



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 04:20 PM JST

PDB ID : 9JPP / pdb_00009jpp
EMDB ID : EMD-61709
Title : Structure of the Bacterial Ribosome with human tRNA Lys(mcm5s2U34) and mRNA(AAG)
Authors : Ishiguro, K.; Mo, Y.; Shirouzu, M.; Suzuki, T.
Deposited on : 2024-09-26
Resolution : 2.26 Å(reported)
Based on initial model : 7y7e

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

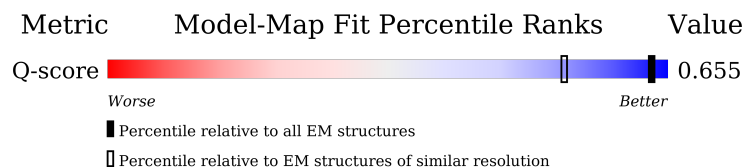
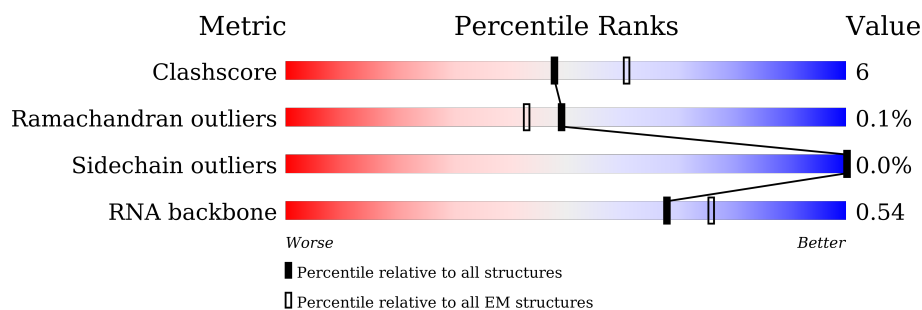
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.26 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	3535 (1.76 - 2.76)

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

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

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

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

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Mol	Chain	Length	Quality of chain
54	Z	77	5% 58% 27% 14%
55	V	76	46% 37% 11%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 142035 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		AltConf
56	A	99	Total	Mg	0
			99	99	
56	a	331	Total	Mg	0
			331	331	
56	b	7	Total	Mg	0
			7	7	
56	c	1	Total	Mg	0
			1	1	
56	d	1	Total	Mg	0
			1	1	
56	Z	3	Total	Mg	0
			3	3	
56	V	1	Total	Mg	0
			1	1	

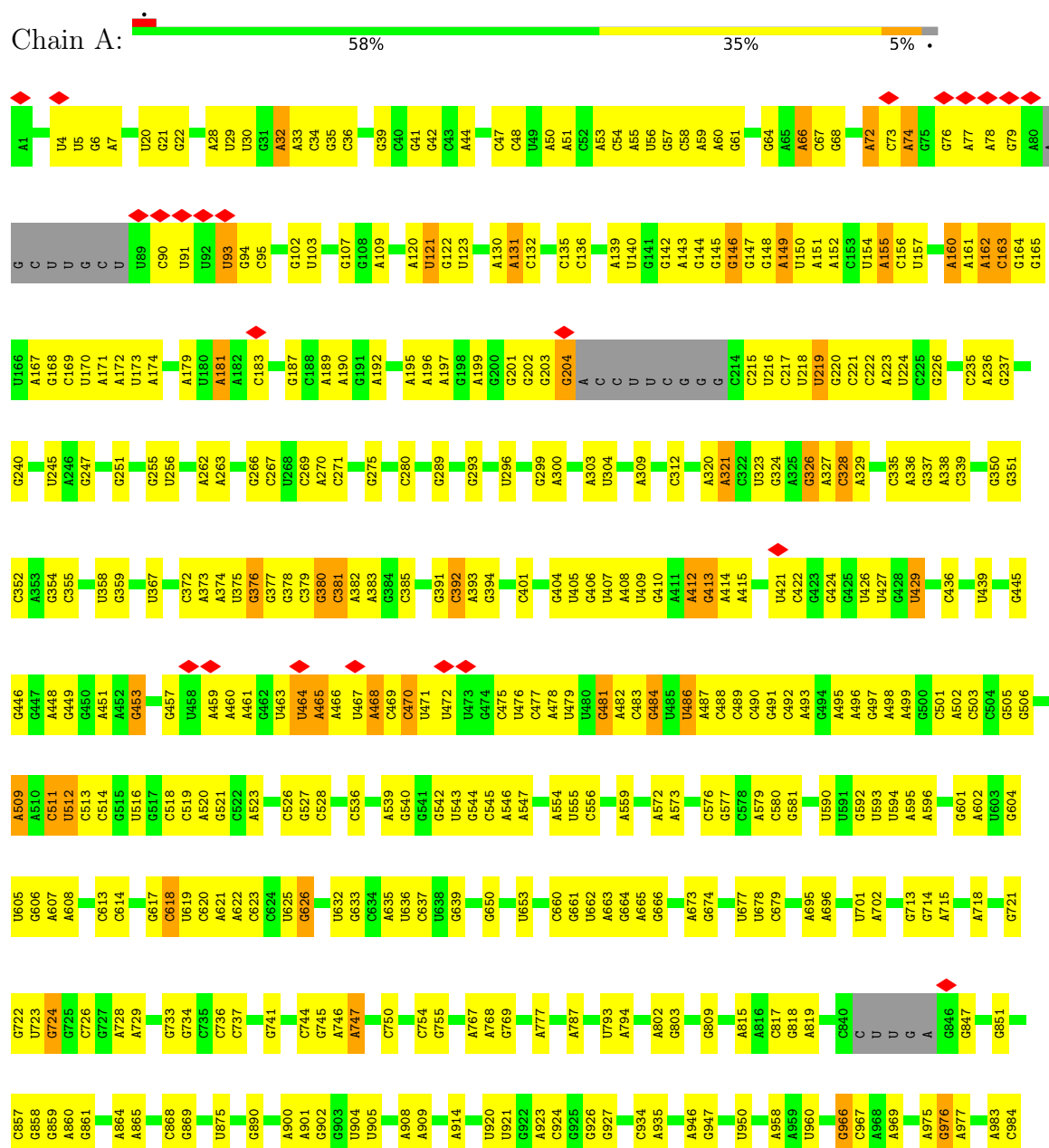
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

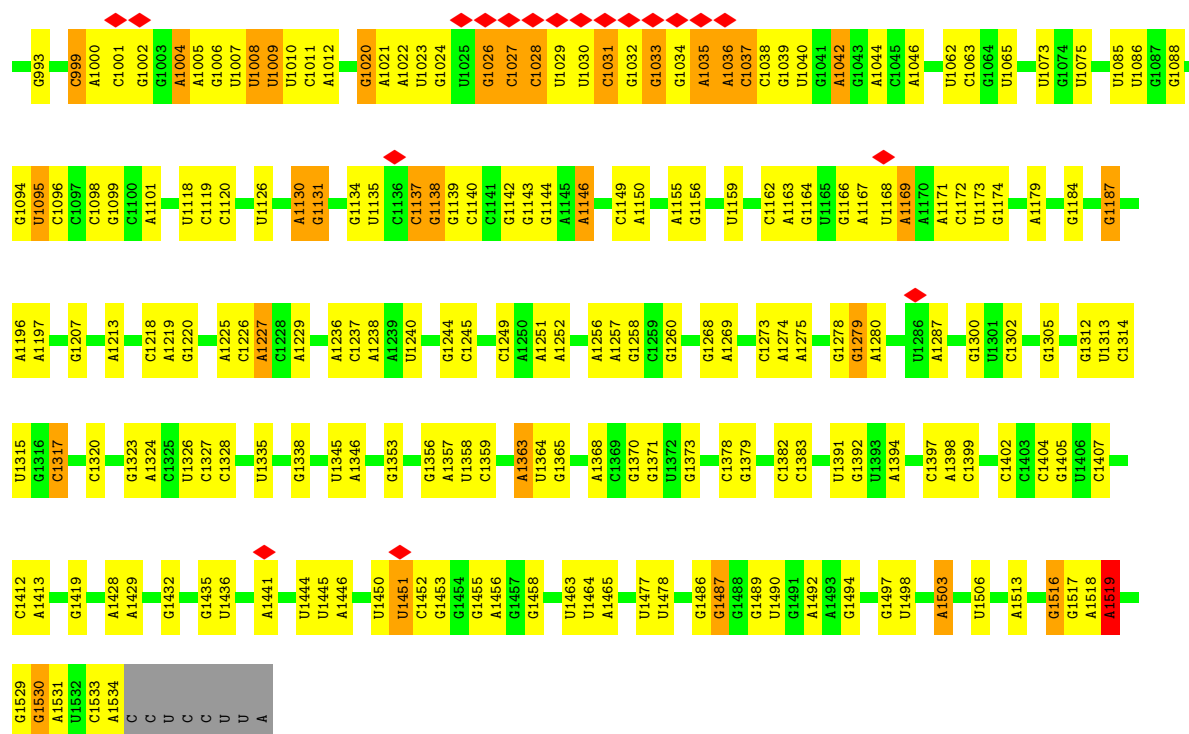
Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

3 Residue-property plots

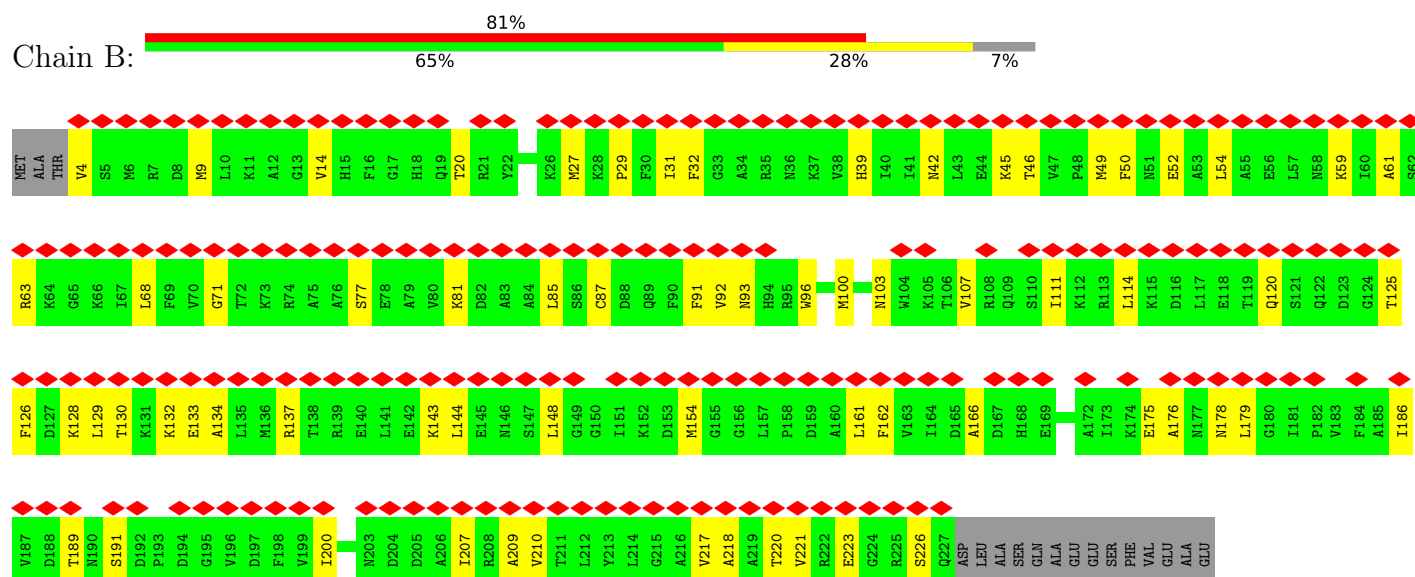
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

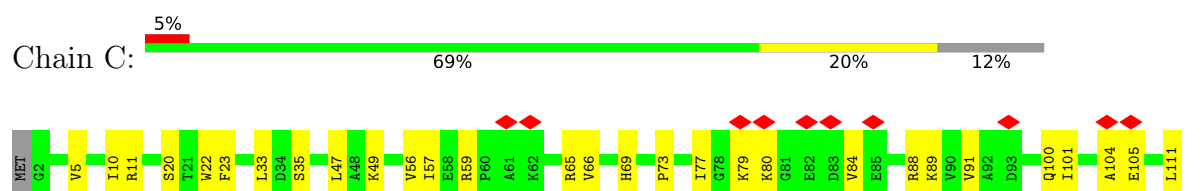


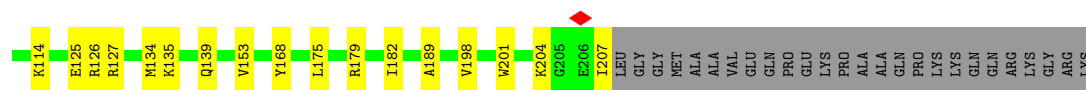


• Molecule 2: 30S ribosomal protein S2

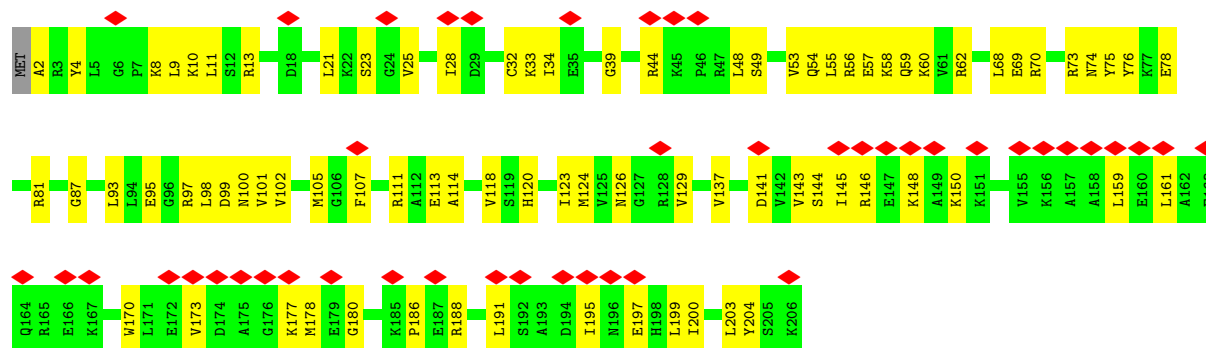


• Molecule 3: 30S ribosomal protein S3

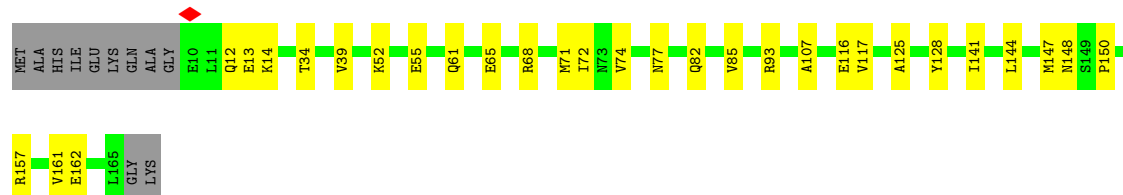
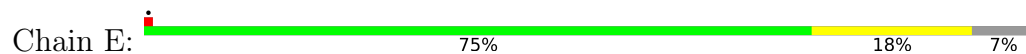




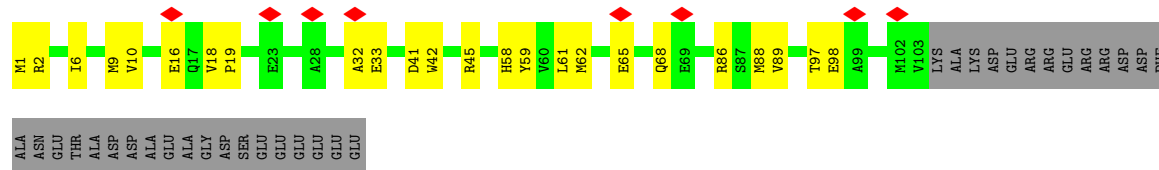
• Molecule 4: 30S ribosomal protein S4



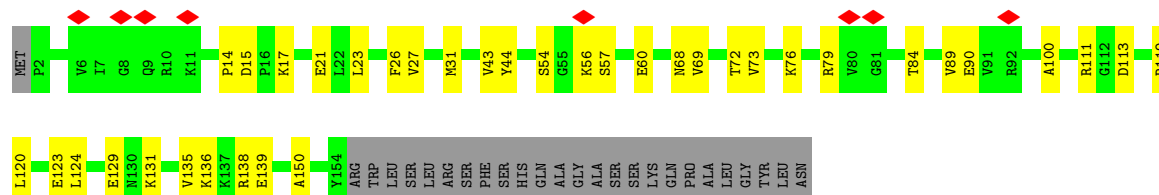
• Molecule 5: 30S ribosomal protein S5



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



• Molecule 7: 30S ribosomal protein S7



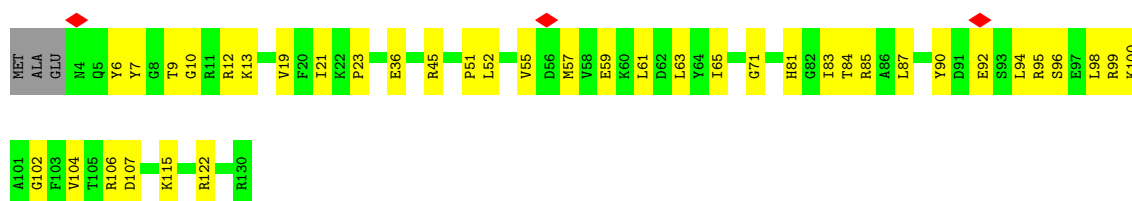
- Molecule 8: 30S ribosomal protein S8

Chain H: 



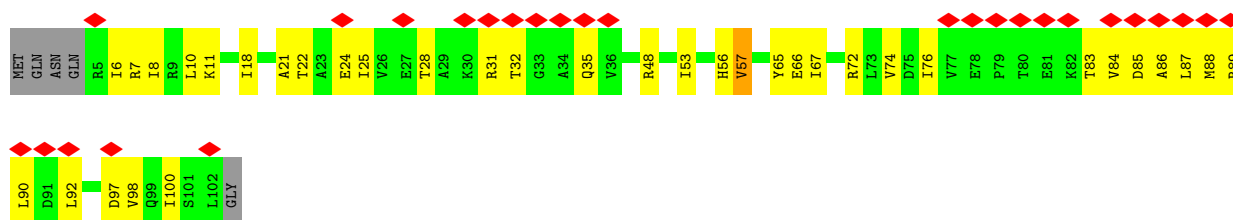
- Molecule 9: 30S ribosomal protein S9

Chain I: 



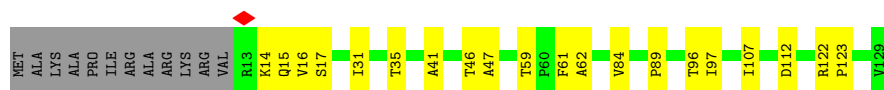
- Molecule 10: 30S ribosomal protein S10

Chain J: 



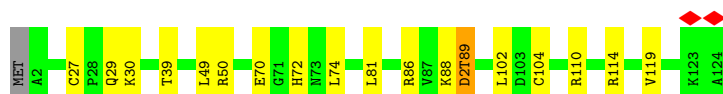
- Molecule 11: 30S ribosomal protein S11

Chain K: 



- Molecule 12: 30S ribosomal protein S12

Chain L: 

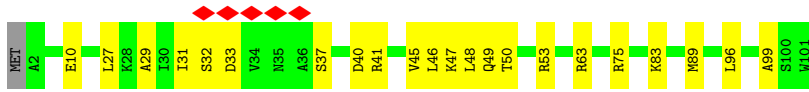
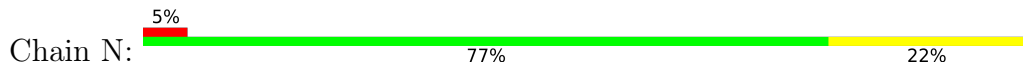


- Molecule 13: 30S ribosomal protein S13

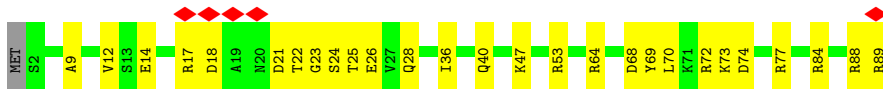
Chain M: 



- Molecule 14: 30S ribosomal protein S14



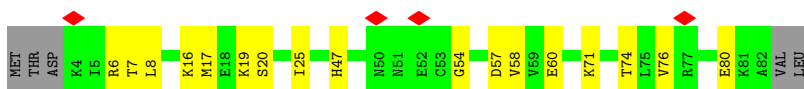
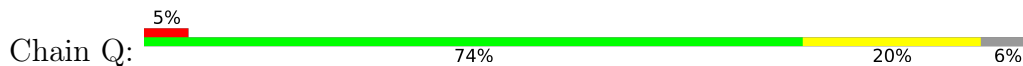
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



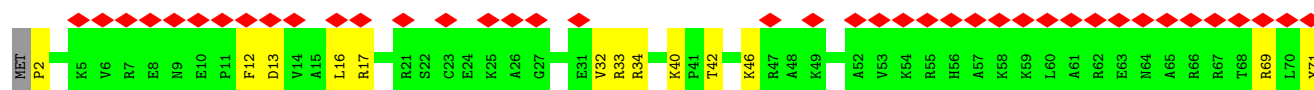
- Molecule 19: 30S ribosomal protein S19



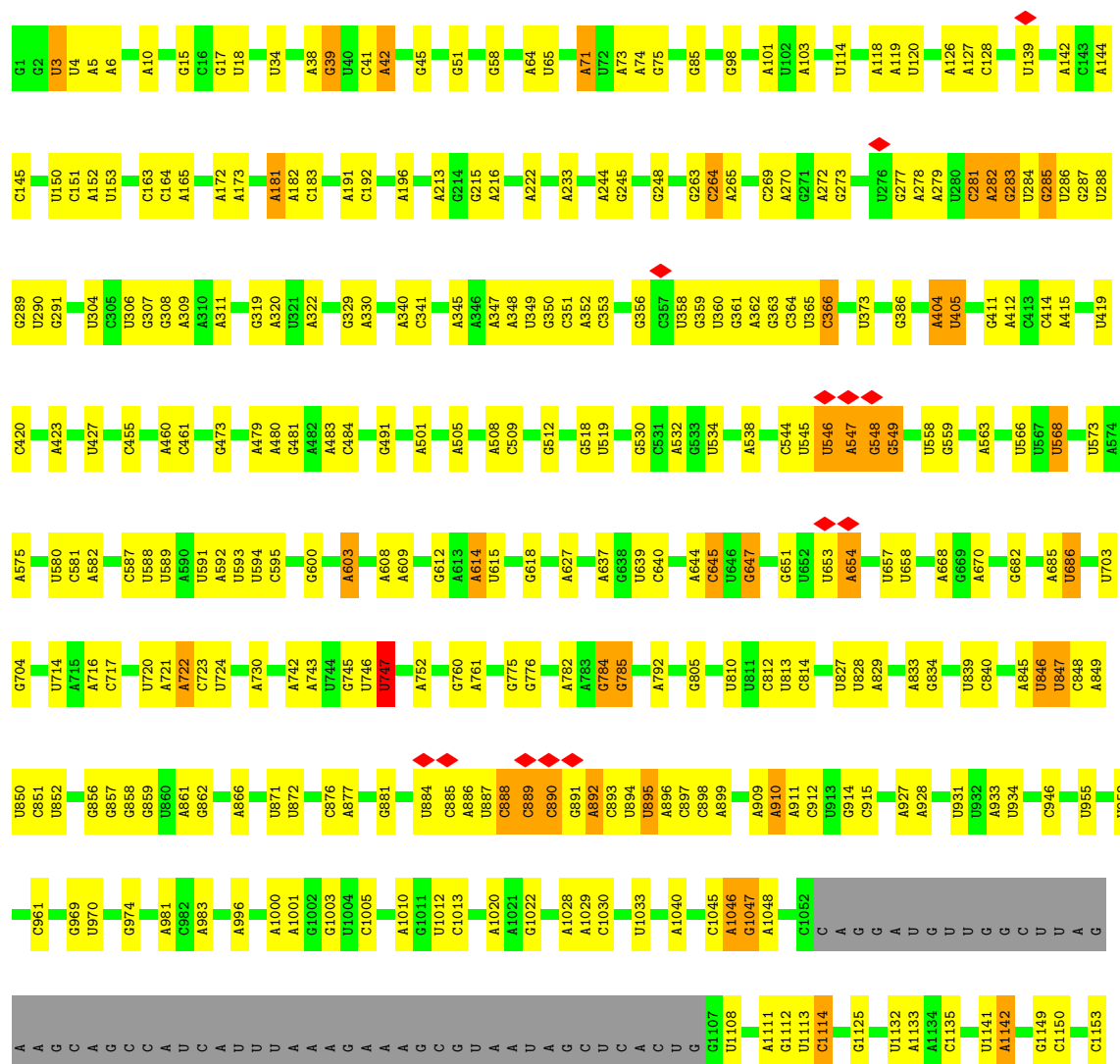
- Molecule 20: 30S ribosomal protein S20



