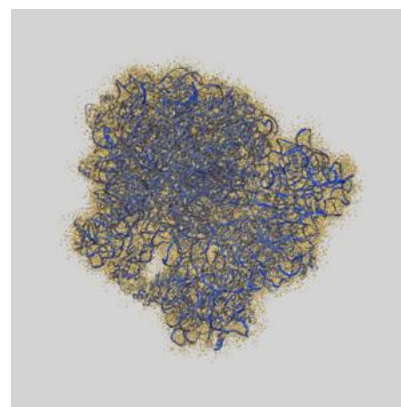
9.1 Map-model overlay [i](#)



X



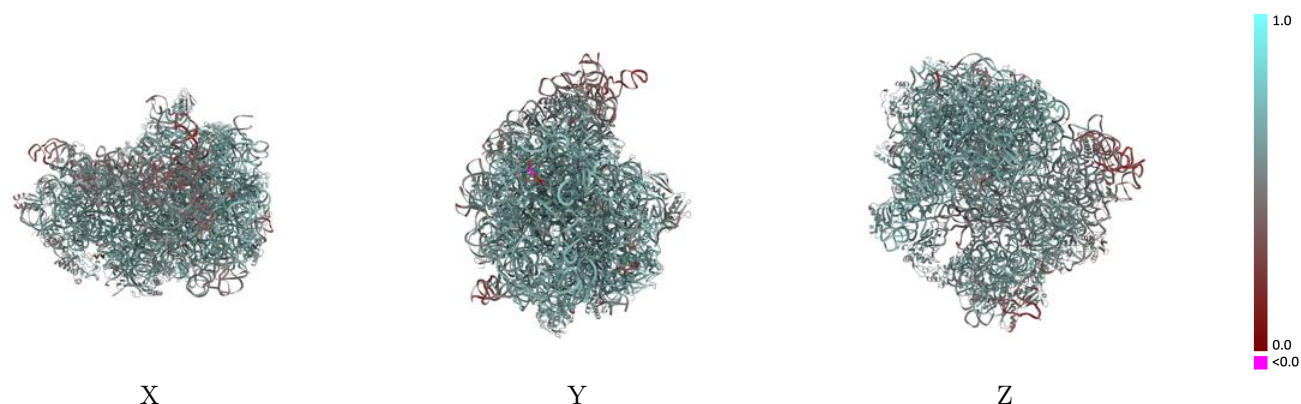
Y



Z

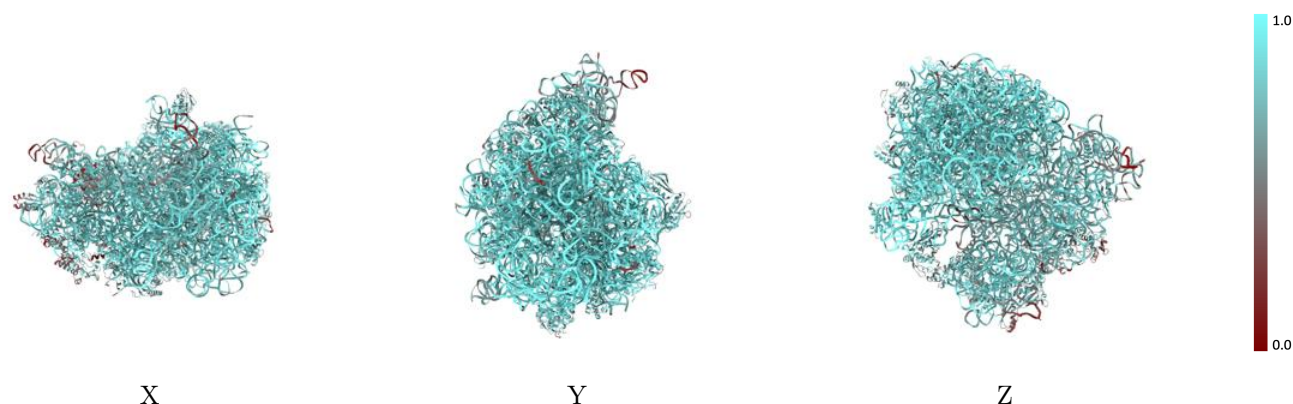
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