- Chain U:  56% 80% 18%



- Chain a:  69% 24% 5%







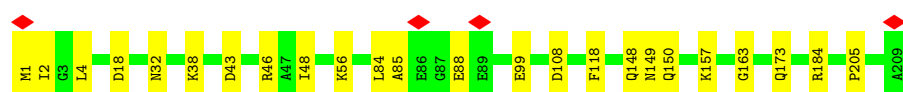
- Molecule 24: 50S ribosomal protein L2

Chain c: 90% 10%



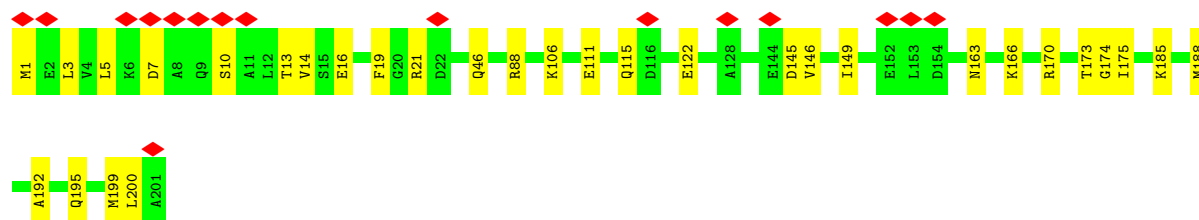
- Molecule 25: 50S ribosomal protein L3

Chain d: 89% 11%



- Molecule 26: 50S ribosomal protein L4

Chain e: 8% 85% 15%



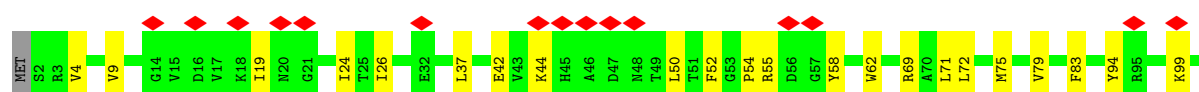
- Molecule 27: 50S ribosomal protein L5

Chain f: 74% 25%



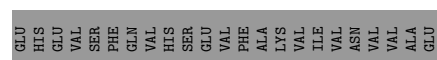
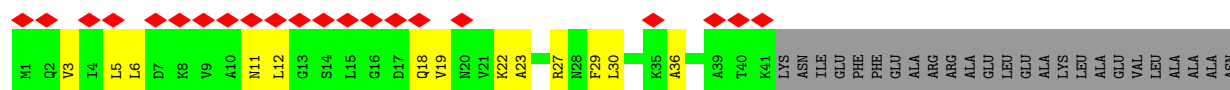
- Molecule 28: 50S ribosomal protein L6

Chain g: 12% 77% 22%

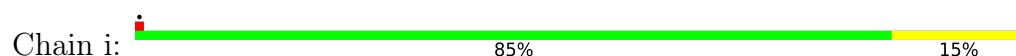




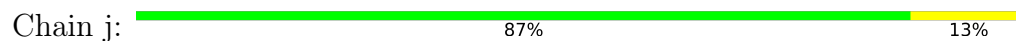
- Molecule 29: 50S ribosomal protein L9



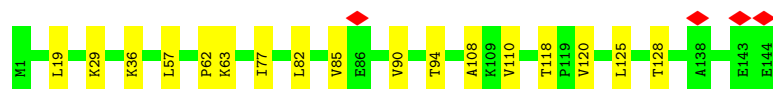
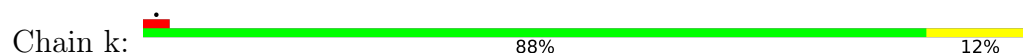
- Molecule 30: 50S ribosomal protein L13



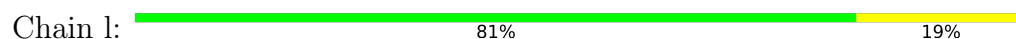
- Molecule 31: 50S ribosomal protein L14



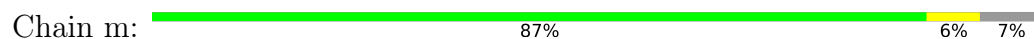
- Molecule 32: 50S ribosomal protein L15



- Molecule 33: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L17





- Molecule 35: 50S ribosomal protein L18

Chain n: 82% 16% ..



- Molecule 36: 50S ribosomal protein L19

Chain o: 81% 18% .



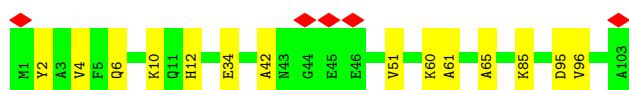
- Molecule 37: 50S ribosomal protein L20

Chain p: 92% 7% .



- Molecule 38: 50S ribosomal protein L21

Chain q: 5% 86% 14%



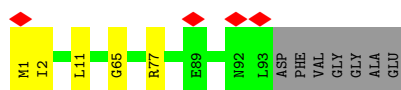
- Molecule 39: 50S ribosomal protein L22

Chain r: 91% 9%

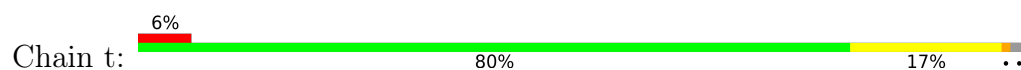


- Molecule 40: 50S ribosomal protein L23

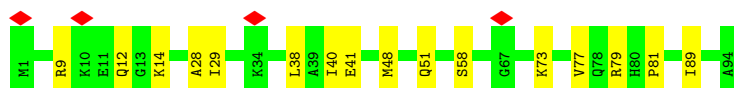
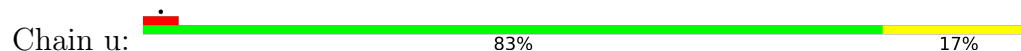
Chain s: 88% 5% 7%



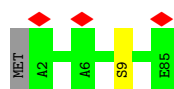
- Molecule 41: 50S ribosomal protein L24



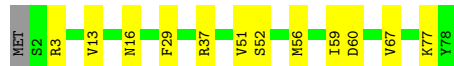
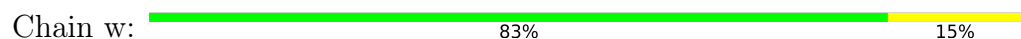
- Molecule 42: 50S ribosomal protein L25



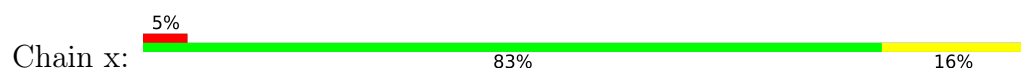
- Molecule 43: 50S ribosomal protein L27



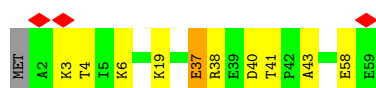
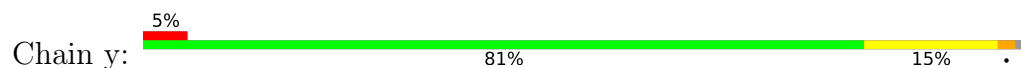
- Molecule 44: 50S ribosomal protein L28



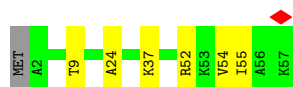
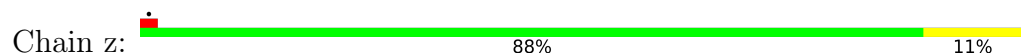
- Molecule 45: 50S ribosomal protein L29



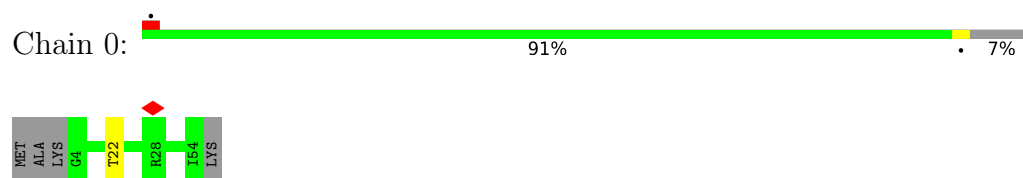
- Molecule 46: 50S ribosomal protein L30



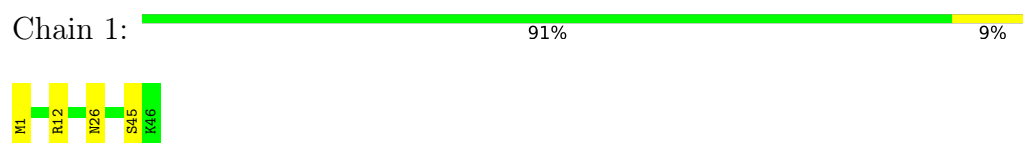
- Molecule 47: 50S ribosomal protein L32



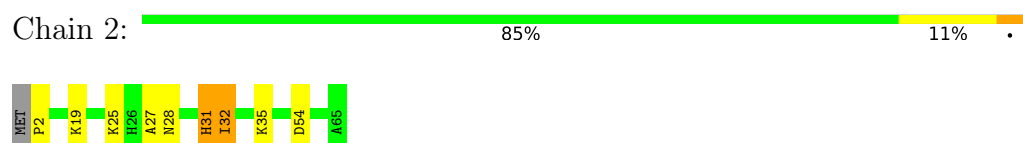
- Molecule 48: 50S ribosomal protein L33



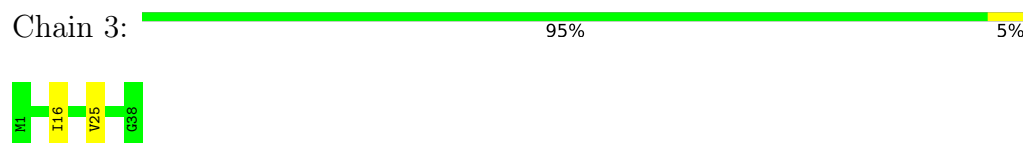
- Molecule 49: 50S ribosomal protein L34



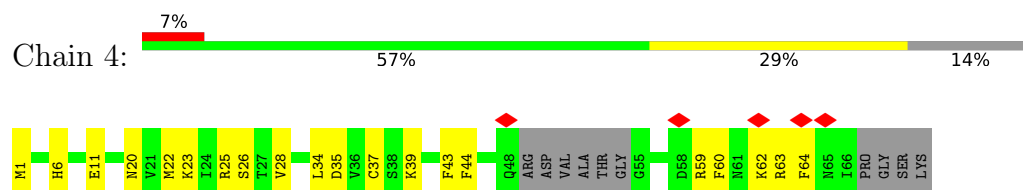
- Molecule 50: 50S ribosomal protein L35



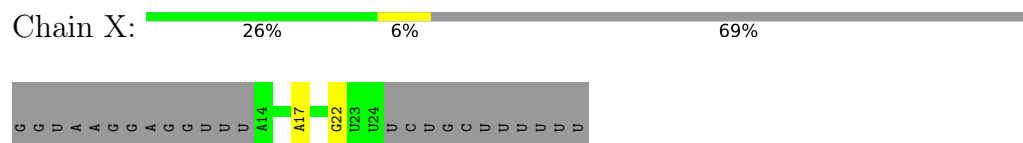
- Molecule 51: 50S ribosomal protein L36



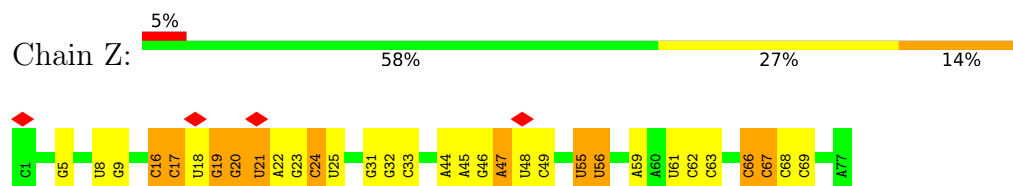
- Molecule 52: 50S ribosomal protein L31



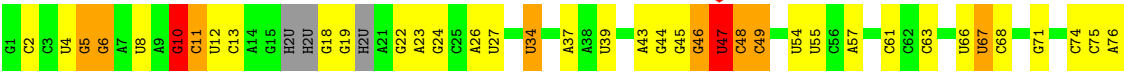
- Molecule 53: mRNA



- Molecule 54: P-site tRNA-fMet



● Molecule 55: A-site tRNA-Lys



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	517738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0169	Depositor
Map size (Å)	439.10498, 439.10498, 439.10498	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8285, 0.8285, 0.8285	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/36073	0.42	0/56264
2	B	0.24	0/1784	0.51	0/2403
3	C	0.39	0/1651	0.54	0/2225
4	D	0.30	0/1665	0.51	0/2227
5	E	0.44	0/1165	0.57	0/1568
6	F	0.35	0/858	0.58	0/1160
7	G	0.34	0/1219	0.53	0/1635
8	H	0.38	0/989	0.49	0/1326
9	I	0.38	0/1034	0.59	0/1375
10	J	0.39	0/796	0.74	4/1077 (0.4%)
11	K	0.37	0/884	0.57	0/1191
12	L	0.35	0/960	0.53	0/1286
13	M	0.37	0/900	0.56	0/1204
14	N	0.40	0/817	0.55	0/1088
15	O	0.38	0/722	0.56	0/964
16	P	0.32	0/653	0.63	0/877
17	Q	0.35	0/650	0.53	0/871
18	R	0.38	0/553	0.56	0/742
19	S	0.35	0/685	0.50	0/922
20	T	0.30	0/676	0.50	0/895
21	U	0.23	0/597	0.51	0/792
22	a	0.60	0/65842	0.47	1/102711 (0.0%)
23	b	0.47	0/2850	0.39	0/4444
24	c	0.46	0/2121	0.54	0/2852
25	d	0.44	0/1576	0.51	0/2119
26	e	0.39	0/1571	0.50	0/2113
27	f	0.34	0/1434	0.49	0/1926
28	g	0.33	0/1343	0.51	0/1816
29	h	0.33	0/306	0.60	0/413
30	i	0.45	0/1152	0.50	0/1551
31	j	0.46	0/955	0.55	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	k	0.46	0/1062	0.54	0/1413
33	l	0.44	0/1073	0.51	0/1433
34	m	0.46	0/958	0.54	0/1281
35	n	0.37	0/902	0.50	0/1209
36	o	0.45	0/929	0.53	0/1242
37	p	0.51	0/960	0.51	0/1278
38	q	0.45	0/829	0.56	0/1107
39	r	0.45	0/864	0.51	0/1156
40	s	0.40	0/744	0.56	0/994
41	t	0.37	0/787	0.61	2/1051 (0.2%)
42	u	0.40	0/766	0.52	0/1025
43	v	0.45	0/642	0.48	0/848
44	w	0.45	0/635	0.50	0/848
45	x	0.38	0/502	0.56	0/667
46	y	0.44	0/453	0.73	1/605 (0.2%)
47	z	0.44	0/450	0.51	0/599
48	0	0.42	0/424	0.52	0/565
49	1	0.49	0/380	0.57	0/498
50	2	0.47	0/513	0.56	0/676
51	3	0.45	0/303	0.52	0/397
52	4	0.30	0/488	0.50	0/649
53	X	0.48	0/261	0.40	0/404
54	Z	0.41	0/1725	0.37	0/2687
55	V	0.35	0/1429	0.40	0/2217
All	All	0.51	0/152560	0.47	8/228165 (0.0%)