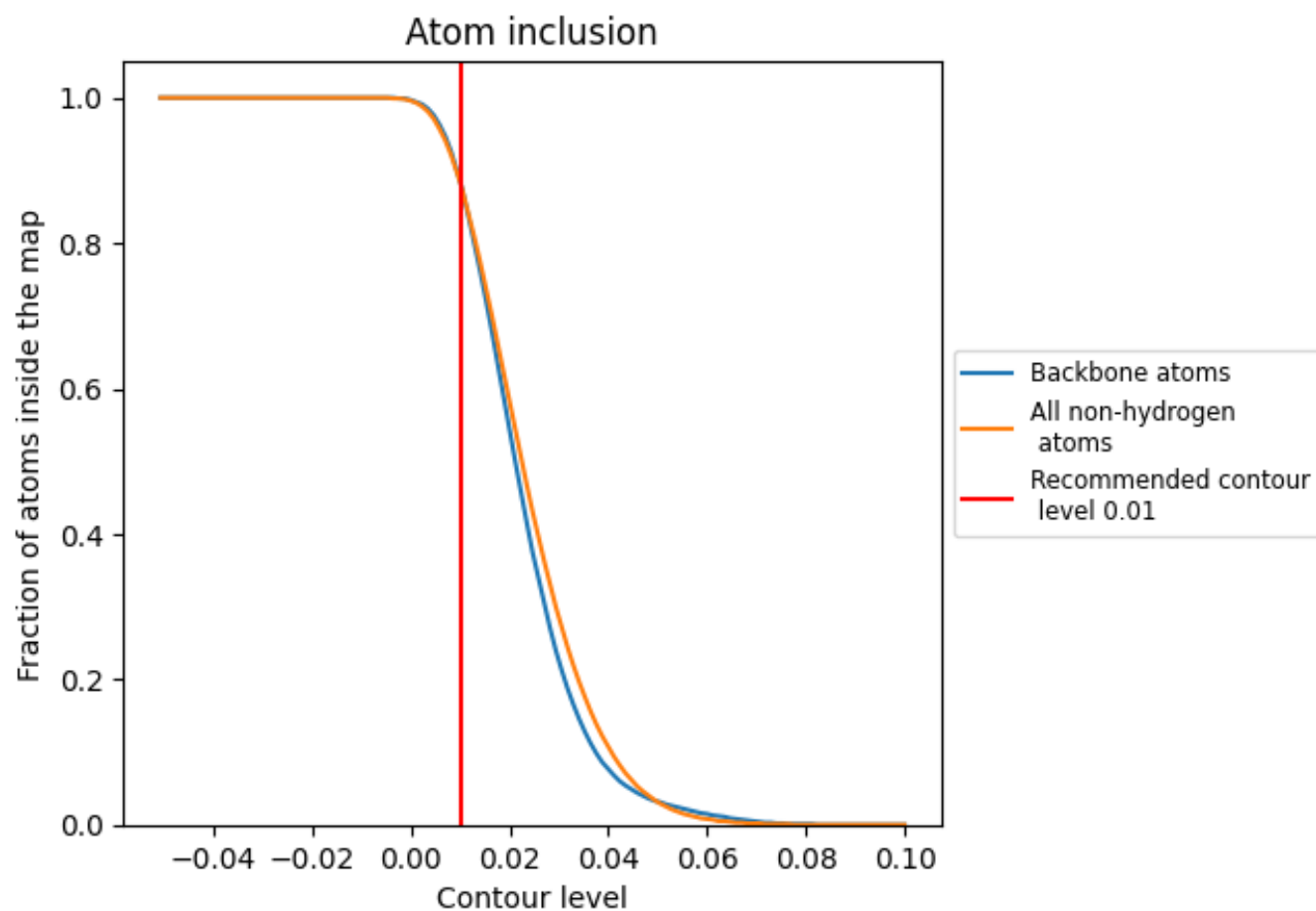
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8840	 0.5940
0	 0.8850	 0.6030
1	 0.9520	 0.6500
2	 0.9590	 0.6550
3	 0.9040	 0.6390
4	 0.5950	 0.4840
8	 0.7370	 0.5030
A	 0.6580	 0.5540
B	 0.8770	 0.5650
C	 0.5800	 0.5210
D	 0.8080	 0.5840
E	 0.5230	 0.4550
F	 0.8380	 0.6070
G	 0.7150	 0.5240
H	 0.6830	 0.5250
I	 0.8340	 0.5970
J	 0.8160	 0.5760
K	 0.6730	 0.5250
L	 0.8040	 0.5860
M	 0.7420	 0.5520
N	 0.7300	 0.5630
O	 0.8310	 0.5780
P	 0.8000	 0.5630
Q	 0.7170	 0.4770
R	 0.7460	 0.5250
S	 0.7900	 0.5700
T	 0.7150	 0.5420
U	 0.7630	 0.4910
V	 0.5870	 0.4900
X	 0.7690	 0.5170
Y	 0.7520	 0.5100
a	 0.9510	 0.6240
b	 0.9500	 0.6120
c	 0.9440	 0.6450
d	 0.9130	 0.6330



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Chain	Atom inclusion	Q-score
e	 0.8160	 0.5920
f	 0.7440	 0.5450
g	 0.7370	 0.5360
h	 0.7930	 0.5480
i	 0.9240	 0.6340
j	 0.8900	 0.6300
k	 0.8940	 0.6180
l	 0.9320	 0.6440
m	 0.9520	 0.6510
n	 0.8770	 0.5930
o	 0.8750	 0.6190
p	 0.9410	 0.6470
q	 0.8490	 0.6000
r	 0.9020	 0.6230
s	 0.8210	 0.5840
t	 0.7760	 0.5600
u	 0.8400	 0.5910
v	 0.9340	 0.6450
w	 0.8950	 0.6280
x	 0.7590	 0.5580
y	 0.8700	 0.6160
z	 0.8880	 0.6210