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

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	512	G	O4'-C1'-N9	6.15	117.42	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	y	37	GLU	CA-CB-CG	6.04	126.17	114.10
10	J	87	LEU	CA-C-N	-5.80	112.23	122.26
10	J	87	LEU	C-N-CA	-5.80	112.23	122.26
41	t	98	SER	CA-C-N	5.73	132.48	121.54
41	t	98	SER	C-N-CA	5.73	132.48	121.54
10	J	53	ILE	CA-C-N	-5.19	107.00	122.71
10	J	53	ILE	C-N-CA	-5.19	107.00	122.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	31	HIS	Peptide
13	M	65	VAL	Peptide
44	w	16	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32466	0	16359	353	0
2	B	1753	0	1780	48	0
3	C	1624	0	1696	30	0
4	D	1643	0	1707	70	0
5	E	1152	0	1196	22	0
6	F	839	0	833	16	0
7	G	1203	0	1254	23	0
8	H	979	0	1031	17	0
9	I	1022	0	1070	29	0
10	J	786	0	828	32	0
11	K	877	0	884	14	0
12	L	957	0	1017	13	0
13	M	891	0	952	19	0
14	N	805	0	844	23	0
15	O	714	0	734	20	0
16	P	643	0	661	17	0
17	Q	641	0	682	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	544	0	565	10	0
19	S	668	0	693	16	0
20	T	670	0	719	14	0
21	U	589	0	629	10	0
22	a	59301	0	29850	340	0
23	b	2549	0	1291	18	0
24	c	2082	0	2154	17	0
25	d	1566	0	1618	19	0
26	e	1552	0	1619	22	0
27	f	1410	0	1444	34	0
28	g	1323	0	1371	29	0
29	h	303	0	327	13	0
30	i	1129	0	1162	15	0
31	j	946	0	1023	11	0
32	k	1053	0	1129	16	0
33	l	1075	0	1144	16	0
34	m	945	0	989	5	0
35	n	892	0	923	16	0
36	o	917	0	962	16	0
37	p	947	0	1019	5	0
38	q	816	0	839	8	0
39	r	857	0	922	7	0
40	s	738	0	807	3	0
41	t	779	0	831	11	0
42	u	753	0	780	10	0
43	v	634	0	653	1	0
44	w	625	0	652	8	0
45	x	501	0	531	7	0
46	y	449	0	488	8	0
47	z	444	0	458	5	0
48	0	417	0	451	1	0
49	1	377	0	418	4	0
50	2	504	0	572	7	0
51	3	302	0	340	1	0
52	4	480	0	478	19	0
53	X	234	0	118	1	0
54	Z	1645	0	842	16	0
55	V	1579	0	820	18	0
56	A	99	0	0	0	0
56	V	1	0	0	0	0
56	Z	3	0	0	0	0
56	a	331	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	b	7	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
57	3	1	0	0	0	0
57	4	1	0	0	0	0
All	All	142035	0	95159	1370	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 (1370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2100:G:H1	22:a:2189:U:H3	1.03	0.98
22:a:2102:G:H1	22:a:2187:U:H3	0.99	0.96
1:A:1009:U:H3	1:A:1020:G:H1	1.09	0.91
23:b:51:G:OP1	35:n:63:LYS:NZ	2.04	0.90
14:N:49:GLN:HE22	19:S:12:ASP:HA	1.37	0.90
1:A:1373:G:H4'	7:G:31:MET:HE1	1.56	0.86
53:X:22:G:H22	55:V:34:70U:HN3	1.20	0.85
1:A:107:G:H1	20:T:6:SER:HG	0.85	0.84
1:A:1086:U:H3	1:A:1099:G:H22	1.24	0.84
7:G:76:LYS:HE3	7:G:89:VAL:HG21	1.60	0.84
1:A:718:A:H2	18:R:38:LYS:HZ2	1.25	0.83
5:E:157:ARG:NH2	8:H:43:GLU:OE2	2.11	0.83
22:a:1417:C:HO2'	22:a:1587:G:HO2'	1.25	0.82
10:J:66:GLU:HG2	14:N:99:ALA:HB2	1.61	0.82
1:A:64:G:OP1	1:A:382:A:N6	2.13	0.81
1:A:4:U:H2'	1:A:5:U:H2'	1.64	0.80
1:A:407:U:O2'	4:D:113:GLU:OE1	1.99	0.80
3:C:168:TYR:OH	5:E:55:GLU:OE2	2.00	0.80
1:A:275:G:H5'	17:Q:16:LYS:HE3	1.63	0.79
22:a:881:G:O6	22:a:895:U:O4	2.00	0.79
1:A:324:G:N1	1:A:327:A:OP2	2.15	0.79
1:A:544:G:OP1	4:D:56:ARG:NH2	2.15	0.79
1:A:1028:C:N4	1:A:1033:G:O6	2.15	0.79
22:a:2100:G:N2	22:a:2189:U:O2	2.14	0.79
42:u:77:VAL:HG12	42:u:89:ILE:HG12	1.65	0.79
10:J:85:ASP:OD1	10:J:86:ALA:N	2.17	0.78
22:a:1800:C:OP2	24:c:182:ARG:NH1	2.17	0.78
28:g:19:ILE:HG12	28:g:24:ILE:HD12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:C:OP2	31:j:98:ARG:NH1	2.17	0.78
25:d:184:ARG:NH1	36:o:11:GLU:OE2	2.17	0.78
22:a:2305:U:H5''	27:f:131:GLY:HA3	1.63	0.78
22:a:881:G:H1	22:a:895:U:H3	0.79	0.76
41:t:18:ASP:OD1	41:t:21:LYS:NZ	2.18	0.76
9:I:106:ARG:NH1	9:I:107:ASP:O	2.17	0.76
1:A:1027:C:H2'	1:A:1028:C:C6	2.21	0.75
46:y:6:LYS:HB2	46:y:58:GLU:HG2	1.66	0.75
1:A:427:U:OP1	4:D:13:ARG:NH2	2.19	0.75
1:A:76:G:H1	1:A:93:U:H3	1.34	0.75
1:A:107:G:N1	20:T:6:SER:OG	2.11	0.75
4:D:28:ILE:HG23	4:D:34:ILE:HD11	1.67	0.75
54:Z:5:G:N1	54:Z:69:C:N3	2.27	0.75
22:a:2830:C:H5''	25:d:56:LYS:HE3	1.68	0.75
31:j:71:ARG:NH2	31:j:123:LEU:O	2.19	0.74
1:A:1229:A:OP2	13:M:113:ARG:NH1	2.20	0.74
1:A:147:G:H2'	1:A:148:G:C8	2.21	0.74
32:k:77:ILE:HD11	32:k:108:ALA:HB1	1.70	0.73
15:O:69:TYR:CZ	15:O:73:LYS:HD2	2.22	0.73
29:h:23:ALA:O	29:h:27:ARG:HG2	1.88	0.73
39:r:4:ILE:HG13	39:r:106:VAL:HG22	1.70	0.73
2:B:68:LEU:HD12	2:B:154:MET:HE1	1.69	0.73
1:A:677:U:H3	1:A:713:G:H22	1.34	0.73
27:f:176:PRO:HB3	52:4:44:PHE:HE1	1.52	0.73
22:a:286:U:H2'	22:a:287:G:H8	1.54	0.73
22:a:1478:G:H1	22:a:1513:U:H3	1.33	0.73
27:f:158:THR:HG22	27:f:160:ALA:H	1.54	0.73
22:a:546:U:H3'	22:a:547:A:H8	1.53	0.72
1:A:309:A:O2'	1:A:607:A:N1	2.23	0.72
47:z:54:VAL:HG23	47:z:55:ILE:HG12	1.70	0.72
14:N:32:SER:O	14:N:41:ARG:NH1	2.23	0.72
1:A:1135:U:O2	1:A:1138:G:N1	2.19	0.72
1:A:664:G:H22	1:A:741:G:H1	1.38	0.71
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.72	0.71
10:J:28:THR:HA	10:J:31:ARG:HE	1.53	0.71
7:G:79:ARG:HB3	7:G:84:THR:HG22	1.70	0.71
17:Q:7:THR:OG1	17:Q:60:GLU:OE2	2.05	0.71
27:f:46:ASP:HB3	27:f:49:LEU:HG	1.72	0.71
3:C:77:ILE:HA	3:C:84:VAL:HG13	1.72	0.71
10:J:88:MET:SD	10:J:89:ARG:NH1	2.63	0.71
14:N:37:SER:OG	14:N:40:ASP:OD2	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2298:A:OP1	27:f:71:ARG:NH2	2.23	0.71
3:C:35:SER:OG	3:C:59:ARG:NH2	2.24	0.70
1:A:477:C:H2'	1:A:478:A:C8	2.26	0.70
7:G:129:GLU:HB2	7:G:131:LYS:HD3	1.74	0.70
10:J:84:VAL:HG22	10:J:88:MET:HE1	1.74	0.70
13:M:77:ILE:HG22	13:M:81:MET:HE2	1.73	0.70
54:Z:5:G:O6	54:Z:69:C:N4	2.17	0.70
1:A:160:A:H2'	1:A:161:A:O4'	1.92	0.70
22:a:1799:G:O2'	24:c:180:GLU:OE2	2.10	0.70
1:A:56:U:H2'	1:A:57:G:C8	2.27	0.69
27:f:176:PRO:HB3	52:4:44:PHE:CE1	2.27	0.69
22:a:612:G:O2'	22:a:614:A:N7	2.20	0.69
22:a:2204:G:OP2	24:c:147:LYS:NZ	2.25	0.69
22:a:1434:A:H2'	22:a:1435:G:C8	2.28	0.68
1:A:673:A:H2'	1:A:674:G:C8	2.29	0.68
24:c:232:HIS:HA	24:c:242:LYS:HE3	1.76	0.68
1:A:476:U:H2'	1:A:477:C:C6	2.29	0.68
9:I:19:VAL:HG22	9:I:65:ILE:HD12	1.76	0.68
1:A:635:A:H2'	1:A:636:U:H6	1.59	0.67
26:e:1:MET:HE2	26:e:16:GLU:HA	1.75	0.67
16:P:18:GLN:CD	16:P:35:ARG:HE	2.03	0.67
1:A:426:U:OP1	4:D:33:LYS:NZ	2.16	0.67
5:E:13:GLU:OE2	5:E:68:ARG:NH2	2.27	0.67
22:a:534:U:O2'	37:p:49:ASP:OD2	2.10	0.67
5:E:14:LYS:NZ	5:E:116:GLU:OE2	2.28	0.67
7:G:113:ASP:HB2	7:G:119:ARG:HG3	1.77	0.67
22:a:1871:A:H2'	22:a:1872:A:C8	2.29	0.67
14:N:49:GLN:NE2	19:S:12:ASP:OD1	2.28	0.66
22:a:1870:C:O2'	22:a:1871:A:O4'	2.14	0.66
40:s:11:LEU:O	45:x:29:ARG:NH2	2.27	0.66
36:o:27:GLU:OE1	36:o:87:LYS:NZ	2.27	0.66
51:3:16:ILE:HD13	51:3:25:VAL:HG22	1.78	0.66
26:e:149:ILE:HB	26:e:188:MET:HG3	1.78	0.66
35:n:16:ARG:NH1	35:n:19:GLN:OE1	2.24	0.66
22:a:2328:A:H2'	22:a:2329:U:C6	2.31	0.66
5:E:12:GLN:NE2	5:E:117:VAL:HA	2.11	0.66
19:S:41:PHE:H	19:S:44:MET:HE3	1.61	0.65
15:O:64:ARG:NH2	15:O:68:ASP:OD1	2.26	0.65
22:a:286:U:H2'	22:a:287:G:C8	2.31	0.65
22:a:1141:U:H4'	22:a:1142:A:O4'	1.96	0.65
37:p:86:ALA:HB2	37:p:116:ALA:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:A:O2'	1:A:296:U:OP1	2.13	0.65
1:A:1038:C:H2'	1:A:1039:G:H8	1.60	0.65
9:I:57:MET:HE2	9:I:61:LEU:HD11	1.79	0.65
30:i:9:GLU:HG2	30:i:10:THR:HG23	1.79	0.65
22:a:2547:A:H2'	22:a:2548:U:C6	2.32	0.65
4:D:95:GLU:HG3	4:D:191:LEU:HD21	1.78	0.65
13:M:107:ARG:NH2	13:M:110:LYS:HE2	2.11	0.65
45:x:13:GLU:HA	45:x:16:THR:HG22	1.79	0.65
1:A:131:A:H2'	1:A:132:C:C6	2.32	0.64
22:a:2095:A:O5'	29:h:11:ASN:ND2	2.30	0.64
28:g:121:ILE:HD12	28:g:141:ILE:HD13	1.77	0.64
30:i:11:VAL:HG21	30:i:50:THR:HA	1.79	0.64
4:D:95:GLU:OE1	4:D:100:ASN:ND2	2.30	0.64
55:V:23:A:H2'	55:V:24:G:C8	2.32	0.64
19:S:11:ILE:HG13	19:S:38:SER:HB3	1.79	0.64
24:c:107:PRO:HD2	24:c:110:LEU:HD22	1.80	0.64
29:h:5:LEU:HD21	29:h:12:LEU:HD11	1.79	0.64
4:D:107:PHE:HD1	4:D:159:LEU:HD11	1.63	0.64
5:E:82:GLN:HG3	5:E:148:ASN:O	1.98	0.64
39:r:73:LYS:HB2	39:r:106:VAL:HB	1.80	0.64
1:A:157:U:H1'	1:A:165:G:N2	2.13	0.64
4:D:73:ARG:NH1	4:D:74:ASN:OD1	2.31	0.64
11:K:35:THR:HG22	11:K:41:ALA:HA	1.78	0.64
25:d:46:ARG:NH1	25:d:85:ALA:O	2.21	0.64
1:A:1031:C:O3'	1:A:1032:G:N2	2.31	0.64
14:N:49:GLN:HE22	19:S:12:ASP:CA	2.11	0.64
1:A:1373:G:H4'	7:G:31:MET:CE	2.28	0.64
4:D:57:GLU:HG2	4:D:60:LYS:HE3	1.80	0.64
4:D:102:VAL:HG23	4:D:107:PHE:HD2	1.63	0.64
1:A:618:C:H5'	1:A:619:U:H5''	1.79	0.63
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.80	0.63
22:a:639:U:H2'	22:a:640:C:C6	2.34	0.63
22:a:1509:A:HO2'	22:a:1510:G:H8	1.47	0.63
10:J:85:ASP:HA	10:J:88:MET:SD	2.38	0.63
12:L:29:GLN:HG2	12:L:81:LEU:HD21	1.80	0.63
54:Z:5:G:N2	54:Z:69:C:O2	2.21	0.63
4:D:87:GLY:HA3	4:D:197:GLU:HG3	1.80	0.63
1:A:459:A:H2'	1:A:460:A:C8	2.34	0.63
1:A:946:A:H2'	1:A:947:G:C8	2.32	0.63
1:A:1530:G:N7	21:U:46:LYS:HE2	2.13	0.63
33:l:14:LYS:O	33:l:71:LYS:NZ	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:A:H2'	1:A:636:U:C6	2.33	0.63
10:J:6:ILE:HB	10:J:76:ILE:HG22	1.81	0.63
1:A:606:G:N2	1:A:632:U:OP1	2.28	0.62
3:C:73:PRO:HG3	3:C:105:GLU:OE1	1.99	0.62
1:A:382:A:H2'	1:A:383:A:C8	2.35	0.62
1:A:1323:G:H2'	1:A:1324:A:C8	2.34	0.62
1:A:1516:2MG:N1	1:A:1519:MA6:OP2	2.32	0.62
1:A:636:U:OP1	17:Q:6:ARG:NH2	2.32	0.62
28:g:55:ARG:HB2	28:g:58:TYR:HD2	1.64	0.62
1:A:350:G:H2'	1:A:351:G:C8	2.34	0.62
4:D:118:VAL:HG22	4:D:123:ILE:HG13	1.80	0.62
5:E:34:THR:HG22	5:E:52:LYS:HG2	1.81	0.62
26:e:46:GLN:O	26:e:88:ARG:NH1	2.33	0.62
4:D:102:VAL:HG13	4:D:114:ALA:HB1	1.80	0.62
22:a:1607:C:N4	22:a:1622:G:OP2	2.22	0.62
28:g:52:PHE:CE2	28:g:72:LEU:HD12	2.35	0.62
41:t:81:ASP:OD1	41:t:82:ARG:N	2.32	0.62
1:A:1023:U:H2'	1:A:1024:G:C8	2.34	0.62
22:a:284:U:H2'	22:a:285:G:C8	2.35	0.62
28:g:52:PHE:HE2	28:g:72:LEU:HD12	1.65	0.62
30:i:125:TYR:OH	30:i:132:HIS:NE2	2.15	0.62
1:A:1004:A:H2'	1:A:1005:A:C8	2.34	0.61
1:A:1359:C:OP2	14:N:75:ARG:NE	2.31	0.61
1:A:392:C:H5'	16:P:13:LYS:HZ2	1.64	0.61
7:G:57:SER:OG	7:G:60:GLU:OE1	2.15	0.61
22:a:153:U:OP1	44:w:77:LYS:NZ	2.25	0.61
1:A:453:G:OP1	16:P:76:LYS:NZ	2.25	0.61
52:4:20:ASN:ND2	52:4:37:CYS:SG	2.73	0.61
1:A:1356:G:H2'	1:A:1357:A:C8	2.36	0.61
11:K:59:THR:HG22	11:K:61:PHE:H	1.64	0.61
22:a:1405:U:H2'	22:a:1406:U:C6	2.36	0.61
14:N:27:LEU:O	14:N:31:ILE:HG12	1.99	0.61
55:V:4:U:O2'	55:V:5:G:H8	1.83	0.61
55:V:43:A:H2'	55:V:44:G:C8	2.36	0.61
22:a:1720:U:H2'	22:a:1721:G:O4'	2.01	0.61
27:f:106:ILE:HD11	52:4:22:MET:HE3	1.82	0.61
12:L:27:CYS:SG	12:L:30:LYS:NZ	2.63	0.61
1:A:1021:A:H2'	1:A:1022:A:H8	1.66	0.61
1:A:1317:C:H4'	14:N:48:LEU:HD21	1.82	0.61
33:l:1:MET:SD	33:l:44:ARG:HD3	2.41	0.60
6:F:61:LEU:HD23	6:F:62:MET:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:44:ILE:HD11	27:f:79:ILE:HG22	1.83	0.60
5:E:82:GLN:NE2	5:E:150:PRO:HD3	2.16	0.60
1:A:745:G:H2'	1:A:746:A:C8	2.36	0.60
22:a:2291:U:H2'	22:a:2292:U:C6	2.36	0.60
7:G:68:ASN:O	7:G:138:ARG:NH1	2.34	0.60
15:O:88:ARG:NH2	22:a:714:U:OP2	2.34	0.60
3:C:134:MET:HE2	3:C:168:TYR:HD1	1.65	0.60
1:A:714:G:H2'	1:A:715:A:C8	2.37	0.60
8:H:77:ARG:NE	8:H:79:SER:O	2.33	0.60
36:o:111:LYS:NZ	36:o:112:GLU:O	2.34	0.60
4:D:100:ASN:OD1	4:D:111:ARG:NH2	2.32	0.60
16:P:40:ASN:HB3	16:P:43:ALA:HB2	1.83	0.60
22:a:126:A:OP1	49:1:45:SER:OG	2.20	0.60
22:a:2327:A:H2'	22:a:2328:A:C8	2.36	0.60
46:y:3:LYS:HE2	46:y:40:ASP:HB3	1.83	0.60
8:H:7:ILE:HB	8:H:77:ARG:NH1	2.17	0.60
22:a:856:G:H2'	22:a:857:G:C8	2.37	0.60
26:e:3:LEU:HD12	26:e:14:VAL:HG11	1.84	0.60
45:x:37:LEU:HD11	45:x:42:LEU:HD12	1.83	0.60
26:e:1:MET:HE1	26:e:19:PHE:C	2.26	0.59
28:g:44:LYS:O	28:g:50:LEU:HA	2.02	0.59
22:a:348:A:H2'	22:a:349:U:O4'	2.01	0.59
1:A:1166:G:N1	1:A:1169:A:OP2	2.34	0.59
16:P:22:ALA:HA	16:P:33:ILE:HD12	1.84	0.59
19:S:12:ASP:OD2	19:S:35:SER:OG	2.16	0.59
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.84	0.59
22:a:85:G:OP2	41:t:7:ARG:NE	2.29	0.59
22:a:876:C:H2'	22:a:877:A:O4'	2.02	0.59
22:a:2193:G:H2'	22:a:2194:U:C6	2.37	0.59
46:y:37:GLU:O	46:y:38:ARG:NH1	2.36	0.59
52:4:20:ASN:HD21	52:4:39:LYS:HB3	1.66	0.59
14:N:49:GLN:NE2	19:S:12:ASP:HA	2.15	0.59
1:A:459:A:H2'	1:A:460:A:H8	1.67	0.59
15:O:14:GLU:CD	15:O:84:ARG:HH21	2.11	0.59
22:a:544:C:H2'	22:a:545:U:O4'	2.02	0.59
22:a:591:U:HO2'	50:2:2:PRO:N	2.00	0.59
1:A:1119:C:OP1	9:I:85:ARG:NH1	2.33	0.59
22:a:2102:G:N2	22:a:2187:U:O2	2.31	0.59
46:y:41:THR:HG22	46:y:43:ALA:H	1.67	0.59
1:A:1273:C:H2'	1:A:1274:A:O4'	2.03	0.59
2:B:61:ALA:HB2	2:B:221:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:21:ILE:HD11	9:I:90:TYR:HB2	1.84	0.59
22:a:365:U:H2'	22:a:366:C:C6	2.38	0.59
22:a:958:U:O2	23:b:89:U:H1'	2.03	0.59
27:f:50:LEU:HD21	27:f:67:ILE:HD12	1.85	0.59
32:k:77:ILE:CD1	32:k:108:ALA:HB1	2.32	0.59
6:F:1:MET:HG3	6:F:65:GLU:OE2	2.03	0.58
2:B:87:CYS:SG	2:B:221:VAL:HG13	2.43	0.58
45:x:9:LYS:HB3	45:x:13:GLU:HG3	1.84	0.58
1:A:1004:A:C6	1:A:1026:G:H1'	2.38	0.58
32:k:57:LEU:HD22	50:2:54:ASP:HB3	1.84	0.58
2:B:54:LEU:HD12	2:B:220:THR:HG21	1.83	0.58
14:N:29:ALA:O	14:N:33:ASP:HB2	2.02	0.58
27:f:29:PRO:HB2	27:f:169:LEU:HD22	1.85	0.58
1:A:76:G:O6	1:A:93:U:O4	2.22	0.58
9:I:6:TYR:HB2	9:I:21:ILE:HG12	1.84	0.58
22:a:2273:A:H2'	22:a:2274:A:C8	2.38	0.58
9:I:12:ARG:HG3	9:I:13:LYS:H	1.68	0.58
11:K:112:ASP:HB3	21:U:2:PRO:HD2	1.85	0.58
22:a:414:C:H2'	22:a:415:A:C8	2.39	0.58
22:a:1187:G:OP1	38:q:85:LYS:NZ	2.30	0.58
35:n:43:ASN:H	35:n:43:ASN:HD22	1.52	0.58
1:A:408:A:O3'	4:D:23:SER:OG	2.21	0.58
1:A:1038:C:H2'	1:A:1039:G:C8	2.39	0.58
1:A:1062:U:H2'	1:A:1063:C:C6	2.38	0.58
2:B:186:ILE:HD13	2:B:200:ILE:HB	1.86	0.58
23:b:118:C:H2'	23:b:119:A:C8	2.39	0.58
55:V:10:2MG:O2'	55:V:11:C:OP1	2.22	0.58
1:A:381:C:H2'	1:A:382:A:O4'	2.04	0.58
3:C:57:ILE:HG12	3:C:66:VAL:HG12	1.86	0.58
9:I:36:GLU:OE1	9:I:36:GLU:N	2.36	0.58
22:a:593:U:H2'	22:a:594:U:C6	2.39	0.58
1:A:1463:U:H2'	1:A:1464:U:C6	2.39	0.57
23:b:29:A:H2'	23:b:30:C:C6	2.39	0.57
1:A:1005:A:O5'	1:A:1005:A:H8	1.84	0.57
33:l:20:LEU:HD13	42:u:81:PRO:HG3	1.85	0.57
42:u:58:SER:O	42:u:73:LYS:NZ	2.37	0.57
1:A:429:U:H3'	4:D:9:LEU:HD12	1.86	0.57
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.84	0.57
22:a:1434:A:H2'	22:a:1435:G:H8	1.67	0.57
4:D:55:LEU:O	4:D:59:GLN:HG2	2.05	0.57
22:a:1182:G:H2'	22:a:1183:U:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1722:A:N6	22:a:1738:G:O2'	2.38	0.57
1:A:1021:A:H2'	1:A:1022:A:C8	2.39	0.57
2:B:32:PHE:HB2	2:B:42:ASN:HB2	1.87	0.57
32:k:108:ALA:HB3	32:k:125:LEU:HD22	1.86	0.57
1:A:1187:G:H5'	9:I:115:LYS:HE3	1.86	0.57
15:O:47:LYS:O	15:O:53:ARG:NH2	2.37	0.57
28:g:54:PRO:HG3	28:g:62:TRP:CE2	2.40	0.57
2:B:107:VAL:O	2:B:111:ILE:HG12	2.05	0.57
19:S:41:PHE:HB2	19:S:44:MET:HE3	1.87	0.57
1:A:1451:U:N3	1:A:1453:G:N7	2.53	0.57
22:a:284:U:H2'	22:a:285:G:H8	1.68	0.57
1:A:613:C:OP1	4:D:81:ARG:NH2	2.32	0.56
4:D:126:ASN:ND2	4:D:141:ASP:OD1	2.38	0.56
9:I:55:VAL:HG11	9:I:94:LEU:HD23	1.86	0.56
1:A:77:A:H2'	1:A:78:A:C8	2.40	0.56
22:a:2092:U:OP2	29:h:27:ARG:NH2	2.35	0.56
55:V:23:A:H2'	55:V:24:G:H8	1.69	0.56
1:A:511:C:O2'	1:A:512:U:OP2	2.21	0.56
22:a:359:G:H2'	22:a:360:U:H6	1.69	0.56
28:g:42:GLU:OE2	28:g:55:ARG:HA	2.05	0.56
34:m:86:ARG:NH2	34:m:117:ASP:OD1	2.18	0.56
39:r:55:ILE:O	39:r:59:GLU:HG3	2.05	0.56
4:D:75:TYR:OH	4:D:97:ARG:NH1	2.30	0.56
9:I:7:TYR:HH	9:I:9:THR:HG1	1.52	0.56
9:I:59:GLU:OE1	9:I:59:GLU:N	2.30	0.56
1:A:67:C:H2'	1:A:68:G:C8	2.40	0.56
1:A:1009:U:O4	1:A:1020:G:O6	2.24	0.56
1:A:1227:A:O2'	13:M:114:LYS:HG3	2.05	0.56
1:A:1135:U:H2'	1:A:1137:C:C5	2.41	0.56
22:a:2100:G:H2'	22:a:2101:A:C8	2.41	0.56
25:d:1:MET:HG2	25:d:2:ILE:H	1.70	0.56
2:B:20:THR:HA	2:B:39:HIS:CE1	2.41	0.56
13:M:66:GLU:OE1	13:M:70:ARG:NH1	2.39	0.56
22:a:849:A:H2'	22:a:850:U:C6	2.41	0.56
1:A:299:G:H2'	1:A:300:A:C8	2.40	0.56
5:E:77:ASN:HB2	5:E:82:GLN:OE1	2.06	0.56
10:J:10:LEU:HD13	10:J:22:THR:HG22	1.87	0.56
1:A:1007:U:H2'	1:A:1008:U:C6	2.40	0.56
1:A:1391:U:H2'	1:A:1392:G:C8	2.41	0.56
8:H:47:GLU:HG2	8:H:64:LYS:HB3	1.88	0.55
22:a:653:U:H5''	22:a:654:A:H5'	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1495:A:H2'	22:a:1496:A:C8	2.41	0.55
30:i:13:ARG:HG3	30:i:51:GLY:O	2.07	0.55
39:r:34:ASP:OD2	47:z:37:LYS:NZ	2.22	0.55
3:C:134:MET:HE2	3:C:168:TYR:CD1	2.41	0.55
22:a:290:U:O2	22:a:350:G:O6	2.24	0.55
22:a:892:A:H2'	22:a:893:C:C6	2.41	0.55
32:k:82:LEU:HD22	32:k:90:VAL:HG21	1.88	0.55
4:D:62:ARG:NH1	4:D:69:GLU:OE1	2.39	0.55
4:D:101:VAL:HG21	4:D:137:VAL:HG21	1.89	0.55
5:E:74:VAL:HG11	5:E:144:LEU:HD22	1.87	0.55
22:a:1794:A:H2'	22:a:1795:C:C6	2.42	0.55
23:b:66:A:N6	23:b:107:G:H2'	2.22	0.55
23:b:66:A:H61	23:b:107:G:H2'	1.70	0.55
30:i:69:ARG:NH1	30:i:90:GLU:OE2	2.40	0.55
1:A:189:A:H8	1:A:189:A:OP2	1.90	0.55
1:A:1001:C:H2'	1:A:1002:G:H8	1.70	0.55
3:C:5:VAL:HG21	3:C:10:ILE:HD12	1.87	0.55
10:J:6:ILE:HB	10:J:76:ILE:CG2	2.36	0.55
22:a:1156:A:C8	37:p:51:ARG:HG2	2.42	0.55
1:A:154:U:O4	1:A:155:A:N6	2.40	0.55
1:A:270:A:H2'	1:A:271:C:C6	2.42	0.55
10:J:18:ILE:O	10:J:22:THR:HG23	2.07	0.55
10:J:22:THR:HG21	10:J:72:ARG:HG2	1.88	0.55
2:B:161:LEU:HD12	2:B:176:ALA:HB2	1.88	0.55
23:b:118:C:H2'	23:b:119:A:H8	1.71	0.55
29:h:3:VAL:O	29:h:18:GLN:HA	2.06	0.55
1:A:1098:C:O2'	21:U:71:TYR:O	2.24	0.55
29:h:27:ARG:HD3	44:w:60:ASP:OD1	2.07	0.55
1:A:77:A:H2'	1:A:78:A:H8	1.72	0.55
6:F:88:MET:HE1	18:R:61:ARG:HG2	1.89	0.55
31:j:76:VAL:HG12	36:o:73:VAL:HB	1.88	0.55
46:y:19:LYS:HD3	46:y:19:LYS:N	2.21	0.55
22:a:703:U:H2'	22:a:704:G:O4'	2.07	0.54
1:A:1179:A:H5''	9:I:104:VAL:HG12	1.89	0.54
14:N:47:LYS:O	14:N:50:THR:OG1	2.25	0.54
22:a:651:G:H5'	50:2:19:LYS:HG3	1.88	0.54
22:a:2790:U:H5'	22:a:2893:A:H62	1.71	0.54
25:d:4:LEU:HD22	25:d:32:ASN:HD22	1.71	0.54
2:B:29:PRO:O	2:B:45:LYS:NZ	2.27	0.54
4:D:54:GLN:HB3	4:D:203:LEU:HD12	1.89	0.54
7:G:56:LYS:HG3	7:G:57:SER:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:167:ARG:HG3	24:c:172:VAL:HG12	1.89	0.54
39:r:72:THR:HG21	39:r:108:SER:HB3	1.90	0.54
41:t:81:ASP:OD2	41:t:96:PHE:HB3	2.08	0.54
46:y:4:THR:HA	46:y:38:ARG:O	2.07	0.54
22:a:181:A:H2'	22:a:182:A:C8	2.43	0.54
29:h:29:PHE:HD2	29:h:30:LEU:HD12	1.72	0.54
1:A:1314:C:H2'	1:A:1315:U:C6	2.43	0.54
22:a:322:A:OP2	26:e:163:ASN:HB2	2.08	0.54
32:k:85:VAL:HB	32:k:94:THR:HG22	1.87	0.54
1:A:102:G:H2'	1:A:103:U:H6	1.72	0.54
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.90	0.54
15:O:18:ASP:HB3	15:O:21:ASP:HB2	1.88	0.54
18:R:35:GLU:OE1	18:R:35:GLU:N	2.41	0.54
20:T:28:MET:O	20:T:32:ILE:HD12	2.08	0.54
22:a:191:A:H2'	22:a:192:C:C6	2.42	0.54
28:g:71:LEU:O	28:g:75:MET:HG3	2.08	0.54
33:l:75:GLU:HG3	33:l:90:GLU:HG3	1.90	0.54
1:A:410:G:H2'	1:A:429:U:C5	2.42	0.54
1:A:488:C:H2'	1:A:489:C:C6	2.43	0.54
3:C:65:ARG:HA	3:C:100:GLN:O	2.07	0.54
22:a:172:A:H2'	22:a:173:A:C8	2.43	0.54
14:N:10:GLU:HG3	14:N:63:ARG:HD2	1.89	0.54
22:a:347:A:H2'	22:a:348:A:C8	2.43	0.54
6:F:9:MET:HE3	6:F:86:ARG:HB3	1.90	0.54
22:a:981:A:N1	22:a:2027:G:O2'	2.38	0.54
1:A:202:G:H1'	1:A:468:A:H2	1.73	0.53
1:A:1001:C:H2'	1:A:1002:G:C8	2.43	0.53
22:a:306:U:H2'	22:a:307:G:O4'	2.07	0.53
47:z:52:ARG:CZ	47:z:54:VAL:HG12	2.38	0.53
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.88	0.53
33:l:66:ARG:NH1	33:l:104:GLU:OE2	2.39	0.53
1:A:35:G:H2'	1:A:36:C:C6	2.43	0.53
1:A:202:G:O2'	1:A:468:A:N3	2.39	0.53
1:A:475:C:H2'	1:A:476:U:C6	2.44	0.53
4:D:49:SER:O	4:D:53:VAL:HG23	2.09	0.53
4:D:146:ARG:O	4:D:150:LYS:HG3	2.08	0.53
12:L:110:ARG:HB3	12:L:119:VAL:HG21	1.89	0.53
22:a:742:A:H2'	22:a:743:A:C8	2.43	0.53
22:a:1509:A:O2'	22:a:1510:G:H8	1.91	0.53
1:A:950:U:O4	13:M:104:THR:HG21	2.09	0.53
7:G:26:PHE:HZ	7:G:120:LEU:HD11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.90	0.53
22:a:1386:C:H2'	22:a:1387:A:C8	2.42	0.53
17:Q:47:HIS:HB3	17:Q:74:THR:HG22	1.90	0.53
1:A:1533:C:H4'	1:A:1534:A:C8	2.44	0.53
22:a:603:A:H8	22:a:654:A:C6	2.26	0.53
22:a:2481:G:HO2'	22:a:2482:A:H8	1.57	0.53
28:g:72:LEU:HD23	28:g:75:MET:SD	2.49	0.53
32:k:29:LYS:O	32:k:29:LYS:HG2	2.09	0.53
35:n:39:VAL:HG12	35:n:48:LEU:HD12	1.90	0.53
36:o:13:MET:HE2	36:o:55:LEU:N	2.24	0.53
52:4:1:MET:HE2	52:4:6:HIS:CD2	2.43	0.53
22:a:545:U:HO2'	22:a:548:G:H1	1.55	0.53
22:a:1469:A:H2'	22:a:1470:A:C8	2.44	0.53
55:V:26:A:H61	55:V:44:G:H1	1.55	0.53
1:A:636:U:H2'	1:A:637:C:C6	2.44	0.53
6:F:32:ALA:O	6:F:33:GLU:HG3	2.08	0.53
22:a:1733:G:H2'	22:a:1734:G:H8	1.73	0.53
31:j:71:ARG:NH1	31:j:106:GLU:OE1	2.42	0.53
36:o:5:ILE:O	36:o:9:GLU:HG2	2.07	0.53
2:B:125:THR:HA	2:B:128:LYS:HZ3	1.73	0.53
2:B:125:THR:HA	2:B:128:LYS:NZ	2.23	0.53
28:g:103:ILE:HD11	28:g:117:LEU:HD21	1.90	0.53
20:T:20:HIS:HE1	20:T:24:ARG:HD2	1.73	0.53
22:a:2102:G:O6	22:a:2187:U:O4	2.27	0.53
22:a:2376:A:N3	35:n:111:ARG:NH1	2.56	0.53
1:A:102:G:H2'	1:A:103:U:C6	2.44	0.52
3:C:175:LEU:HD23	3:C:182:ILE:HD13	1.91	0.52
1:A:1035:A:C4	1:A:1036:A:H2	2.26	0.52
4:D:57:GLU:O	4:D:60:LYS:HG3	2.09	0.52
7:G:150:ALA:O	11:K:59:THR:HG21	2.09	0.52
1:A:412:A:O2'	1:A:413:G:H4'	2.10	0.52
1:A:439:U:O4'	4:D:120:HIS:HA	2.10	0.52
23:b:1:U:H2'	23:b:2:G:H8	1.75	0.52
31:j:14:SER:OG	31:j:86:LEU:HD12	2.09	0.52
52:4:59:ARG:HA	52:4:62:LYS:HE3	1.90	0.52
1:A:56:U:H2'	1:A:57:G:H8	1.73	0.52
10:J:8:ILE:CD1	10:J:100:ILE:HG22	2.40	0.52
1:A:337:G:H2'	1:A:338:A:C8	2.45	0.52
22:a:2299:U:OP1	27:f:72:LYS:NZ	2.42	0.52
1:A:521:G:H4'	12:L:70:GLU:HG3	1.91	0.52
22:a:558:U:OP1	30:i:113:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:V:11:C:H2'	55:V:12:U:C6	2.44	0.52
1:A:545:C:H5'	4:D:69:GLU:HG2	1.92	0.52
1:A:728:A:H2'	1:A:729:A:C8	2.44	0.52
22:a:892:A:H2'	22:a:893:C:H6	1.74	0.52
33:l:111:GLU:CD	33:l:111:GLU:H	2.18	0.52
1:A:382:A:H2'	1:A:383:A:H8	1.72	0.52
1:A:736:C:H2'	1:A:737:C:C6	2.44	0.52
22:a:1864:U:OP1	22:a:2410:G:O2'	2.26	0.52
33:l:111:GLU:O	33:l:115:GLU:HG2	2.09	0.52
36:o:100:LEU:HD11	36:o:110:ILE:HD11	1.92	0.52
37:p:61:TRP:CZ2	37:p:93:LYS:HD3	2.45	0.52
1:A:488:C:H2'	1:A:489:C:H6	1.75	0.52
8:H:10:MET:HG3	8:H:27:MET:HE2	1.91	0.52
22:a:887:U:O2'	22:a:889:C:OP2	2.28	0.52
22:a:1242:U:H2'	22:a:1243:C:C6	2.45	0.52
30:i:114:LEU:HG	30:i:118:MET:HE3	1.91	0.52
1:A:376:G:O3'	16:P:5:ARG:NH1	2.41	0.52
1:A:769:G:H4'	1:A:1513:A:H4'	1.91	0.52
2:B:54:LEU:HD12	2:B:220:THR:CG2	2.39	0.52
4:D:99:ASP:OD1	4:D:100:ASN:N	2.43	0.52
3:C:66:VAL:HG22	3:C:101:ILE:HG22	1.91	0.51
15:O:24:SER:O	15:O:28:GLN:HG3	2.10	0.51
28:g:99:LYS:O	28:g:102:VAL:HG12	2.09	0.51
1:A:539:A:H2'	1:A:540:G:C8	2.46	0.51
22:a:3:U:H2'	22:a:4:U:C6	2.45	0.51
25:d:1:MET:HE2	25:d:205:PRO:HG2	1.92	0.51
54:Z:66:C:H2'	54:Z:67:C:C6	2.45	0.51
1:A:216:U:H2'	1:A:217:C:C6	2.45	0.51
22:a:1178:C:H2'	22:a:1179:G:C8	2.46	0.51
4:D:58:LYS:HA	4:D:200:ILE:HD11	1.92	0.51
41:t:94:ARG:HB3	41:t:103:ILE:HD12	1.93	0.51
1:A:131:A:H2'	1:A:132:C:H6	1.76	0.51
22:a:1178:C:H2'	22:a:1179:G:H8	1.75	0.51
1:A:269:C:H2'	1:A:270:A:H8	1.76	0.51
1:A:404:G:O2'	1:A:498:A:N1	2.35	0.51
21:U:40:LYS:HD2	21:U:42:THR:HG22	1.93	0.51
22:a:668:A:H2'	22:a:670:A:H62	1.75	0.51
27:f:147:ASP:OD1	27:f:148:ARG:N	2.39	0.51
28:g:113:VAL:HG21	28:g:151:TYR:CE1	2.45	0.51
30:i:31:GLU:HG2	30:i:142:ILE:HG23	1.92	0.51
1:A:1032:G:C6	1:A:1033:G:H1'	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:45:ARG:HD3	6:F:59:TYR:CD1	2.45	0.51
1:A:618:C:N4	1:A:621:A:OP2	2.42	0.51
6:F:59:TYR:CE2	18:R:67:LEU:HD21	2.46	0.51
11:K:16:VAL:O	11:K:17:SER:OG	2.29	0.51
22:a:1856:U:H2'	22:a:1857:G:O4'	2.11	0.51
22:a:2193:G:H2'	22:a:2194:U:H6	1.73	0.51
1:A:470:C:H2'	1:A:471:U:C6	2.46	0.50
1:A:1218:C:H2'	1:A:1219:A:C8	2.46	0.50
11:K:97:ILE:HD11	21:U:16:LEU:HD13	1.92	0.50
1:A:983:A:H5'	1:A:984:C:OP2	2.11	0.50
12:L:39:THR:HG21	12:L:49:LEU:HB3	1.93	0.50
22:a:927:A:H2'	22:a:928:A:C8	2.47	0.50
22:a:1168:G:H2'	22:a:1169:A:H8	1.75	0.50
22:a:1311:G:H21	22:a:1603:A:H62	1.58	0.50
39:r:65:ASP:OD1	39:r:65:ASP:N	2.44	0.50
11:K:96:THR:HG23	11:K:97:ILE:HG23	1.93	0.50
22:a:871:U:H2'	22:a:872:U:C6	2.47	0.50
22:a:1030:C:OP2	33:l:127:LYS:HE2	2.12	0.50
22:a:1361:G:H2'	22:a:1362:C:C6	2.46	0.50
3:C:23:PHE:CD1	10:J:97:ASP:HB2	2.45	0.50
3:C:47:LEU:C	3:C:49:LYS:H	2.18	0.50
10:J:92:LEU:HG	10:J:98:VAL:HG21	1.94	0.50
16:P:21:VAL:HG11	16:P:60:TRP:CE2	2.46	0.50
22:a:17:G:H2'	22:a:18:U:C6	2.46	0.50
22:a:784:G:H5'	22:a:785:G:OP1	2.11	0.50
22:a:2243:U:H2'	22:a:2244:U:C6	2.46	0.50
31:j:121:GLU:OE1	36:o:65:SER:OG	2.27	0.50
1:A:33:A:H2'	1:A:34:C:C6	2.46	0.50
1:A:151:A:C2	1:A:152:A:H1'	2.46	0.50
1:A:1530:G:H2'	1:A:1531:A:C8	2.46	0.50
22:a:282:A:H2'	22:a:283:G:C8	2.47	0.50
24:c:199:GLU:H	24:c:199:GLU:CD	2.18	0.50
25:d:18:ASP:OD1	25:d:18:ASP:N	2.43	0.50
25:d:38:LYS:HG2	25:d:43:ASP:OD2	2.12	0.50
41:t:97:LYS:O	41:t:98:SER:OG	2.26	0.50
1:A:1035:A:H8	1:A:1037:C:H41	1.59	0.50
1:A:1162:C:H2'	1:A:1163:A:H8	1.77	0.50
6:F:41:ASP:OD1	6:F:58:HIS:NE2	2.44	0.50
22:a:414:C:H2'	22:a:415:A:H8	1.76	0.50
22:a:2557:G:H2'	22:a:2558:C:C6	2.46	0.50
22:a:2788:C:H2'	22:a:2789:C:C6	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:t:7:ARG:HG2	41:t:27:ASN:HA	1.92	0.50
2:B:71:GLY:O	2:B:93:ASN:HA	2.12	0.50
22:a:2537:U:H2'	22:a:2538:C:C6	2.47	0.50
1:A:1010:U:H2'	1:A:1011:C:C6	2.46	0.50
20:T:59:ASP:OD1	20:T:76:LYS:NZ	2.35	0.50
22:a:1141:U:H2'	30:i:65:THR:HG21	1.94	0.50
27:f:65:PRO:HA	27:f:89:VAL:HG12	1.94	0.50
35:n:111:ARG:NH2	35:n:117:PHE:OXT	2.45	0.50
54:Z:16:C:H3'	54:Z:17:C:C6	2.46	0.50
1:A:404:G:N7	4:D:2:ALA:HB3	2.27	0.50
1:A:1326:U:H2'	1:A:1327:C:C6	2.46	0.50
3:C:111:LEU:O	3:C:204:LYS:NZ	2.45	0.50
20:T:20:HIS:CE1	20:T:24:ARG:HD2	2.47	0.50
22:a:181:A:H2'	22:a:182:A:H8	1.75	0.50
22:a:1484:U:H2'	22:a:1485:U:C6	2.47	0.50
23:b:2:G:H2'	23:b:3:C:C6	2.47	0.50
28:g:105:LEU:HB2	28:g:113:VAL:HG13	1.93	0.50
36:o:2:SER:OG	36:o:3:ASN:N	2.43	0.50
42:u:48:MET:HE3	42:u:51:GLN:NE2	2.27	0.49
1:A:722:G:N3	1:A:722:G:H2'	2.27	0.49
1:A:328:C:H4'	1:A:329:A:H5'	1.94	0.49
22:a:1113:U:O2'	22:a:1114:C:H5'	2.13	0.49
1:A:195:A:H2'	1:A:196:A:C8	2.48	0.49
1:A:555:U:H2'	1:A:556:C:C6	2.46	0.49
2:B:9:MET:HE1	2:B:46:THR:HG22	1.93	0.49
13:M:49:SER:O	13:M:53:ILE:HG12	2.12	0.49
22:a:1723:G:H2'	22:a:1724:G:O4'	2.12	0.49
25:d:1:MET:HG2	25:d:2:ILE:N	2.27	0.49
27:f:116:GLY:HA3	27:f:178:ARG:HB3	1.93	0.49
35:n:41:ALA:HB3	35:n:43:ASN:ND2	2.27	0.49
1:A:490:C:H2'	1:A:491:G:C8	2.47	0.49
1:A:512:U:P	4:D:44:ARG:HH12	2.35	0.49
2:B:129:LEU:HB2	2:B:134:ALA:HB2	1.93	0.49
5:E:39:VAL:HG13	5:E:71:MET:HE1	1.95	0.49
17:Q:17:MET:HG3	17:Q:20:SER:OG	2.13	0.49
22:a:2086:U:H2'	22:a:2087:G:C8	2.47	0.49
22:a:2567:G:H2'	22:a:2568:U:C6	2.48	0.49
22:a:2845:U:H5''	36:o:52:ASN:O	2.12	0.49
1:A:695:A:H2'	1:A:696:A:C8	2.48	0.49
1:A:1119:C:H2'	1:A:1120:C:H6	1.76	0.49
15:O:17:ARG:HD2	15:O:17:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:1:U:H2'	23:b:2:G:C8	2.48	0.49
26:e:1:MET:O	26:e:13:THR:HA	2.13	0.49
1:A:1073:U:O2'	2:B:103:ASN:OD1	2.10	0.49
1:A:1130:A:H2'	1:A:1131:G:C8	2.48	0.49
22:a:2071:A:H2'	22:a:2072:C:C6	2.47	0.49
26:e:5:LEU:HD13	26:e:10:SER:HB2	1.94	0.49
28:g:37:LEU:HD11	28:g:72:LEU:HD11	1.95	0.49
36:o:57:SER:HB2	36:o:76:THR:HG21	1.95	0.49
1:A:625:U:O2'	1:A:626:G:H5'	2.13	0.49
2:B:50:PHE:O	2:B:54:LEU:HD23	2.12	0.49
5:E:82:GLN:HE21	5:E:150:PRO:HD3	1.78	0.49
7:G:14:PRO:HG3	7:G:21:GLU:HG3	1.95	0.49
22:a:548:G:H2'	22:a:549:G:O4'	2.12	0.49
27:f:60:ILE:HG13	27:f:141:ILE:HD11	1.95	0.49
55:V:67:U:H2'	55:V:68:C:C6	2.48	0.49
4:D:129:VAL:HG22	4:D:146:ARG:HD3	1.95	0.49
3:C:125:GLU:HG3	3:C:189:ALA:HB1	1.93	0.48
9:I:52:LEU:HD11	9:I:63:LEU:HD11	1.93	0.48
15:O:12:VAL:HG21	15:O:22:THR:HG22	1.94	0.48
22:a:361:G:H8	22:a:361:G:OP2	1.96	0.48
22:a:2799:A:O2'	22:a:2800:A:H5''	2.13	0.48
38:q:61:ALA:HB1	38:q:96:VAL:HG22	1.95	0.48
1:A:1444:U:H2'	1:A:1445:U:C6	2.48	0.48
22:a:1655:A:H1'	25:d:118:PHE:CE2	2.49	0.48
23:b:79:G:N7	42:u:14:LYS:NZ	2.59	0.48
45:x:9:LYS:O	45:x:60:LYS:HE2	2.12	0.48
1:A:451:A:H61	1:A:481:G:H5'	1.78	0.48
24:c:145:GLU:HB2	24:c:188:CYS:HB3	1.95	0.48
26:e:188:MET:HG2	26:e:192:ALA:HB3	1.95	0.48
28:g:9:VAL:CG1	28:g:50:LEU:HB2	2.43	0.48
54:Z:19:G:O2'	54:Z:20:G:H5''	2.13	0.48
55:V:18:G:HO2'	55:V:57:A:H2	1.61	0.48
1:A:1155:A:H2'	1:A:1156:G:O4'	2.13	0.48
2:B:68:LEU:HB3	2:B:161:LEU:HD23	1.94	0.48
5:E:85:VAL:HG11	5:E:147:MET:HB3	1.95	0.48
7:G:54:SER:OG	7:G:56:LYS:HG2	2.14	0.48
22:a:723:C:H2'	22:a:724:U:O4'	2.13	0.48
22:a:1809:A:H2'	22:a:1810:A:C8	2.49	0.48
1:A:269:C:H2'	1:A:270:A:C8	2.48	0.48
1:A:999:C:N3	1:A:1042:A:N6	2.62	0.48
2:B:59:LYS:O	2:B:63:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1028:A:H2'	22:a:1029:A:C8	2.48	0.48
22:a:1168:G:H2'	22:a:1169:A:C8	2.48	0.48
22:a:1210:G:OP1	22:a:1211:C:O2'	2.20	0.48
22:a:2469:A:H2'	22:a:2470:G:O4'	2.13	0.48
23:b:42:C:C5	27:f:66:LEU:HD22	2.49	0.48
2:B:126:PHE:HE1	2:B:137:ARG:NE	2.11	0.48
16:P:1:MET:O	16:P:24:SER:N	2.43	0.48
18:R:32:TYR:CG	18:R:55:LEU:HD21	2.47	0.48
22:a:279:A:O5'	22:a:279:A:H8	1.96	0.48
22:a:833:A:H2'	22:a:834:G:C8	2.48	0.48
1:A:604:G:H2'	1:A:605:U:O4'	2.14	0.48
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.96	0.48
9:I:92:GLU:O	9:I:95:ARG:HG3	2.13	0.48
22:a:588:U:H2'	22:a:589:U:C6	2.48	0.48
22:a:2636:C:H2'	22:a:2637:U:C6	2.48	0.48
24:c:155:ALA:HB2	24:c:162:VAL:HG23	1.95	0.48
1:A:408:A:H2'	1:A:409:U:C6	2.48	0.48
1:A:481:G:O2'	1:A:483:C:N4	2.47	0.48
1:A:736:C:H2'	1:A:737:C:H6	1.79	0.48
1:A:1098:C:OP2	2:B:143:LYS:HE2	2.14	0.48
8:H:113:ASP:OD1	8:H:114:ARG:N	2.46	0.48
13:M:107:ARG:HH22	13:M:110:LYS:HE2	1.79	0.48
15:O:64:ARG:HH12	15:O:89:ARG:C	2.22	0.48
27:f:106:ILE:HD12	52:4:34:LEU:CD1	2.43	0.48
35:n:4:LYS:O	35:n:8:ILE:HG12	2.14	0.48
1:A:139:A:H2'	1:A:140:U:C6	2.47	0.48
1:A:1268:G:H2'	1:A:1269:A:C8	2.49	0.48
2:B:92:VAL:HG21	2:B:100:MET:HE1	1.95	0.48
5:E:13:GLU:HG3	5:E:39:VAL:HG23	1.96	0.48
9:I:83:ILE:O	9:I:87:LEU:HG	2.14	0.48
10:J:8:ILE:HB	10:J:74:VAL:CG2	2.44	0.48
22:a:347:A:H2'	22:a:348:A:H8	1.79	0.48
22:a:419:U:H2'	22:a:420:C:C6	2.49	0.48
22:a:1746:A:H2'	22:a:1747:U:C6	2.48	0.48
9:I:10:GLY:HA2	9:I:81:HIS:ND1	2.29	0.48
20:T:43:ASP:CG	20:T:46:ALA:H	2.22	0.48
22:a:1509:A:N3	22:a:1510:G:C8	2.81	0.48
27:f:142:ASP:O	27:f:146:VAL:HG13	2.13	0.48
34:m:66:ALA:O	34:m:69:ARG:O	2.32	0.48
1:A:255:G:H2'	1:A:256:U:C6	2.49	0.47
1:A:513:C:H2'	1:A:514:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:U:O2'	8:H:15:ARG:HD2	2.14	0.47
1:A:1162:C:H2'	1:A:1163:A:C8	2.49	0.47
8:H:59:LEU:HD12	8:H:60:GLU:H	1.79	0.47
22:a:1794:A:H2'	22:a:1795:C:H6	1.78	0.47
4:D:8:LYS:HB3	4:D:21:LEU:CD2	2.45	0.47
7:G:72:THR:HG22	7:G:73:VAL:HG13	1.96	0.47
16:P:39:PHE:HD1	16:P:50:THR:OG1	1.96	0.47
22:a:857:G:H2'	22:a:858:G:O4'	2.15	0.47
22:a:2657:A:O2'	28:g:160:LYS:NZ	2.47	0.47
28:g:94:TYR:HA	28:g:106:SER:O	2.15	0.47
1:A:378:G:H2'	1:A:379:C:C6	2.48	0.47
2:B:14:VAL:HG12	2:B:209:ALA:HB1	1.96	0.47
2:B:120:GLN:HB3	2:B:137:ARG:HH21	1.78	0.47
2:B:129:LEU:HD23	2:B:133:GLU:HB3	1.96	0.47
6:F:42:TRP:HZ2	6:F:61:LEU:HD12	1.79	0.47
10:J:10:LEU:CD1	10:J:22:THR:HG22	2.44	0.47
17:Q:20:SER:HB3	17:Q:71:LYS:NZ	2.28	0.47
17:Q:54:GLY:N	17:Q:57:ASP:OD2	2.32	0.47
24:c:122:ALA:HB1	24:c:128:ASN:HD22	1.78	0.47
25:d:108:ASP:OD1	25:d:173:GLN:HA	2.15	0.47
29:h:3:VAL:CG2	29:h:36:ALA:HB1	2.44	0.47
31:j:80:ASP:OD2	36:o:69:GLY:HA3	2.14	0.47
4:D:8:LYS:HB3	4:D:21:LEU:HD22	1.95	0.47
4:D:57:GLU:OE1	4:D:200:ILE:HG12	2.14	0.47
22:a:1441:G:H2'	22:a:1442:U:C6	2.50	0.47
22:a:2780:G:OP2	30:i:120:ARG:HD3	2.13	0.47
28:g:26:ILE:HG22	28:g:79:VAL:HG21	1.97	0.47
31:j:63:VAL:HG12	31:j:107:LEU:HD11	1.96	0.47
1:A:323:U:H2'	1:A:324:G:O4'	2.15	0.47
22:a:2892:G:H5''	22:a:2894:G:N2	2.29	0.47
25:d:99:GLU:OE1	25:d:99:GLU:N	2.48	0.47
32:k:118:THR:O	32:k:120:VAL:HG23	2.15	0.47
1:A:613:C:H2'	1:A:614:C:C6	2.50	0.47
1:A:927:G:O2'	1:A:1503:A:N7	2.40	0.47
8:H:5:ASP:OD1	8:H:77:ARG:NH1	2.40	0.47
8:H:54:ASP:OD1	8:H:54:ASP:N	2.47	0.47
16:P:6:LEU:HD22	16:P:17:TYR:HB3	1.97	0.47
22:a:1199:U:H2'	22:a:1200:C:C6	2.49	0.47
22:a:2074:U:H2'	22:a:2075:U:C6	2.49	0.47
22:a:2698:U:H2'	22:a:2699:C:C6	2.50	0.47
4:D:60:LYS:NZ	4:D:195:ILE:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:12:ARG:O	9:I:13:LYS:C	2.57	0.47
10:J:11:LYS:HB2	10:J:97:ASP:HB3	1.97	0.47
22:a:1149:G:H2'	22:a:1150:C:C6	2.50	0.47
22:a:1296:G:OP1	22:a:2709:G:O2'	2.29	0.47
22:a:1703:G:H2'	22:a:1704:C:C6	2.50	0.47
22:a:2052:A:H4'	25:d:148:GLN:O	2.14	0.47
22:a:2796:U:H3	22:a:2799:A:H61	1.63	0.47
26:e:145:ASP:HB2	26:e:166:LYS:HE3	1.96	0.47
28:g:42:GLU:OE2	28:g:55:ARG:HD3	2.15	0.47
1:A:61:G:N7	20:T:6:SER:HB2	2.29	0.47
1:A:666:G:H5'	1:A:726:C:H1'	1.96	0.47
1:A:1004:A:O2'	1:A:1036:A:N6	2.48	0.47
9:I:96:SER:O	9:I:100:LYS:HG2	2.14	0.47
15:O:69:TYR:OH	15:O:73:LYS:HD2	2.14	0.47
22:a:580:U:H2'	22:a:581:C:C6	2.50	0.47
44:w:13:VAL:HG22	44:w:29:PHE:HB2	1.97	0.47
1:A:377:G:H2'	1:A:378:G:C8	2.50	0.47
1:A:590:U:OP1	8:H:31:LYS:HG2	2.15	0.47
1:A:746:A:H2'	1:A:747:A:C8	2.50	0.47
1:A:976:G:OP2	1:A:1358:U:O2'	2.32	0.47
1:A:1032:G:N2	1:A:1033:G:N3	2.63	0.47
3:C:135:LYS:O	3:C:139:GLN:HG3	2.15	0.47
6:F:1:MET:N	6:F:65:GLU:OE2	2.44	0.47
7:G:17:LYS:HD3	7:G:44:TYR:CD2	2.50	0.47
1:A:187:G:N2	1:A:189:A:H5''	2.29	0.47
12:L:74:LEU:HD21	12:L:104:CYS:SG	2.55	0.47
22:a:594:U:H2'	22:a:595:C:C6	2.50	0.47
22:a:2657:A:O3'	28:g:160:LYS:NZ	2.40	0.47
1:A:1412:C:H2'	1:A:1413:A:C8	2.50	0.46
14:N:33:ASP:C	14:N:41:ARG:HH12	2.22	0.46
22:a:2825:G:H5''	22:a:2825:G:N3	2.29	0.46
23:b:2:G:H2'	23:b:3:C:H6	1.80	0.46
44:w:51:VAL:HG22	44:w:52:SER:O	2.15	0.46
1:A:78:A:H2'	1:A:79:G:C8	2.50	0.46
1:A:464:U:O4	1:A:468:A:N7	2.48	0.46
1:A:546:A:OP1	4:D:69:GLU:HB3	2.15	0.46
22:a:1197:G:H2'	22:a:1198:U:H6	1.80	0.46
23:b:48:U:H2'	23:b:49:C:C6	2.50	0.46
29:h:30:LEU:HB3	29:h:36:ALA:HB3	1.97	0.46
35:n:25:ARG:HG2	35:n:27:VAL:HG22	1.96	0.46
1:A:120:A:H4'	1:A:121:U:OP1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:63:LEU:HB3	9:I:65:ILE:HD11	1.97	0.46
18:R:26:ILE:O	18:R:30:LYS:HG2	2.15	0.46
22:a:848:C:H2'	22:a:849:A:C8	2.50	0.46
22:a:933:A:H5'	22:a:934:U:OP2	2.15	0.46
1:A:73:C:O2'	1:A:74:A:H8	1.99	0.46
1:A:204:G:H1'	1:A:465:A:C2	2.50	0.46
1:A:546:A:P	4:D:69:GLU:HB3	2.55	0.46
2:B:166:ALA:HB3	2:B:191:SER:OG	2.16	0.46
3:C:88:ARG:HH22	3:C:89:LYS:HE3	1.79	0.46
4:D:124:MET:O	4:D:143:VAL:HG23	2.15	0.46
22:a:752:A:P	49:1:1:MET:HE1	2.56	0.46
22:a:861:A:H2'	22:a:862:G:O4'	2.16	0.46
22:a:894:U:H2'	22:a:895:U:O4'	2.16	0.46
26:e:146:VAL:HA	26:e:185:LYS:O	2.15	0.46
27:f:143:TYR:O	27:f:146:VAL:HG22	2.16	0.46
55:V:75:C:H2'	55:V:76:A:C8	2.50	0.46
1:A:72:A:H2'	1:A:73:C:H5'	1.97	0.46
4:D:124:MET:HB3	4:D:144:SER:HB2	1.96	0.46
13:M:71:ARG:NH2	27:f:113:ASP:OD1	2.45	0.46
22:a:657:U:H2'	22:a:658:U:C6	2.51	0.46
22:a:889:C:H2'	22:a:890:C:O4'	2.16	0.46
22:a:1365:A:OP1	44:w:3:ARG:NH2	2.42	0.46
22:a:2680:U:O2'	22:a:2681:C:H5'	2.15	0.46
34:m:29:VAL:HG11	34:m:75:ILE:HG23	1.97	0.46
1:A:236:A:H2'	1:A:237:G:C8	2.51	0.46
1:A:358:U:H2'	1:A:359:G:H8	1.81	0.46
1:A:1477:U:H2'	1:A:1478:U:C6	2.50	0.46
4:D:60:LYS:HZ3	4:D:195:ILE:HA	1.80	0.46
5:E:144:LEU:O	5:E:147:MET:HG2	2.14	0.46
22:a:359:G:H2'	22:a:360:U:C6	2.50	0.46
1:A:109:A:C6	1:A:326:G:C6	3.03	0.46
1:A:475:C:H2'	1:A:476:U:H6	1.80	0.46
1:A:713:G:H2'	1:A:714:G:C8	2.50	0.46
1:A:999:C:H2'	1:A:1000:A:C8	2.50	0.46
1:A:1163:A:H2'	1:A:1164:G:C8	2.51	0.46
5:E:12:GLN:HE21	5:E:117:VAL:HG22	1.80	0.46
15:O:26:GLU:CD	15:O:77:ARG:HH21	2.23	0.46
22:a:1045:C:O2	22:a:1047:G:N2	2.49	0.46
30:i:111:LYS:HD2	30:i:111:LYS:N	2.30	0.46
1:A:448:A:H3'	1:A:449:G:H8	1.81	0.46
22:a:144:A:H2'	22:a:145:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:150:U:H2'	22:a:151:C:C6	2.51	0.46
22:a:308:G:H2'	22:a:309:A:C8	2.51	0.46
1:A:701:U:OP1	1:A:702:A:O2'	2.26	0.46
1:A:744:C:H2'	1:A:745:G:H8	1.81	0.46
7:G:136:LYS:O	7:G:139:GLU:HG3	2.16	0.46
23:b:75:G:H5''	42:u:12:GLN:OE1	2.15	0.46
30:i:65:THR:HG22	30:i:66:GLY:N	2.31	0.46
41:t:54:GLN:N	41:t:55:PRO:HD2	2.30	0.46
45:x:19:LEU:HD23	45:x:19:LEU:HA	1.72	0.46
2:B:114:LEU:HD12	2:B:144:LEU:HB3	1.97	0.46
3:C:11:ARG:NH2	3:C:175:LEU:O	2.48	0.46
13:M:71:ARG:HH22	27:f:113:ASP:CG	2.24	0.46
22:a:1181:U:H2'	22:a:1182:G:C8	2.51	0.46
22:a:2820:A:N3	22:a:2820:A:H2'	2.31	0.46
28:g:55:ARG:HB2	28:g:58:TYR:CD2	2.47	0.46
50:2:31:HIS:ND1	50:2:32:ILE:HD12	2.31	0.46
1:A:20:U:H2'	1:A:21:G:O4'	2.16	0.45
1:A:580:C:H2'	1:A:581:G:O4'	2.17	0.45
1:A:745:G:H2'	1:A:746:A:H8	1.80	0.45
2:B:96:TRP:NE1	2:B:175:GLU:OE1	2.45	0.45
22:a:2094:A:P	29:h:22:LYS:HD2	2.57	0.45
5:E:12:GLN:HE21	5:E:117:VAL:HA	1.81	0.45
5:E:93:ARG:HG3	5:E:128:TYR:HB2	1.98	0.45
15:O:14:GLU:O	15:O:84:ARG:NH2	2.48	0.45
15:O:74:ASP:OD2	15:O:77:ARG:HG2	2.17	0.45
17:Q:58:VAL:HB	17:Q:80:GLU:HB3	1.98	0.45
22:a:320:A:N3	26:e:163:ASN:ND2	2.58	0.45
22:a:639:U:H2'	22:a:640:C:H6	1.80	0.45
22:a:1594:U:H2'	22:a:1595:C:C6	2.51	0.45
22:a:1796:U:H2'	22:a:1797:G:H8	1.81	0.45
1:A:78:A:H2'	1:A:79:G:H8	1.81	0.45
1:A:744:C:H2'	1:A:745:G:C8	2.51	0.45
1:A:802:A:H2'	1:A:803:G:O4'	2.17	0.45
7:G:73:VAL:HG12	7:G:90:GLU:HA	1.97	0.45
22:a:1269:A:H2'	22:a:1270:C:C6	2.52	0.45
22:a:2896:C:H2'	22:a:2897:U:C6	2.51	0.45
1:A:320:A:H2'	1:A:321:A:O4'	2.17	0.45
1:A:859:G:H2'	1:A:860:A:C8	2.52	0.45
1:A:1010:U:H2'	1:A:1011:C:H6	1.82	0.45
1:A:1075:U:OP1	2:B:178:ASN:ND2	2.49	0.45
1:A:1244:G:H2'	1:A:1245:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1464:U:H2'	1:A:1465:A:H8	1.81	0.45
12:L:86:ARG:NH1	12:L:88:LYS:HG3	2.32	0.45
20:T:79:LEU:HD23	20:T:79:LEU:HA	1.73	0.45
22:a:64:A:H2'	22:a:65:U:C6	2.51	0.45
22:a:846:U:H5'	22:a:847:U:OP1	2.17	0.45
22:a:1496:A:H2'	22:a:1498:C:C5	2.50	0.45
31:j:7:MET:HE1	31:j:44:LYS:HG3	1.98	0.45
33:l:110:GLU:OE2	33:l:114:ARG:NH2	2.49	0.45
1:A:303:A:H2'	1:A:304:U:O4'	2.17	0.45
1:A:554:A:H2'	1:A:555:U:C6	2.52	0.45
4:D:107:PHE:CG	4:D:145:ILE:HD11	2.52	0.45
4:D:146:ARG:HH22	4:D:148:LYS:HD3	1.81	0.45
5:E:161:VAL:HG23	5:E:162:GLU:CD	2.41	0.45
12:L:72:HIS:ND1	12:L:74:LEU:HB2	2.31	0.45
16:P:1:MET:HE3	16:P:2:VAL:O	2.17	0.45
22:a:1180:U:H2'	22:a:1181:U:O4'	2.16	0.45
22:a:1446:C:H2'	22:a:1447:C:C6	2.51	0.45
22:a:1526:C:H2'	22:a:1527:G:O4'	2.16	0.45
22:a:1590:A:H2'	22:a:1591:A:H8	1.82	0.45
26:e:111:GLU:O	26:e:115:GLN:HG3	2.17	0.45
38:q:34:GLU:HG2	38:q:60:LYS:HG2	1.99	0.45
55:V:43:A:H2'	55:V:44:G:H8	1.80	0.45
2:B:31:ILE:HG21	2:B:39:HIS:HD2	1.82	0.45
22:a:2038:G:H2'	22:a:2039:U:O4'	2.16	0.45
22:a:2101:A:H2'	22:a:2102:G:O4'	2.17	0.45
22:a:2514:U:H2'	22:a:2515:C:C6	2.52	0.45
36:o:63:LYS:HE2	36:o:65:SER:HB2	1.99	0.45
40:s:65:GLY:HA3	40:s:77:ARG:O	2.16	0.45
1:A:324:G:N2	1:A:327:A:C8	2.85	0.45
8:H:96:MET:SD	8:H:130:ALA:HB1	2.56	0.45
18:R:47:THR:HG22	18:R:48:ARG:N	2.32	0.45
22:a:1733:G:H2'	22:a:1734:G:C8	2.52	0.45
22:a:2278:A:OP1	33:l:10:ARG:NH1	2.49	0.45
22:a:2899:A:H2'	22:a:2900:A:C8	2.51	0.45
24:c:261:LYS:HA	24:c:264:ASP:OD2	2.16	0.45
25:d:48:ILE:HG23	25:d:84:LEU:HD11	1.99	0.45
29:h:3:VAL:HG12	29:h:19:VAL:O	2.17	0.45
1:A:235:C:H2'	1:A:236:A:C8	2.52	0.45
1:A:393:A:C2	1:A:394:G:C8	3.05	0.45
1:A:601:G:H2'	1:A:602:A:H8	1.82	0.45
16:P:8:ARG:HB2	16:P:17:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1046:A:H3'	22:a:1047:G:H5'	1.97	0.45
23:b:41:G:O6	27:f:69:LYS:NZ	2.42	0.45
45:x:27:ASN:O	45:x:31:GLN:HG3	2.17	0.45
52:4:59:ARG:O	52:4:63:ARG:HB2	2.16	0.45
54:Z:9:G:N3	54:Z:46:G:H2'	2.32	0.45
55:V:44:G:H2'	55:V:45:G:O4'	2.16	0.45
1:A:41:G:H2'	1:A:42:G:H8	1.82	0.45
1:A:477:C:H2'	1:A:478:A:H8	1.81	0.45
1:A:1251:A:H2'	1:A:1252:A:C8	2.51	0.45
4:D:191:LEU:HD23	4:D:191:LEU:HA	1.81	0.45
22:a:848:C:H2'	22:a:849:A:H8	1.82	0.45
32:k:85:VAL:HG21	32:k:90:VAL:HG22	1.98	0.45
38:q:2:TYR:CZ	38:q:42:ALA:HB3	2.52	0.45
1:A:377:G:H2'	1:A:378:G:H8	1.82	0.45
1:A:512:U:H2'	1:A:513:C:C6	2.52	0.45
1:A:636:U:H2'	1:A:637:C:H6	1.83	0.45
1:A:1225:A:H2'	1:A:1226:C:C5	2.51	0.45
1:A:1363:A:O2'	1:A:1365:G:N7	2.43	0.45
1:A:1428:A:H2'	1:A:1429:A:O4'	2.17	0.45
2:B:4:VAL:HG11	2:B:50:PHE:CE2	2.51	0.45
2:B:162:PHE:CE1	2:B:217:VAL:HG11	2.51	0.45
14:N:27:LEU:HD13	14:N:48:LEU:HB2	1.98	0.45
20:T:43:ASP:OD1	20:T:45:ALA:N	2.50	0.45
22:a:363:G:H2'	22:a:364:C:H6	1.82	0.45
22:a:404:A:H1'	22:a:405:U:OP2	2.17	0.45
22:a:839:U:H2'	22:a:840:C:C6	2.52	0.45
22:a:1537:G:H2'	22:a:1538:G:O4'	2.17	0.45
22:a:2810:A:H2'	22:a:2811:G:O4'	2.17	0.45
26:e:7:ASP:CG	26:e:122:GLU:H	2.24	0.45
26:e:170:ARG:HD3	26:e:174:GLY:O	2.17	0.45
27:f:105:THR:HG22	27:f:106:ILE:HD13	1.99	0.45
33:l:53:MET:HE1	33:l:103:TYR:CG	2.52	0.45
42:u:28:ALA:HB3	42:u:40:ILE:HG13	1.98	0.45
54:Z:24:C:H2'	54:Z:25:U:C6	2.52	0.45
1:A:724:G:H8	1:A:724:G:OP2	2.01	0.44
1:A:750:C:O2	15:O:23:GLY:HA3	2.18	0.44
15:O:36:ILE:O	15:O:40:GLN:HG2	2.17	0.44
22:a:286:U:C2	22:a:287:G:C8	3.04	0.44
22:a:1000:A:H2'	22:a:1001:A:C8	2.52	0.44
42:u:29:ILE:HD12	42:u:38:LEU:O	2.17	0.44
1:A:142:G:H3'	1:A:143:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:A:H2'	1:A:156:C:H6	1.81	0.44
1:A:409:U:H5''	4:D:25:VAL:HG21	1.99	0.44
4:D:78:GLU:OE1	4:D:93:LEU:HD11	2.18	0.44
7:G:15:ASP:OD2	7:G:23:LEU:HD23	2.17	0.44
22:a:645:C:H2'	22:a:647:G:C8	2.53	0.44
27:f:103:LEU:HA	27:f:107:ALA:HB3	1.98	0.44
39:r:23:LEU:HD22	47:z:24:ALA:HB2	1.99	0.44
1:A:168:G:H2'	1:A:169:C:C6	2.52	0.44
1:A:392:C:H2'	1:A:393:A:C8	2.53	0.44
2:B:223:GLU:HA	2:B:226:SER:HB2	1.98	0.44
13:M:105:ASN:O	13:M:106:ALA:HB3	2.16	0.44
15:O:9:ALA:HA	15:O:12:VAL:HG12	1.99	0.44
22:a:813:U:H2'	22:a:814:C:C6	2.53	0.44
22:a:909:A:H2'	22:a:912:C:C5	2.52	0.44
42:u:9:ARG:HG2	42:u:41:GLU:HG3	1.99	0.44
1:A:123:U:OP1	1:A:312:C:H5'	2.17	0.44
1:A:223:A:H2'	1:A:224:U:C6	2.53	0.44
2:B:129:LEU:HD21	2:B:137:ARG:HH11	1.83	0.44
9:I:57:MET:HE2	9:I:61:LEU:CD1	2.46	0.44
22:a:288:U:H2'	22:a:289:G:O4'	2.17	0.44
36:o:57:SER:HB2	36:o:76:THR:CG2	2.48	0.44
1:A:145:G:H2'	1:A:146:G:O4'	2.18	0.44
2:B:77:SER:HB3	2:B:93:ASN:HB2	1.99	0.44
17:Q:60:GLU:OE1	17:Q:76:VAL:HB	2.17	0.44
20:T:35:VAL:HG22	20:T:50:ALA:HB1	2.00	0.44
22:a:479:A:H4'	22:a:480:A:OP1	2.17	0.44
22:a:608:A:H2'	22:a:609:A:C8	2.52	0.44
22:a:851:C:H2'	22:a:852:U:C6	2.53	0.44
22:a:1870:C:HO2'	22:a:1871:A:H8	1.65	0.44
22:a:2796:U:H3	22:a:2799:A:N6	2.15	0.44
38:q:65:ALA:HB3	38:q:95:ASP:HB2	2.00	0.44
10:J:24:GLU:HG3	10:J:90:LEU:HD21	1.99	0.44
10:J:32:THR:HG21	10:J:83:THR:HA	2.00	0.44
20:T:55:GLN:HB3	20:T:56:PRO:HD3	1.99	0.44
22:a:2082:A:H2'	22:a:2083:G:O4'	2.18	0.44
28:g:154:PRO:HA	28:g:160:LYS:O	2.18	0.44
44:w:56:MET:HE2	44:w:56:MET:HB3	1.77	0.44
55:V:44:G:O2'	55:V:45:G:H5'	2.18	0.44
1:A:32:A:H2'	1:A:33:A:C8	2.53	0.44
1:A:374:A:H2'	1:A:375:U:C6	2.53	0.44
1:A:542:G:H5'	4:D:39:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:U:O3'	8:H:31:LYS:NZ	2.51	0.44
1:A:868:C:H2'	1:A:869:G:O4'	2.18	0.44
1:A:958:A:OP1	19:S:55:ARG:NH1	2.48	0.44
2:B:111:ILE:HD13	2:B:148:LEU:HD13	1.99	0.44
11:K:84:VAL:HG11	11:K:97:ILE:HG21	2.00	0.44
12:L:102:LEU:H	12:L:102:LEU:HG	1.58	0.44
22:a:888:C:H2'	22:a:889:C:C6	2.52	0.44
22:a:1432:G:H2'	22:a:1433:A:C8	2.53	0.44
22:a:1747:U:H2'	22:a:1748:C:C6	2.53	0.44
28:g:4:VAL:O	28:g:69:ARG:HD2	2.18	0.44
30:i:65:THR:HG22	30:i:66:GLY:H	1.83	0.44
1:A:662:U:H2'	1:A:663:A:C8	2.53	0.44
1:A:1011:C:H2'	1:A:1012:A:C8	2.52	0.44
10:J:22:THR:O	10:J:25:ILE:HG22	2.18	0.44
22:a:581:C:H2'	22:a:582:A:C8	2.52	0.44
22:a:1003:G:O2'	22:a:1010:A:N1	2.48	0.44
22:a:1028:A:N6	22:a:1125:G:H2'	2.33	0.44
22:a:1357:C:H2'	22:a:1358:G:O4'	2.18	0.44
38:q:4:VAL:HA	38:q:12:HIS:O	2.18	0.44
46:y:3:LYS:HB2	46:y:40:ASP:HB3	1.99	0.44
54:Z:59:A:O2'	54:Z:61:U:OP2	2.32	0.44
1:A:146:G:N1	1:A:147:G:C5	2.86	0.44
1:A:380:G:H5'	1:A:381:C:OP2	2.18	0.44
1:A:1486:G:H2'	1:A:1487:G:O4'	2.18	0.44
4:D:58:LYS:NZ	4:D:69:GLU:OE1	2.51	0.44
10:J:66:GLU:HG2	14:N:99:ALA:CB	2.39	0.44
22:a:38:A:H2'	22:a:39:G:O4'	2.17	0.44
22:a:263:G:H2'	22:a:264:C:O4'	2.17	0.44
22:a:1417:C:O2'	22:a:1587:G:O2'	2.08	0.44
22:a:2455:G:H2'	22:a:2456:C:C6	2.53	0.44
1:A:594:U:H2'	1:A:595:A:C8	2.53	0.43
1:A:864:A:H2'	1:A:865:A:C8	2.53	0.43
10:J:21:ALA:O	10:J:24:GLU:HG2	2.18	0.43
13:M:33:ILE:HD11	13:M:63:PHE:HE2	1.82	0.43
14:N:45:VAL:HG12	14:N:46:LEU:HD22	2.00	0.43
19:S:80:TYR:CZ	19:S:82:GLY:HA2	2.53	0.43
22:a:483:A:C8	41:t:45:HIS:HD2	2.35	0.43
22:a:546:U:H3'	22:a:547:A:C8	2.43	0.43
22:a:1590:A:H2'	22:a:1591:A:C8	2.53	0.43
22:a:1904:G:O2'	22:a:1928:A:N1	2.47	0.43
22:a:2591:C:H2'	22:a:2592:G:C8	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:m:117:ASP:OD1	34:m:117:ASP:C	2.61	0.43
38:q:6:GLN:HG2	38:q:10:LYS:O	2.18	0.43
41:t:10:GLU:OE2	41:t:22:ARG:HB3	2.19	0.43
54:Z:21:H2U:H2'	54:Z:21:H2U:H61	1.74	0.43
1:A:492:C:H2'	1:A:493:A:C8	2.53	0.43
1:A:678:U:H2'	1:A:679:C:C6	2.53	0.43
1:A:1118:U:H2'	1:A:1119:C:C6	2.54	0.43
3:C:88:ARG:HA	3:C:91:VAL:HG22	1.99	0.43
13:M:71:ARG:NH2	27:f:115:ARG:HD3	2.33	0.43
18:R:10:PHE:CZ	18:R:12:ARG:HG2	2.53	0.43
22:a:340:A:H2'	22:a:341:C:O4'	2.19	0.43
22:a:352:A:H2'	22:a:353:C:O4'	2.17	0.43
31:j:105:ARG:HG2	31:j:108:ARG:HD2	2.00	0.43
32:k:62:PRO:HG2	50:2:25:LYS:HB3	1.99	0.43
41:t:74:ASN:C	41:t:76:ALA:H	2.26	0.43
1:A:155:A:H2'	1:A:156:C:C6	2.53	0.43
1:A:923:A:O2'	1:A:1399:C:OP2	2.31	0.43
10:J:22:THR:HA	10:J:25:ILE:HG22	2.00	0.43
10:J:65:TYR:HB3	14:N:96:LEU:HD11	2.00	0.43
22:a:460:A:H2'	22:a:461:C:O4'	2.18	0.43
22:a:1292:G:H2'	22:a:1293:C:C6	2.54	0.43
22:a:1682:G:H2'	22:a:1683:U:C6	2.52	0.43
22:a:2849:U:H4'	22:a:2868:A:C2	2.53	0.43
26:e:149:ILE:HG12	26:e:175:ILE:HD11	2.00	0.43
1:A:908:A:H2'	1:A:909:A:C8	2.53	0.43
1:A:1229:A:O2'	54:Z:31:G:OP1	2.35	0.43
14:N:89:MET:HE2	14:N:89:MET:HA	2.00	0.43
20:T:28:MET:HE1	20:T:67:ILE:HG21	2.01	0.43
22:a:2047:C:H2'	22:a:2048:G:H8	1.84	0.43
22:a:2100:G:H2'	22:a:2101:A:H8	1.82	0.43
22:a:2314:A:OP1	27:f:88:LYS:NZ	2.52	0.43
22:a:2419:U:H4'	48:0:22:THR:HG21	2.00	0.43
25:d:118:PHE:CE1	25:d:163:GLY:HA2	2.54	0.43
27:f:36:LEU:HD22	27:f:154:ILE:HG12	2.01	0.43
52:4:11:GLU:HA	52:4:25:ARG:HA	2.01	0.43
1:A:501:C:H2'	1:A:502:A:C8	2.54	0.43
1:A:512:U:OP1	4:D:44:ARG:NH1	2.52	0.43
1:A:860:A:H2'	1:A:861:G:O4'	2.17	0.43
17:Q:19:LYS:O	17:Q:19:LYS:HG2	2.17	0.43
22:a:1180:U:H2'	22:a:1181:U:C6	2.53	0.43
23:b:110:C:H2'	23:b:111:U:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:164:TYR:HB2	28:g:167:GLU:HB2	2.00	0.43
29:h:3:VAL:HG21	29:h:36:ALA:HB1	2.00	0.43
35:n:36:TYR:HD1	35:n:52:SER:HB2	1.84	0.43
1:A:157:U:H1'	1:A:165:G:H22	1.84	0.43
1:A:161:A:H2'	1:A:162:A:C8	2.53	0.43
1:A:391:G:P	16:P:28:ARG:HH12	2.42	0.43
1:A:754:C:OP1	15:O:72:ARG:NH2	2.48	0.43
3:C:56:VAL:O	3:C:66:VAL:HA	2.17	0.43
5:E:72:ILE:HD11	5:E:141:ILE:HG23	2.00	0.43
10:J:8:ILE:HD12	10:J:100:ILE:HG22	2.00	0.43
10:J:48:ARG:HG2	10:J:66:GLU:HB3	2.01	0.43
13:M:11:ASP:HA	13:M:45:ILE:HB	2.00	0.43
22:a:1482:G:H1'	22:a:1509:A:H61	1.84	0.43
22:a:1599:U:H2'	22:a:1600:C:C6	2.54	0.43
22:a:1870:C:O2'	22:a:1871:A:O5'	2.36	0.43
22:a:2199:A:OP1	44:w:37:ARG:NH1	2.52	0.43
22:a:2251:OMG:HM23	22:a:2251:OMG:H1'	1.83	0.43
35:n:41:ALA:HB3	35:n:43:ASN:HD21	1.82	0.43
50:2:27:ALA:O	50:2:28:ASN:HB2	2.18	0.43
1:A:904:U:H2'	1:A:905:U:C6	2.54	0.43
1:A:999:C:H2'	1:A:1000:A:H8	1.84	0.43
1:A:1039:G:H2'	1:A:1040:U:C6	2.53	0.43
2:B:218:ALA:HA	2:B:221:VAL:HG12	2.00	0.43
4:D:102:VAL:CG1	4:D:114:ALA:HB1	2.48	0.43
13:M:71:ARG:CZ	27:f:115:ARG:HD3	2.49	0.43
22:a:566:U:OP1	32:k:29:LYS:HE2	2.18	0.43
1:A:502:A:H2'	1:A:503:C:O4'	2.19	0.43
22:a:1790:C:H2'	22:a:1791:A:C5	2.53	0.43
22:a:2228:G:H2'	22:a:2229:U:C6	2.53	0.43
22:a:2430:A:N3	22:a:2430:A:H2'	2.34	0.43
22:a:2481:G:O2'	22:a:2482:A:H8	2.02	0.43
33:l:8:LYS:HG3	33:l:9:PHE:CD2	2.53	0.43
33:l:39:GLY:HA3	33:l:126:ILE:HD11	2.01	0.43
1:A:660:C:H2'	1:A:661:G:O4'	2.19	0.43
1:A:1149:C:H2'	1:A:1150:A:C8	2.54	0.43
4:D:105:MET:SD	4:D:180:GLY:HA3	2.59	0.43
4:D:107:PHE:CD1	4:D:159:LEU:HD11	2.50	0.43
22:a:1883:U:H2'	22:a:1884:G:O4'	2.19	0.43
1:A:130:A:H1'	1:A:263:A:O2'	2.19	0.43
1:A:542:G:OP1	4:D:10:LYS:NZ	2.51	0.43
1:A:900:A:H2'	1:A:901:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:U:O2	2:B:103:ASN:ND2	2.49	0.43
1:A:1455:G:H2'	1:A:1456:A:O4'	2.19	0.43
6:F:16:GLU:O	6:F:19:PRO:HD2	2.19	0.43
10:J:67:ILE:HG13	14:N:96:LEU:HD13	2.00	0.43
11:K:107:ILE:HD13	21:U:12:PHE:CE1	2.54	0.43
13:M:104:THR:O	13:M:105:ASN:O	2.37	0.43
22:a:151:C:H2'	22:a:152:A:C8	2.54	0.43
22:a:2025:C:H2'	22:a:2026:U:C6	2.53	0.43
1:A:34:C:H2'	1:A:35:G:H8	1.84	0.42
1:A:56:U:H6	1:A:56:U:O5'	2.02	0.42
1:A:90:C:H2'	1:A:91:U:C6	2.54	0.42
1:A:464:U:H2'	1:A:466:A:OP2	2.19	0.42
1:A:526:C:P	12:L:88:LYS:HE3	2.59	0.42
4:D:76:TYR:CE2	4:D:204:TYR:HB3	2.54	0.42
8:H:5:ASP:OD2	8:H:77:ARG:NH1	2.52	0.42
9:I:55:VAL:HG23	9:I:57:MET:HB3	2.01	0.42
17:Q:8:LEU:HD13	17:Q:25:ILE:HD13	2.00	0.42
22:a:1655:A:H1'	25:d:118:PHE:HE2	1.83	0.42
22:a:1796:U:H2'	22:a:1797:G:C8	2.54	0.42
22:a:1873:G:H2'	22:a:1874:C:C6	2.54	0.42
22:a:2065:C:H2'	22:a:2066:C:C6	2.54	0.42
30:i:31:GLU:OE2	30:i:34:ARG:HD3	2.19	0.42
52:4:26:SER:OG	52:4:28:VAL:HG12	2.19	0.42
1:A:155:A:N6	1:A:167:A:H61	2.17	0.42
3:C:79:LYS:O	3:C:80:LYS:HG2	2.19	0.42
22:a:1153:C:H2'	22:a:1154:G:O4'	2.19	0.42
32:k:110:VAL:O	32:k:128:THR:HG23	2.19	0.42
35:n:26:LEU:HD23	35:n:92:PHE:HD1	1.84	0.42
1:A:72:A:H2'	1:A:72:A:N3	2.34	0.42
1:A:150:U:C4	1:A:170:U:C5	3.08	0.42
1:A:155:A:N6	1:A:167:A:N6	2.67	0.42
4:D:98:LEU:HD13	4:D:137:VAL:HG11	2.01	0.42
16:P:5:ARG:NH2	16:P:26:ASN:O	2.46	0.42
16:P:18:GLN:OE1	16:P:35:ARG:NE	2.52	0.42
22:a:2723:C:H2'	22:a:2724:U:O4'	2.19	0.42
52:4:59:ARG:HA	52:4:62:LYS:HG2	2.02	0.42
1:A:1088:G:H21	1:A:1167:A:H61	1.66	0.42
1:A:1404:C:H2'	1:A:1405:G:C8	2.54	0.42
3:C:33:LEU:HA	3:C:33:LEU:HD23	1.77	0.42
7:G:27:VAL:HG22	7:G:43:VAL:HG21	2.00	0.42
21:U:33:ARG:HB3	21:U:34:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:278:A:H2	22:a:361:G:N2	2.16	0.42
22:a:810:U:C4	32:k:29:LYS:O	2.72	0.42
22:a:1048:A:H2'	22:a:1048:A:N3	2.34	0.42
22:a:1183:U:H2'	22:a:1184:U:C6	2.54	0.42
22:a:1199:U:H2'	22:a:1200:C:H6	1.84	0.42
26:e:7:ASP:OD1	26:e:7:ASP:N	2.49	0.42
26:e:200:LEU:HA	26:e:200:LEU:HD23	1.75	0.42
54:Z:62:C:H2'	54:Z:63:C:H6	1.84	0.42
1:A:445:G:H2'	1:A:446:G:O4'	2.20	0.42
1:A:601:G:H2'	1:A:602:A:C8	2.54	0.42
1:A:920:U:H2'	1:A:921:U:C6	2.55	0.42
4:D:68:LEU:HD23	4:D:68:LEU:HA	1.84	0.42
16:P:73:ALA:O	16:P:76:LYS:HG2	2.19	0.42
19:S:9:PRO:HD3	52:4:64:PHE:CG	2.55	0.42
22:a:41:C:H2'	22:a:42:A:O4'	2.19	0.42
22:a:127:A:H5''	22:a:128:C:C6	2.55	0.42
22:a:265:A:N1	22:a:427:U:O2'	2.45	0.42
22:a:909:A:H2'	22:a:912:C:H5	1.85	0.42
22:a:2331:G:O2'	22:a:2336:A:N1	2.45	0.42
52:4:11:GLU:OE2	52:4:23:LYS:HB3	2.20	0.42
54:Z:45:A:H2'	54:Z:46:G:C8	2.54	0.42
1:A:67:C:H2'	1:A:68:G:H8	1.83	0.42
1:A:401:C:OP2	4:D:70:ARG:NH1	2.50	0.42
1:A:620:C:H2'	1:A:621:A:O4'	2.19	0.42
1:A:857:C:H2'	1:A:858:G:O4'	2.20	0.42
1:A:1144:G:N2	1:A:1146:A:H62	2.17	0.42
1:A:1172:C:H2'	1:A:1173:U:C6	2.55	0.42
2:B:81:LYS:HG3	2:B:91:PHE:CE2	2.55	0.42
2:B:207:ILE:HA	2:B:210:VAL:HG12	2.02	0.42
4:D:178:MET:HE3	4:D:178:MET:HB2	1.91	0.42
6:F:10:VAL:HG21	6:F:18:VAL:HG22	2.02	0.42
8:H:13:ARG:NH1	8:H:26:THR:O	2.53	0.42
9:I:23:PRO:HA	9:I:61:LEU:HD23	2.01	0.42
18:R:70:TYR:HB2	18:R:74:HIS:CE1	2.55	0.42
22:a:2554:U:H2'	22:a:2555:U:C6	2.55	0.42
37:p:76:TYR:CZ	37:p:80:ILE:HG13	2.54	0.42
1:A:216:U:H2'	1:A:217:C:H6	1.83	0.42
1:A:483:C:H5''	1:A:484:G:OP2	2.19	0.42
4:D:188:ARG:HA	4:D:188:ARG:HD2	1.85	0.42
12:L:39:THR:HA	12:L:50:ARG:O	2.20	0.42
22:a:2394:C:H5''	32:k:63:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2784:U:H4'	25:d:43:ASP:OD1	2.19	0.42
23:b:66:A:OP2	23:b:108:A:N6	2.52	0.42
33:l:136:MET:O	42:u:79:ARG:NH2	2.43	0.42
21:U:69:ARG:HH21	21:U:71:TYR:C	2.27	0.42
22:a:720:U:H2'	22:a:721:A:H8	1.85	0.42
22:a:1020:A:C2	22:a:1141:U:C2	3.07	0.42
22:a:1932:A:H2'	22:a:1933:G:O4'	2.19	0.42
1:A:501:C:OP1	12:L:114:ARG:NH2	2.47	0.42
1:A:1130:A:H2'	1:A:1131:G:H8	1.84	0.42
1:A:1489:G:H2'	1:A:1490:U:O4'	2.19	0.42
3:C:114:LYS:HD2	3:C:114:LYS:HA	1.80	0.42
4:D:48:LEU:HD12	4:D:48:LEU:HA	1.85	0.42
4:D:161:LEU:HD23	4:D:161:LEU:HA	1.77	0.42
10:J:35:GLN:O	10:J:76:ILE:HD12	2.20	0.42
27:f:132:VAL:HB	27:f:152:LEU:HD23	2.02	0.42
1:A:149:A:C4	1:A:150:U:C5	3.08	0.42
1:A:195:A:O2'	1:A:196:A:O4'	2.29	0.42
1:A:490:C:H2'	1:A:491:G:H8	1.85	0.42
1:A:1126:U:OP1	10:J:7:ARG:NH2	2.50	0.42
1:A:1464:U:H2'	1:A:1465:A:C8	2.55	0.42
2:B:27:MET:O	2:B:31:ILE:HG12	2.19	0.42
3:C:153:VAL:HG22	3:C:198:VAL:HG22	2.02	0.42
22:a:363:G:H2'	22:a:364:C:C6	2.55	0.42
22:a:2255:G:H21	43:v:9:SER:HB3	1.85	0.42
22:a:2902:C:H3'	22:a:2903:U:C6	2.54	0.42
25:d:46:ARG:NH2	25:d:88:GLU:O	2.52	0.42
54:Z:19:G:O6	54:Z:56:PSU:H1'	2.20	0.42
1:A:135:C:H2'	1:A:136:C:H5'	2.01	0.41
1:A:335:C:H2'	1:A:336:A:H8	1.85	0.41
1:A:460:A:H2'	1:A:461:A:H8	1.84	0.41
1:A:519:C:H2'	1:A:520:A:O4'	2.20	0.41
3:C:20:SER:OG	3:C:22:TRP:NE1	2.53	0.41
22:a:290:U:O2	22:a:350:G:C6	2.74	0.41
22:a:614:A:H2	26:e:173:THR:HB	1.83	0.41
22:a:829:A:N7	22:a:2247:A:O2'	2.46	0.41
22:a:1315:C:O2'	22:a:1392:A:N3	2.51	0.41
27:f:29:PRO:HB3	27:f:160:ALA:HB2	2.02	0.41
40:s:1:MET:HG2	40:s:2:ILE:N	2.35	0.41
55:V:47:H2U:O2'	55:V:47:H2U:H61	2.18	0.41
1:A:221:C:H2'	1:A:222:C:H6	1.85	0.41
1:A:471:U:H2'	1:A:472:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:U:H2'	1:A:1119:C:H6	1.85	0.41
1:A:1236:A:H2'	1:A:1237:C:C6	2.55	0.41
3:C:175:LEU:HD21	3:C:201:TRP:CD1	2.56	0.41
4:D:9:LEU:HD13	4:D:32:CYS:HB3	2.01	0.41
7:G:69:VAL:HG12	7:G:135:VAL:HG22	2.01	0.41
10:J:8:ILE:HB	10:J:74:VAL:HG23	2.02	0.41
16:P:1:MET:SD	16:P:2:VAL:N	2.94	0.41
22:a:5:A:H2'	22:a:6:A:C8	2.56	0.41
22:a:71:A:H5''	22:a:73:A:C8	2.55	0.41
22:a:1808:A:H3'	22:a:1809:A:C8	2.56	0.41
50:2:32:ILE:HG21	50:2:35:LYS:HE3	2.01	0.41
1:A:219:U:C2	1:A:220:G:C8	3.08	0.41
1:A:464:U:C2	1:A:466:A:N7	2.88	0.41
1:A:523:A:N6	12:L:89:D2T:OD2	2.42	0.41
1:A:718:A:H2	18:R:38:LYS:NZ	2.06	0.41
3:C:179:ARG:HD2	3:C:207:ILE:HG12	2.01	0.41
4:D:170:TRP:CD2	4:D:186:PRO:HB3	2.55	0.41
17:Q:19:LYS:HG2	17:Q:47:HIS:CE1	2.55	0.41
22:a:714:U:O2'	22:a:716:A:N7	2.48	0.41
22:a:2859:G:H2'	22:a:2860:A:C8	2.55	0.41
24:c:93:LEU:HD13	24:c:103:TYR:CE1	2.55	0.41
28:g:164:TYR:N	28:g:167:GLU:OE2	2.52	0.41
36:o:114:LEU:O	36:o:114:LEU:HD12	2.20	0.41
1:A:380:G:H8	1:A:380:G:H5''	1.86	0.41
1:A:407:U:H2'	1:A:408:A:H8	1.84	0.41
22:a:1327:A:H2'	22:a:1328:A:O4'	2.20	0.41
22:a:1980:G:O2'	22:a:1982:U:OP2	2.37	0.41
35:n:88:LYS:O	35:n:88:LYS:HG3	2.20	0.41
1:A:53:A:H2'	1:A:54:C:O4'	2.20	0.41
1:A:818:G:O2'	1:A:819:A:H5'	2.20	0.41
4:D:105:MET:HA	4:D:173:VAL:HG21	2.03	0.41
5:E:61:GLN:O	5:E:65:GLU:OE1	2.38	0.41
7:G:69:VAL:HG23	7:G:100:ALA:HB1	2.02	0.41
11:K:89:PRO:HG3	21:U:32:VAL:HG11	2.02	0.41
22:a:587:C:C2	32:k:19:LEU:HD12	2.56	0.41
22:a:644:A:H2'	22:a:645:C:O4'	2.21	0.41
22:a:760:G:H2'	22:a:761:A:O4'	2.20	0.41
22:a:1902:C:H4'	24:c:242:LYS:O	2.21	0.41
24:c:272:SER:O	24:c:272:SER:OG	2.38	0.41
27:f:134:GLU:HG3	27:f:136:ILE:HG12	2.03	0.41
32:k:85:VAL:HB	32:k:94:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:m:44:LEU:O	34:m:48:VAL:HG12	2.20	0.41
1:A:1006:G:C5	1:A:1007:U:C5	3.08	0.41
1:A:1313:U:O4	19:S:2:PRO:HD2	2.19	0.41
5:E:107:ALA:HB2	5:E:125:ALA:HB3	2.02	0.41
11:K:47:ALA:HB1	11:K:62:ALA:HB1	2.03	0.41
22:a:1558:C:O4'	22:a:1560:G:C8	2.74	0.41
22:a:2482:A:H4'	55:V:63:C:HO2'	1.85	0.41
22:a:2552:OMU:HM23	22:a:2554:U:C6	2.56	0.41
28:g:127:THR:HG22	28:g:128:GLN:N	2.35	0.41
29:h:5:LEU:O	29:h:6:LEU:HD23	2.21	0.41
35:n:63:LYS:HE3	35:n:63:LYS:HB3	1.75	0.41
36:o:57:SER:O	36:o:76:THR:HG22	2.20	0.41
1:A:162:A:H2'	1:A:163:C:O4'	2.20	0.41
1:A:218:U:H2'	1:A:219:U:O4'	2.21	0.41
1:A:405:U:H1'	1:A:498:A:H2'	2.01	0.41
1:A:486:U:H2'	1:A:487:A:H8	1.86	0.41
1:A:946:A:H2'	1:A:947:G:H8	1.80	0.41
1:A:1021:A:C4	1:A:1022:A:C8	3.09	0.41
4:D:4:TYR:CE2	4:D:11:LEU:HD11	2.56	0.41
9:I:99:ARG:O	9:I:102:GLY:N	2.54	0.41
22:a:319:G:H2'	22:a:320:A:O4'	2.20	0.41
22:a:1240:U:O2'	22:a:1241:A:O5'	2.37	0.41
22:a:2299:U:H2'	22:a:2300:C:C6	2.56	0.41
22:a:2373:G:H2'	22:a:2374:C:C6	2.56	0.41
22:a:2900:A:H2'	22:a:2901:C:C6	2.55	0.41
24:c:76:ALA:HB2	24:c:96:TYR:CD1	2.55	0.41
27:f:42:GLU:H	27:f:42:GLU:CD	2.28	0.41
31:j:66:LYS:HB3	31:j:66:LYS:HE2	1.58	0.41
54:Z:9:G:H21	54:Z:46:G:H3'	1.86	0.41
54:Z:9:G:N2	54:Z:47:A:OP2	2.53	0.41
1:A:482:A:H2'	1:A:483:C:O4'	2.21	0.41
1:A:622:A:C8	1:A:623:C:C6	3.09	0.41
1:A:1085:U:H3'	1:A:1086:U:C5	2.56	0.41
13:M:57:ARG:NH1	52:4:35:ASP:HA	2.36	0.41
14:N:47:LYS:O	14:N:50:THR:N	2.54	0.41
15:O:26:GLU:OE2	15:O:77:ARG:NH2	2.52	0.41
19:S:20:GLU:HA	19:S:23:VAL:HG22	2.03	0.41
22:a:291:G:O6	22:a:349:U:O2	2.39	0.41
22:a:373:U:O2'	22:a:423:A:H1'	2.21	0.41
22:a:969:G:H2'	22:a:970:U:C6	2.56	0.41
1:A:57:G:H2'	1:A:58:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:A:C4	1:A:461:A:C8	3.09	0.41
1:A:539:A:H2'	1:A:540:G:H8	1.86	0.41
1:A:607:A:H2'	1:A:608:A:C8	2.56	0.41
3:C:126:ARG:O	3:C:127:ARG:HB2	2.20	0.41
4:D:102:VAL:HG23	4:D:107:PHE:CD2	2.50	0.41
6:F:42:TRP:CZ2	6:F:61:LEU:HD12	2.55	0.41
7:G:124:LEU:HA	7:G:124:LEU:HD23	1.82	0.41
9:I:45:ARG:HH11	9:I:45:ARG:HD2	1.76	0.41
13:M:49:SER:OG	13:M:50:GLU:N	2.54	0.41
14:N:83:LYS:HA	14:N:83:LYS:HD3	1.91	0.41
22:a:281:C:H3'	22:a:282:A:H8	1.84	0.41
22:a:284:U:O2	22:a:356:G:O6	2.39	0.41
22:a:358:U:N3	22:a:359:G:N7	2.69	0.41
22:a:558:U:H2'	22:a:559:G:H8	1.86	0.41
22:a:747:5MU:O2	22:a:2014:A:H1'	2.21	0.41
22:a:1230:A:H2'	22:a:1231:U:C6	2.56	0.41
22:a:1508:A:H2	22:a:1509:A:N6	2.19	0.41
22:a:1607:C:H4'	22:a:1608:A:O5'	2.21	0.41
22:a:1853:A:N1	22:a:2087:G:H1'	2.36	0.41
22:a:2482:A:H4'	55:V:63:C:O2'	2.19	0.41
22:a:2795:C:H2'	22:a:2796:U:C6	2.55	0.41
22:a:2895:G:H2'	22:a:2896:C:C6	2.56	0.41
28:g:121:ILE:HD11	28:g:140:VAL:HG12	2.02	0.41
35:n:43:ASN:HD22	35:n:43:ASN:N	2.17	0.41
46:y:19:LYS:HE2	46:y:19:LYS:HB2	1.93	0.41
52:4:43:PHE:HD1	52:4:44:PHE:CD1	2.38	0.41
1:A:187:G:H1'	1:A:190:A:N6	2.36	0.41
1:A:1134:G:N3	1:A:1134:G:H2'	2.36	0.41
1:A:1435:G:H2'	1:A:1436:U:C6	2.56	0.41
3:C:69:HIS:HA	3:C:104:ALA:HB3	2.03	0.41
9:I:51:PRO:O	9:I:55:VAL:HG22	2.21	0.41
22:a:285:G:H2'	22:a:286:U:H5'	2.03	0.41
22:a:1484:U:H2'	22:a:1485:U:H6	1.85	0.41
22:a:1989:G:H2'	22:a:1990:C:O4'	2.21	0.41
1:A:181:A:C6	1:A:195:A:C5	3.09	0.40
1:A:464:U:O2'	1:A:465:A:H3'	2.20	0.40
4:D:57:GLU:OE1	4:D:199:LEU:HB2	2.20	0.40
11:K:122:ARG:HA	11:K:123:PRO:HD3	1.91	0.40
22:a:269:C:H2'	22:a:270:A:O4'	2.21	0.40
22:a:518:G:H2'	22:a:519:U:C6	2.56	0.40
22:a:885:C:H2'	22:a:886:A:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2585:U:H6	22:a:2585:U:H2'	1.75	0.40
22:a:2661:G:H8	22:a:2661:G:OP2	2.03	0.40
26:e:21:ARG:HD3	26:e:106:LYS:HB3	2.02	0.40
26:e:195:GLN:O	26:e:199:MET:HG2	2.21	0.40
1:A:172:A:N7	1:A:174:A:N7	2.70	0.40
1:A:509:A:N3	1:A:543:U:O2'	2.48	0.40
1:A:923:A:H2'	1:A:924:C:O4'	2.21	0.40
1:A:1095:U:H2'	1:A:1096:C:C6	2.55	0.40
1:A:1458:G:OP1	20:T:30:THR:OG1	2.24	0.40
2:B:27:MET:HG3	2:B:189:THR:O	2.21	0.40
2:B:179:LEU:HA	2:B:179:LEU:HD23	1.86	0.40
6:F:6:ILE:HG12	6:F:89:VAL:HG22	2.03	0.40
7:G:111:ARG:HD2	7:G:123:GLU:OE1	2.21	0.40
11:K:14:LYS:HD3	11:K:15:GLN:H	1.86	0.40
19:S:16:LEU:O	19:S:19:VAL:HG12	2.20	0.40
22:a:244:A:H2'	22:a:245:G:O4'	2.22	0.40
22:a:1181:U:H2'	22:a:1182:G:H8	1.86	0.40
22:a:2700:A:H2'	22:a:2701:U:C6	2.57	0.40
27:f:40:VAL:HG12	27:f:43:ALA:HB2	2.02	0.40
35:n:9:ARG:O	35:n:12:THR:HG22	2.21	0.40
1:A:34:C:H2'	1:A:35:G:C8	2.56	0.40
1:A:592:G:H2'	1:A:593:U:C6	2.56	0.40
1:A:1278:G:O5'	1:A:1279:G:H5'	2.22	0.40
1:A:1345:U:OP1	9:I:122:ARG:NH1	2.48	0.40
6:F:2:ARG:NH1	6:F:68:GLN:OE1	2.54	0.40
22:a:722:A:H2'	22:a:723:C:C6	2.56	0.40
22:a:881:G:O6	22:a:895:U:C4	2.73	0.40
22:a:910:A:H2'	22:a:911:A:C8	2.57	0.40
28:g:83:PHE:CE1	28:g:138:LYS:HB2	2.56	0.40
38:q:51:VAL:HG23	38:q:51:VAL:O	2.22	0.40
44:w:59:ILE:HG12	44:w:67:VAL:HG21	2.04	0.40
1:A:29:U:O2'	1:A:30:U:H5'	2.21	0.40
1:A:66:A:H4'	1:A:173:U:C4	2.56	0.40
1:A:235:C:H2'	1:A:236:A:H8	1.87	0.40
1:A:767:A:H2'	1:A:768:A:O4'	2.22	0.40
1:A:1142:G:H2'	1:A:1143:G:O4'	2.21	0.40
1:A:1328:C:OP1	13:M:28:THR:HG21	2.21	0.40
1:A:1371:G:O3'	9:I:71:GLY:HA3	2.22	0.40
2:B:130:THR:C	2:B:132:LYS:H	2.29	0.40
11:K:31:ILE:HG12	11:K:46:THR:HG22	2.03	0.40
19:S:63:THR:HG22	19:S:64:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:13:ASP:O	21:U:17:ARG:HG2	2.22	0.40
22:a:183:C:N4	22:a:213:A:H61	2.20	0.40
22:a:682:G:H5'	49:1:26:ASN:ND2	2.37	0.40
22:a:686:U:O4	49:1:12:ARG:HB2	2.22	0.40
22:a:1418:G:O2'	22:a:1580:A:N6	2.51	0.40
22:a:1549:A:H2'	22:a:1550:C:O4'	2.21	0.40
22:a:2020:A:H5'	47:z:9:THR:CG2	2.52	0.40
22:a:2030:6MZ:C2	22:a:2499:C:H5''	2.51	0.40
24:c:145:GLU:HG2	24:c:151:GLY:C	2.46	0.40
25:d:157:LYS:HG2	30:i:80:HIS:CE1	2.56	0.40
27:f:102:ARG:NH2	52:4:25:ARG:O	2.55	0.40
33:l:26:VAL:HG13	33:l:104:GLU:OE1	2.21	0.40
33:l:41:LEU:HD23	33:l:41:LEU:HA	1.96	0.40
52:4:60:PHE:C	52:4:60:PHE:CD1	2.98	0.40
1:A:150:U:H2'	1:A:151:A:H8	1.86	0.40
1:A:1220:G:P	14:N:53:ARG:HH12	2.44	0.40
2:B:49:MET:HA	2:B:52:GLU:OE1	2.22	0.40
2:B:85:LEU:HD23	2:B:85:LEU:HA	1.96	0.40
2:B:220:THR:O	2:B:223:GLU:HG2	2.22	0.40
4:D:177:LYS:HD3	4:D:177:LYS:O	2.22	0.40
6:F:97:THR:O	6:F:98:GLU:HB2	2.22	0.40
10:J:56:HIS:CG	10:J:57:VAL:H	2.38	0.40
10:J:85:ASP:OD1	10:J:85:ASP:C	2.63	0.40
22:a:351:C:H2'	22:a:352:A:C8	2.56	0.40
22:a:548:G:O5'	22:a:548:G:H8	2.03	0.40
22:a:1319:C:O2'	22:a:1320:C:H5'	2.22	0.40
22:a:1778:U:H2'	22:a:1784:A:N6	2.35	0.40
26:e:7:ASP:OD2	26:e:122:GLU:N	2.55	0.40
52:4:23:LYS:HA	52:4:23:LYS:HD2	1.96	0.40
55:V:66:U:H2'	55:V:67:U:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	206 (93%)	16 (7%)	0	100	100
3	C	204/233 (88%)	192 (94%)	12 (6%)	0	100	100
4	D	203/206 (98%)	193 (95%)	10 (5%)	0	100	100
5	E	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
6	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
7	G	151/179 (84%)	138 (91%)	13 (9%)	0	100	100
8	H	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
9	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
10	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	10
11	K	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
12	L	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
13	M	113/118 (96%)	107 (95%)	5 (4%)	1 (1%)	14	12
14	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	P	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
17	Q	77/84 (92%)	69 (90%)	8 (10%)	0	100	100
18	R	64/75 (85%)	59 (92%)	4 (6%)	1 (2%)	7	4
19	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
20	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	U	68/71 (96%)	63 (93%)	5 (7%)	0	100	100
24	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
25	d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	24
26	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	f	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
28	g	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
29	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
30	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
31	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
32	k	142/144 (99%)	134 (94%)	7 (5%)	1 (1%)	18	17
33	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
35	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
36	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
37	p	115/118 (98%)	115 (100%)	0	0	100	100
38	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
39	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
40	s	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
41	t	100/104 (96%)	92 (92%)	7 (7%)	1 (1%)	12	10
42	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
43	v	82/85 (96%)	80 (98%)	2 (2%)	0	100	100
44	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
45	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	54 (100%)	0	0	100	100
48	0	49/55 (89%)	49 (100%)	0	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	4
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/70 (80%)	50 (89%)	6 (11%)	0	100	100
All	All	5487/5913 (93%)	5240 (96%)	240 (4%)	7 (0%)	49	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL
13	M	105	ASN
50	2	32	ILE
25	d	149	ASN
32	k	36	LYS
41	t	99	ASN
18	R	23	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	89/98 (91%)	89 (100%)	0	100	100
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
24	c	216/218 (99%)	216 (100%)	0	100	100
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	137/138 (99%)	137 (100%)	0	100	100
29	h	32/114 (28%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	i	116/116 (100%)	116 (100%)	0	100	100
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	107/107 (100%)	107 (100%)	0	100	100
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	85 (99%)	1 (1%)	63	74
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100
39	r	93/93 (100%)	93 (100%)	0	100	100
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	83 (100%)	0	100	100
42	u	78/78 (100%)	78 (100%)	0	100	100
43	v	62/63 (98%)	62 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	54 (100%)	0	100	100
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100
48	0	46/49 (94%)	46 (100%)	0	100	100
49	1	38/38 (100%)	38 (100%)	0	100	100
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	55/62 (89%)	55 (100%)	0	100	100
All	All	4576/4825 (95%)	4575 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	n	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	39	HIS
2	B	177	ASN
3	C	102	ASN
4	D	40	GLN
4	D	136	GLN
5	E	12	GLN
5	E	121	HIS
6	F	94	HIS
7	G	68	ASN
9	I	50	GLN
11	K	24	HIS
11	K	101	ASN
13	M	12	HIS
14	N	49	GLN
15	O	28	GLN
15	O	35	GLN
16	P	40	ASN
20	T	20	HIS
24	c	53	HIS
24	c	115	GLN
25	d	32	ASN
25	d	58	ASN
25	d	126	ASN
25	d	173	GLN
26	e	94	GLN
27	f	5	HIS
30	i	80	HIS
31	j	5	GLN
33	l	97	GLN
34	m	9	GLN
37	p	71	GLN
38	q	6	GLN
41	t	53	ASN
42	u	5	ASN
44	w	36	HIS
45	x	15	ASN
49	1	26	ASN
50	2	28	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1542 (97%)	235 (15%)	6 (0%)
22	a	2757/2904 (94%)	329 (11%)	0
23	b	118/120 (98%)	13 (11%)	0
53	X	10/35 (28%)	1 (10%)	0
54	Z	76/77 (98%)	17 (22%)	1 (1%)
55	V	70/76 (92%)	16 (22%)	1 (1%)
All	All	4539/4754 (95%)	611 (13%)	8 (0%)

All (611) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	A
1	A	22	G
1	A	32	A
1	A	39	G
1	A	44	A
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	55	A
1	A	59	A
1	A	60	A
1	A	66	A
1	A	72	A
1	A	74	A
1	A	93	U
1	A	94	G
1	A	95	C
1	A	121	U
1	A	122	G
1	A	131	A
1	A	144	G
1	A	146	G
1	A	149	A
1	A	155	A
1	A	160	A
1	A	162	A
1	A	163	C
1	A	164	G

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Mol	Chain	Res	Type
1	A	171	A
1	A	179	A
1	A	181	A
1	A	183	C
1	A	192	A
1	A	197	A
1	A	199	A
1	A	201	G
1	A	203	G
1	A	204	G
1	A	215	C
1	A	219	U
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	262	A
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	293	G
1	A	321	A
1	A	326	G
1	A	328	C
1	A	352	C
1	A	354	G
1	A	355	C
1	A	367	U
1	A	372	C
1	A	373	A
1	A	376	G
1	A	380	G
1	A	381	C
1	A	385	C
1	A	392	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A

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Mol	Chain	Res	Type
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	436	C
1	A	453	G
1	A	457	G
1	A	463	U
1	A	464	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	470	C
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	497	G
1	A	499	A
1	A	505	G
1	A	506	G
1	A	509	A
1	A	511	C
1	A	512	U
1	A	518	C
1	A	528	C
1	A	536	C
1	A	547	A
1	A	559	A
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	596	A
1	A	617	G
1	A	618	C
1	A	626	G
1	A	633	G

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Mol	Chain	Res	Type
1	A	639	G
1	A	650	G
1	A	653	U
1	A	665	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	733	G
1	A	734	G
1	A	747	A
1	A	755	G
1	A	777	A
1	A	787	A
1	A	793	U
1	A	794	A
1	A	809	G
1	A	815	A
1	A	817	C
1	A	847	G
1	A	851	G
1	A	890	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	993	G
1	A	999	C
1	A	1004	A
1	A	1008	U
1	A	1009	U
1	A	1020	G
1	A	1027	C
1	A	1028	C
1	A	1029	U
1	A	1030	U

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Mol	Chain	Res	Type
1	A	1031	C
1	A	1033	G
1	A	1034	G
1	A	1035	A
1	A	1036	A
1	A	1037	C
1	A	1042	A
1	A	1044	A
1	A	1046	A
1	A	1065	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1159	U
1	A	1168	U
1	A	1169	A
1	A	1171	A
1	A	1174	G
1	A	1184	G
1	A	1187	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1227	A
1	A	1238	A
1	A	1249	C
1	A	1256	A
1	A	1257	A
1	A	1258	G
1	A	1260	G
1	A	1275	A
1	A	1279	G
1	A	1280	A
1	A	1287	A
1	A	1300	G

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Mol	Chain	Res	Type
1	A	1302	C
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1320	C
1	A	1335	U
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1364	U
1	A	1368	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1382	C
1	A	1383	C
1	A	1394	A
1	A	1397	C
1	A	1398	A
1	A	1419	G
1	A	1432	G
1	A	1441	A
1	A	1446	A
1	A	1450	U
1	A	1451	U
1	A	1452	C
1	A	1487	G
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1519	MA6
1	A	1529	G
1	A	1530	G
22	a	3	U
22	a	10	A
22	a	15	G
22	a	34	U
22	a	39	G

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Mol	Chain	Res	Type
22	a	42	A
22	a	45	G
22	a	51	G
22	a	58	G
22	a	71	A
22	a	74	A
22	a	75	G
22	a	98	G
22	a	101	A
22	a	103	A
22	a	114	U
22	a	118	A
22	a	119	A
22	a	120	U
22	a	139	U
22	a	142	A
22	a	163	C
22	a	164	C
22	a	165	A
22	a	181	A
22	a	196	A
22	a	215	G
22	a	216	A
22	a	222	A
22	a	233	A
22	a	248	G
22	a	264	C
22	a	272	A
22	a	273	G
22	a	277	G
22	a	281	C
22	a	282	A
22	a	283	G
22	a	285	G
22	a	304	U
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	362	A
22	a	366	C
22	a	386	G

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Mol	Chain	Res	Type
22	a	404	A
22	a	405	U
22	a	411	G
22	a	412	A
22	a	455	C
22	a	473	G
22	a	481	G
22	a	484	C
22	a	491	G
22	a	501	A
22	a	505	A
22	a	508	A
22	a	509	C
22	a	530	G
22	a	532	A
22	a	538	A
22	a	546	U
22	a	547	A
22	a	548	G
22	a	549	G
22	a	563	A
22	a	568	U
22	a	573	U
22	a	575	A
22	a	592	A
22	a	600	G
22	a	603	A
22	a	614	A
22	a	615	U
22	a	618	G
22	a	627	A
22	a	637	A
22	a	645	C
22	a	647	G
22	a	654	A
22	a	685	A
22	a	686	U
22	a	717	C
22	a	722	A
22	a	730	A
22	a	747	5MU
22	a	775	G

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Mol	Chain	Res	Type
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	792	A
22	a	805	G
22	a	812	C
22	a	827	U
22	a	828	U
22	a	845	A
22	a	846	U
22	a	847	U
22	a	859	G
22	a	866	A
22	a	884	U
22	a	888	C
22	a	889	C
22	a	890	C
22	a	891	G
22	a	892	A
22	a	895	U
22	a	896	A
22	a	897	C
22	a	898	C
22	a	899	A
22	a	910	A
22	a	914	G
22	a	915	C
22	a	931	U
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	996	A
22	a	1005	C
22	a	1012	U
22	a	1013	C
22	a	1022	G
22	a	1033	U
22	a	1040	A
22	a	1046	A
22	a	1047	G

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Mol	Chain	Res	Type
22	a	1108	U
22	a	1111	A
22	a	1112	G
22	a	1114	C
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1172	C
22	a	1178	C
22	a	1241	A
22	a	1253	A
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1273	U
22	a	1275	A
22	a	1300	G
22	a	1301	A
22	a	1321	A
22	a	1329	U
22	a	1343	G
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1416	G
22	a	1420	A
22	a	1427	A
22	a	1428	C
22	a	1434	A
22	a	1437	C
22	a	1452	G
22	a	1453	A
22	a	1459	G
22	a	1482	G
22	a	1485	U
22	a	1493	C
22	a	1497	U
22	a	1508	A
22	a	1509	A
22	a	1510	G

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Mol	Chain	Res	Type
22	a	1515	A
22	a	1523	U
22	a	1529	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1560	G
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1586	A
22	a	1608	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1715	G
22	a	1724	G
22	a	1726	C
22	a	1729	U
22	a	1730	C
22	a	1731	G
22	a	1738	G
22	a	1744	A
22	a	1764	C
22	a	1773	A
22	a	1782	U
22	a	1791	A
22	a	1800	C
22	a	1801	A
22	a	1807	G
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1848	A
22	a	1855	U
22	a	1858	A
22	a	1869	G

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Mol	Chain	Res	Type
22	a	1871	A
22	a	1872	A
22	a	1873	G
22	a	1906	G
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1965	C
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2023	C
22	a	2030	6MZ
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2063	C
22	a	2069	G7M
22	a	2093	G
22	a	2191	A
22	a	2198	A
22	a	2204	G
22	a	2211	A
22	a	2212	A
22	a	2223	G
22	a	2225	A
22	a	2238	G
22	a	2268	A
22	a	2273	A
22	a	2279	G
22	a	2283	C
22	a	2287	A

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Mol	Chain	Res	Type
22	a	2305	U
22	a	2308	G
22	a	2310	C
22	a	2319	G
22	a	2321	U
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2335	A
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2366	A
22	a	2372	U
22	a	2383	G
22	a	2385	C
22	a	2396	G
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2410	G
22	a	2425	A
22	a	2429	G
22	a	2430	A
22	a	2431	U
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2470	G
22	a	2475	C
22	a	2476	A
22	a	2478	A
22	a	2482	A
22	a	2491	U
22	a	2494	G
22	a	2501	C
22	a	2502	G
22	a	2505	G
22	a	2518	A
22	a	2525	G
22	a	2529	G
22	a	2547	A

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Mol	Chain	Res	Type
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2586	U
22	a	2602	A
22	a	2609	U
22	a	2613	U
22	a	2629	U
22	a	2630	G
22	a	2663	G
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2726	A
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2765	A
22	a	2778	A
22	a	2797	U
22	a	2798	U
22	a	2820	A
22	a	2821	A
22	a	2835	A
22	a	2861	U
22	a	2873	A
22	a	2874	C
22	a	2880	C
22	a	2884	U
22	a	2900	A
23	b	13	G
23	b	35	C
23	b	36	C
23	b	37	C
23	b	42	C
23	b	44	G
23	b	56	G
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	105	G

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Mol	Chain	Res	Type
23	b	109	A
53	X	17	A
54	Z	16	C
54	Z	17	C
54	Z	18	U
54	Z	19	G
54	Z	20	G
54	Z	22	A
54	Z	23	G
54	Z	24	C
54	Z	32	G
54	Z	44	A
54	Z	47	A
54	Z	48	U
54	Z	49	C
54	Z	55	5MU
54	Z	66	C
54	Z	67	C
54	Z	68	C
55	V	2	C
55	V	5	G
55	V	6	2MG
55	V	8	U
55	V	11	C
55	V	13	C
55	V	19	G
55	V	22	G
55	V	46	G7M
55	V	47	H2U
55	V	48	5MC
55	V	49	5MC
55	V	61	C
55	V	67	U
55	V	71	G
55	V	74	C

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	199	A
1	A	464	U
1	A	1026	G

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Mol	Chain	Res	Type
1	A	1034	G
1	A	1035	A
1	A	1240	U
54	Z	67	C
55	V	10	2MG

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	G7M	V	46	55	23,26,27	2.78	8 (34%)	35,39,42	1.77	8 (22%)
22	H2U	a	2449	22	18,21,22	1.25	2 (11%)	21,30,33	0.89	0
22	PSU	a	2504	22	18,21,22	1.05	1 (5%)	22,30,33	1.64	3 (13%)
22	3TD	a	1915	22	18,22,23	3.98	7 (38%)	22,32,35	1.63	3 (13%)
22	2MG	a	2445	22	23,26,27	2.41	7 (30%)	32,38,41	2.13	9 (28%)
1	MA6	A	1519	1	23,26,27	1.52	5 (21%)	34,38,41	2.27	12 (35%)
54	4SU	Z	8	54	18,21,22	4.01	8 (44%)	26,30,33	2.24	4 (15%)
54	H2U	Z	21	54,56	18,21,22	1.11	2 (11%)	21,30,33	0.74	1 (4%)
55	1MA	V	58	55	21,25,26	0.57	0	31,37,40	0.77	0
55	2MU	V	54	55	20,23,24	1.40	5 (25%)	28,33,36	2.03	9 (32%)
22	OMU	a	2552	22	19,22,23	2.58	6 (31%)	26,31,34	1.82	5 (19%)
22	5MC	a	1962	22	18,22,23	3.26	7 (38%)	26,32,35	1.10	2 (7%)
1	G7M	A	527	1	23,26,27	2.78	8 (34%)	35,39,42	1.72	7 (20%)
54	PSU	Z	56	54	18,21,22	1.03	1 (5%)	22,30,33	1.83	3 (13%)
1	UR3	A	1498	1	19,22,23	2.59	6 (31%)	26,32,35	1.36	2 (7%)
1	MA6	A	1518	1	23,26,27	1.42	5 (21%)	34,38,41	2.33	12 (35%)
22	5MU	a	747	22	19,22,23	4.52	7 (36%)	28,32,35	3.65	9 (32%)
33	4D4	l	81	33	9,11,12	1.51	1 (11%)	8,13,15	2.19	5 (62%)
1	2MG	A	1516	1	23,26,27	2.49	7 (30%)	32,38,41	2.21	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MC	V	48	55	18,22,23	3.64	7 (38%)	26,32,35	1.07	2 (7%)
22	5MU	a	1939	22	19,22,23	4.47	7 (36%)	28,32,35	3.78	9 (32%)
22	PSU	a	2457	22	18,21,22	1.25	2 (11%)	22,30,33	2.06	5 (22%)
22	2MA	a	2503	56,22	22,25,26	3.80	10 (45%)	33,37,40	2.82	11 (33%)
22	PSU	a	2604	22	18,21,22	1.12	1 (5%)	22,30,33	1.88	4 (18%)
22	6MZ	a	1618	22	23,25,26	2.65	4 (17%)	29,36,39	2.38	9 (31%)
55	PSU	V	39	55	18,21,22	1.05	1 (5%)	22,30,33	1.82	4 (18%)
1	2MG	A	1207	1	23,26,27	2.56	7 (30%)	32,38,41	2.11	10 (31%)
55	H2U	V	47	55	18,21,22	1.06	2 (11%)	21,30,33	0.85	1 (4%)
1	5MC	A	967	1	18,22,23	3.48	7 (38%)	26,32,35	1.06	2 (7%)
1	2MG	A	966	1	23,26,27	2.54	6 (26%)	32,38,41	2.21	9 (28%)
55	2MG	V	6	55	23,26,27	2.62	7 (30%)	32,38,41	2.25	9 (28%)
1	4OC	A	1402	1,56	20,23,24	2.88	8 (40%)	26,32,35	1.10	2 (7%)
1	PSU	A	516	1,56	18,21,22	1.07	3 (16%)	22,30,33	1.66	4 (18%)
1	5MC	A	1407	1	18,22,23	3.42	7 (38%)	26,32,35	0.96	1 (3%)
25	MEQ	d	150	25	8,9,10	1.53	1 (12%)	5,10,12	1.43	1 (20%)
22	1MG	a	745	22	22,26,27	2.46	7 (31%)	33,39,42	1.65	5 (15%)
22	PSU	a	2605	22	18,21,22	1.13	1 (5%)	22,30,33	2.04	5 (22%)
55	2MG	V	10	55	23,26,27	2.64	7 (30%)	32,38,41	2.26	10 (31%)
55	70U	V	34	55,53	22,26,27	1.11	1 (4%)	28,37,40	0.94	1 (3%)
55	5MC	V	49	55	18,22,23	3.61	8 (44%)	26,32,35	1.03	2 (7%)
22	OMC	a	2498	56,22	19,22,23	2.60	8 (42%)	26,31,34	1.00	1 (3%)
22	PSU	a	2580	22	18,21,22	1.26	2 (11%)	22,30,33	1.91	5 (22%)
22	PSU	a	1911	22	18,21,22	1.08	1 (5%)	22,30,33	1.79	2 (9%)
22	PSU	a	746	56,22	18,21,22	1.10	3 (16%)	22,30,33	1.80	4 (18%)
22	OMG	a	2251	54,22	23,26,27	2.51	8 (34%)	33,38,41	2.08	8 (24%)
55	PSU	V	55	55	18,21,22	1.08	1 (5%)	22,30,33	1.98	5 (22%)
22	PSU	a	955	22	18,21,22	1.17	1 (5%)	22,30,33	1.87	3 (13%)
22	PSU	a	1917	22	18,21,22	1.10	3 (16%)	22,30,33	2.02	5 (22%)
11	IAS	K	119	11	6,7,8	1.00	0	6,8,10	1.20	0
54	OMC	Z	33	54	19,22,23	2.73	7 (36%)	26,31,34	0.68	0
22	2MG	a	1835	22	23,26,27	2.53	7 (30%)	32,38,41	2.19	9 (28%)
22	6MZ	a	2030	22	23,25,26	2.53	4 (17%)	29,36,39	2.43	10 (34%)
22	G7M	a	2069	22	23,26,27	2.62	8 (34%)	35,39,42	1.78	9 (25%)
54	5MU	Z	55	54	19,22,23	4.65	7 (36%)	28,32,35	3.75	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	MS6	l	82	33	5,7,8	1.25	1 (20%)	2,7,9	1.97	1 (50%)
55	12A	V	37	55,56	33,36,37	0.92	1 (3%)	47,52,55	1.28	6 (12%)
55	PSU	V	27	55	18,21,22	1.00	1 (5%)	22,30,33	1.70	4 (18%)
12	D2T	L	89	12	7,9,10	1.55	1 (14%)	6,11,13	1.31	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	G7M	V	46	55	-	3/7/25/26	0/3/3/3
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
22	PSU	a	2504	22	-	1/7/25/26	0/2/2/2
22	3TD	a	1915	22	-	2/7/25/26	0/2/2/2
22	2MG	a	2445	22	-	1/9/27/28	0/3/3/3
1	MA6	A	1519	1	-	3/11/29/30	0/3/3/3
54	4SU	Z	8	54	-	0/7/25/26	0/2/2/2
54	H2U	Z	21	54,56	-	4/7/38/39	0/2/2/2
55	1MA	V	58	55	-	2/7/25/26	0/3/3/3
55	2MU	V	54	55	-	0/9/27/28	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
22	5MC	a	1962	22	-	1/7/25/26	0/2/2/2
1	G7M	A	527	1	-	1/7/25/26	0/3/3/3
54	PSU	Z	56	54	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
22	5MU	a	747	22	-	1/7/25/26	0/2/2/2
33	4D4	l	81	33	-	1/11/12/14	-
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
55	5MC	V	48	55	-	2/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	2MA	a	2503	56,22	-	1/7/25/26	0/3/3/3
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
55	PSU	V	39	55	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
55	H2U	V	47	55	-	7/7/38/39	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	966	1	-	2/9/27/28	0/3/3/3
55	2MG	V	6	55	-	2/9/27/28	0/3/3/3
1	4OC	A	1402	1,56	-	0/9/29/30	0/2/2/2
1	PSU	A	516	1,56	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
25	MEQ	d	150	25	-	4/8/9/11	-
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
55	2MG	V	10	55	-	0/9/27/28	0/3/3/3
55	70U	V	34	55,53	-	2/13/31/32	0/2/2/2
55	5MC	V	49	55	-	2/7/25/26	0/2/2/2
22	OMC	a	2498	56,22	-	0/9/27/28	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	PSU	a	746	56,22	-	2/7/25/26	0/2/2/2
22	OMG	a	2251	54,22	-	1/9/27/28	0/3/3/3
55	PSU	V	55	55	-	0/7/25/26	0/2/2/2
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1917	22	-	2/7/25/26	0/2/2/2
11	IAS	K	119	11	-	0/7/7/8	-
54	OMC	Z	33	54	-	0/9/27/28	0/2/2/2
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
22	G7M	a	2069	22	-	1/7/25/26	0/3/3/3
54	5MU	Z	55	54	-	2/7/25/26	0/2/2/2
33	MS6	l	82	33	-	1/4/6/8	-
55	12A	V	37	55,56	-	8/25/43/44	0/3/3/3
55	PSU	V	27	55	-	0/7/25/26	0/2/2/2
12	D2T	L	89	12	-	1/7/12/14	-

All (261) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C6-C5	12.09	1.49	1.35
22	a	2503	2MA	C4-N3	12.02	1.49	1.34
22	a	1618	6MZ	C6-N6	11.01	1.46	1.34
54	Z	55	5MU	C6-N1	10.68	1.56	1.38
54	Z	55	5MU	C2-N1	10.44	1.55	1.38
22	a	2030	6MZ	C6-N6	10.35	1.45	1.34
22	a	747	5MU	C6-N1	10.16	1.55	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1939	5MU	C2-N1	9.87	1.54	1.38
22	a	747	5MU	C2-N1	9.57	1.53	1.38
22	a	1939	5MU	C6-N1	9.38	1.54	1.38
55	V	48	5MC	C6-C5	9.11	1.49	1.34
55	V	49	5MC	C6-C5	9.06	1.49	1.34
22	a	747	5MU	C4-C5	9.06	1.59	1.44
1	A	1407	5MC	C6-C5	9.00	1.49	1.34
54	Z	8	4SU	C4-N3	8.90	1.47	1.37
1	A	967	5MC	C6-C5	8.76	1.49	1.34
54	Z	55	5MU	C4-C5	8.71	1.59	1.44
22	a	1939	5MU	C4-C5	8.47	1.58	1.44
22	a	1915	3TD	C2-N1	8.40	1.48	1.37
22	a	1939	5MU	C4-N3	-8.23	1.23	1.38
22	a	1962	5MC	C6-C5	8.22	1.48	1.34
55	V	10	2MG	C2-N3	7.69	1.46	1.31
22	a	747	5MU	C4-N3	-7.68	1.24	1.38
54	Z	55	5MU	C4-N3	-7.62	1.24	1.38
55	V	6	2MG	C2-N3	7.54	1.46	1.31
54	Z	8	4SU	C2-N1	7.35	1.50	1.38
1	A	966	2MG	C2-N3	7.19	1.45	1.31
55	V	48	5MC	C4-N3	6.98	1.45	1.34
22	a	2503	2MA	C2-N3	6.97	1.46	1.34
55	V	49	5MC	C4-N3	6.96	1.45	1.34
1	A	1516	2MG	C2-N3	6.93	1.45	1.31
1	A	1207	2MG	C2-N3	6.85	1.45	1.31
22	a	1835	2MG	C2-N3	6.79	1.44	1.31
22	a	2251	OMG	C4-N3	6.67	1.50	1.34
1	A	967	5MC	C4-N3	6.54	1.45	1.34
22	a	2445	2MG	C2-N3	6.47	1.44	1.31
55	V	10	2MG	C4-N3	6.46	1.49	1.34
22	a	1962	5MC	C4-N3	6.45	1.45	1.34
54	Z	55	5MU	C6-C5	6.43	1.45	1.34
55	V	6	2MG	C4-N3	6.42	1.49	1.34
1	A	1207	2MG	C4-N3	6.39	1.49	1.34
1	A	966	2MG	C4-N3	6.38	1.49	1.34
55	V	48	5MC	C2-N3	6.34	1.49	1.36
55	V	46	G7M	C2-N2	6.28	1.49	1.34
54	Z	8	4SU	C2-N3	6.27	1.49	1.38
1	A	527	G7M	C2-N2	6.18	1.48	1.34
1	A	1498	UR3	C2-N1	6.17	1.47	1.38
55	V	49	5MC	C2-N3	6.15	1.48	1.36
1	A	1402	4OC	C6-C5	6.13	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C4-N3	6.10	1.43	1.32
1	A	1516	2MG	C4-N3	6.09	1.48	1.34
22	a	747	5MU	C6-C5	6.09	1.44	1.34
55	V	46	G7M	C4-N3	6.08	1.48	1.34
1	A	527	G7M	C4-N3	6.05	1.48	1.34
1	A	967	5MC	C2-N3	5.97	1.48	1.36
1	A	1407	5MC	C4-N3	5.93	1.44	1.34
22	a	1835	2MG	C4-N3	5.90	1.48	1.34
54	Z	8	4SU	C6-C5	5.89	1.48	1.35
22	a	2503	2MA	C2-N1	5.89	1.44	1.34
22	a	2552	OMU	C2-N1	5.78	1.47	1.38
22	a	1939	5MU	C6-C5	5.74	1.44	1.34
1	A	1498	UR3	C6-C5	5.70	1.48	1.35
54	Z	33	OMC	C6-C5	5.69	1.48	1.35
22	a	1962	5MC	C2-N3	5.65	1.47	1.36
54	Z	8	4SU	C4-S4	-5.65	1.57	1.68
22	a	2445	2MG	C4-N3	5.64	1.47	1.34
22	a	1915	3TD	C6-N1	5.58	1.45	1.36
22	a	2069	G7M	C2-N2	5.57	1.47	1.34
54	Z	33	OMC	C2-N3	5.57	1.47	1.36
22	a	2069	G7M	C4-N3	5.50	1.47	1.34
55	V	46	G7M	C2-N3	5.48	1.46	1.33
22	a	745	1MG	C4-N3	5.47	1.47	1.34
1	A	527	G7M	C2-N3	5.44	1.46	1.33
22	a	2069	G7M	C5-N7	-5.43	1.32	1.39
22	a	2498	OMC	C6-C5	5.25	1.47	1.35
1	A	1407	5MC	C2-N3	5.21	1.46	1.36
22	a	2552	OMU	C6-C5	5.17	1.47	1.35
54	Z	8	4SU	C5-C4	5.17	1.49	1.42
1	A	527	G7M	C5-N7	-5.15	1.33	1.39
22	a	2552	OMU	C2-N3	5.14	1.47	1.38
22	a	2503	2MA	C6-N6	-5.13	1.21	1.34
22	a	2498	OMC	C2-N3	5.07	1.46	1.36
22	a	745	1MG	C2-N3	5.04	1.43	1.34
1	A	1402	4OC	C2-N3	5.02	1.46	1.36
22	a	2251	OMG	C2-N3	4.99	1.45	1.33
22	a	745	1MG	C2-N2	4.99	1.43	1.34
1	A	1407	5MC	C6-N1	4.96	1.46	1.38
55	V	10	2MG	C2-N1	4.95	1.44	1.36
22	a	2503	2MA	C5-C6	4.86	1.54	1.41
55	V	48	5MC	C6-N1	4.85	1.46	1.38
55	V	49	5MC	C6-N1	4.79	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	46	G7M	C5-N7	-4.79	1.33	1.39
55	V	6	2MG	C2-N1	4.72	1.44	1.36
1	A	967	5MC	C6-N1	4.61	1.45	1.38
54	Z	33	OMC	C4-N4	4.58	1.44	1.33
1	A	1207	2MG	C2-N1	4.56	1.44	1.36
22	a	2069	G7M	C2-N3	4.55	1.44	1.33
22	a	1835	2MG	C2-N1	4.49	1.43	1.36
54	Z	33	OMC	C4-N3	4.38	1.43	1.34
22	a	2251	OMG	C2-N2	4.38	1.44	1.34
1	A	966	2MG	C2-N1	4.36	1.43	1.36
1	A	1498	UR3	C2-N3	4.35	1.47	1.39
22	a	2498	OMC	C2-N1	4.14	1.49	1.40
22	a	2498	OMC	C4-N4	4.12	1.43	1.33
55	V	49	5MC	C2-N1	4.07	1.48	1.40
1	A	1516	2MG	C2-N1	4.05	1.43	1.36
22	a	1962	5MC	C6-N1	4.04	1.44	1.38
55	V	34	70U	C2-S2	-3.92	1.61	1.67
1	A	527	G7M	C5-C6	3.92	1.54	1.43
55	V	49	5MC	C4-N4	3.91	1.44	1.34
1	A	1402	4OC	C4-N4	3.90	1.43	1.35
55	V	48	5MC	C4-N4	3.88	1.44	1.34
55	V	46	G7M	C5-C6	3.87	1.54	1.43
55	V	48	5MC	C2-N1	3.85	1.48	1.40
22	a	2251	OMG	O6-C6	-3.83	1.16	1.23
1	A	967	5MC	C2-N1	3.82	1.48	1.40
22	a	2251	OMG	C5-N7	-3.78	1.31	1.39
22	a	1835	2MG	C5-N7	-3.75	1.31	1.39
22	a	1915	3TD	C2-N3	3.75	1.46	1.38
22	a	2552	OMU	O2-C2	-3.74	1.16	1.23
22	a	2498	OMC	C4-N3	3.74	1.42	1.34
1	A	1402	4OC	C2-N1	3.73	1.48	1.40
1	A	1402	4OC	O2-C2	-3.73	1.16	1.23
1	A	967	5MC	C4-N4	3.72	1.43	1.34
22	a	2445	2MG	C2-N1	3.71	1.42	1.36
22	a	2552	OMU	O4-C4	-3.69	1.17	1.24
22	a	745	1MG	C5-N7	-3.68	1.31	1.39
54	Z	33	OMC	C2-N1	3.67	1.47	1.40
22	a	2503	2MA	C5-N7	-3.66	1.32	1.39
1	A	1207	2MG	C5-N7	-3.63	1.32	1.39
22	a	2498	OMC	O2-C2	-3.62	1.17	1.23
1	A	1407	5MC	C4-N4	3.59	1.43	1.34
22	a	2445	2MG	C5-N7	-3.59	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	5MC	C2-N1	3.54	1.47	1.40
1	A	966	2MG	C5-N7	-3.52	1.32	1.39
54	Z	8	4SU	O2-C2	-3.51	1.16	1.23
1	A	1519	MA6	C5-C4	-3.50	1.32	1.39
22	a	745	1MG	C4-N9	-3.46	1.29	1.38
22	a	2069	G7M	C5-C6	3.46	1.53	1.43
1	A	1402	4OC	C5-C4	3.45	1.48	1.40
22	a	2069	G7M	O6-C6	-3.44	1.17	1.23
22	a	1962	5MC	C4-N4	3.40	1.42	1.34
33	l	81	4D4	OB-CB	-3.38	1.36	1.43
22	a	1835	2MG	O6-C6	-3.38	1.17	1.23
1	A	1518	MA6	C5-C4	-3.36	1.32	1.39
55	V	6	2MG	C5-N7	-3.35	1.32	1.39
54	Z	33	OMC	O2-C2	-3.29	1.17	1.23
22	a	1939	5MU	O2-C2	-3.26	1.17	1.23
22	a	2445	2MG	O6-C6	-3.26	1.17	1.23
1	A	1407	5MC	O2-C2	-3.23	1.17	1.23
1	A	1516	2MG	C5-N7	-3.21	1.32	1.39
22	a	2449	H2U	C2-N3	-3.18	1.32	1.38
55	V	55	PSU	C6-C5	3.17	1.39	1.35
1	A	1516	2MG	O6-C6	-3.17	1.17	1.23
1	A	1498	UR3	O2-C2	-3.15	1.16	1.22
12	L	89	D2T	CB-SB	3.14	1.85	1.82
22	a	1618	6MZ	C5-C4	-3.11	1.33	1.39
54	Z	8	4SU	C6-N1	3.08	1.45	1.38
1	A	1498	UR3	O4-C4	-3.05	1.17	1.23
54	Z	56	PSU	C6-C5	3.05	1.38	1.35
1	A	527	G7M	C2-N1	3.02	1.45	1.37
22	a	2449	H2U	C4-N3	-3.01	1.32	1.37
22	a	2030	6MZ	C5-C4	-3.01	1.33	1.39
22	a	1962	5MC	O2-C2	-3.01	1.18	1.23
1	A	1519	MA6	C5-N7	-2.99	1.33	1.39
22	a	1939	5MU	O4-C4	-2.99	1.17	1.23
22	a	2030	6MZ	C5-N7	-2.99	1.33	1.39
22	a	1618	6MZ	C5-N7	-2.98	1.33	1.39
22	a	2457	PSU	C6-C5	2.98	1.38	1.35
22	a	745	1MG	O6-C6	-2.97	1.16	1.23
55	V	27	PSU	C6-C5	2.94	1.38	1.35
55	V	10	2MG	C5-N7	-2.91	1.33	1.39
1	A	966	2MG	O6-C6	-2.90	1.18	1.23
22	a	2503	2MA	C6-N1	2.90	1.39	1.35
22	a	2504	PSU	C6-C5	2.89	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	39	PSU	C6-C5	2.88	1.38	1.35
22	a	2030	6MZ	C8-N9	-2.87	1.32	1.37
55	V	47	H2U	C2-N3	-2.87	1.32	1.38
55	V	54	2MU	C4-N3	-2.85	1.33	1.38
55	V	47	H2U	C4-N3	-2.82	1.32	1.37
54	Z	21	H2U	C2-N3	-2.81	1.33	1.38
22	a	745	1MG	C5-C6	2.81	1.52	1.45
22	a	2445	2MG	C4-N9	-2.81	1.30	1.38
1	A	1519	MA6	C8-N9	-2.79	1.32	1.37
1	A	1518	MA6	C5-N7	-2.79	1.33	1.39
22	a	1962	5MC	C2-N1	2.78	1.46	1.40
22	a	747	5MU	O2-C2	-2.78	1.18	1.23
55	V	46	G7M	C6-N1	2.77	1.44	1.38
54	Z	21	H2U	C4-N3	-2.77	1.32	1.37
1	A	1402	4OC	C6-N1	2.76	1.44	1.38
55	V	46	G7M	C2-N1	2.76	1.44	1.37
22	a	1911	PSU	C6-C5	2.75	1.38	1.35
55	V	6	2MG	O6-C6	-2.74	1.18	1.23
1	A	1519	MA6	C6-N6	2.74	1.44	1.36
22	a	2604	PSU	C6-C5	2.74	1.38	1.35
22	a	2498	OMC	C6-N1	2.73	1.44	1.38
1	A	1498	UR3	C6-N1	2.73	1.44	1.38
1	A	1518	MA6	C6-N6	2.72	1.44	1.36
1	A	967	5MC	O2-C2	-2.71	1.18	1.23
54	Z	33	OMC	C6-N1	2.71	1.44	1.38
1	A	1207	2MG	O6-C6	-2.70	1.18	1.23
33	l	82	MS6	CB-CA	2.68	1.57	1.53
55	V	46	G7M	O6-C6	-2.68	1.18	1.23
55	V	48	5MC	O2-C2	-2.68	1.18	1.23
22	a	1917	PSU	C6-C5	2.66	1.38	1.35
22	a	2580	PSU	C6-C5	2.65	1.38	1.35
1	A	1519	MA6	C4-N9	-2.64	1.31	1.37
22	a	955	PSU	C6-C5	2.63	1.38	1.35
1	A	516	PSU	C6-C5	2.62	1.38	1.35
1	A	527	G7M	O6-C6	-2.61	1.18	1.23
25	d	150	MEQ	CG-CD	-2.58	1.46	1.51
55	V	54	2MU	C2-N1	2.57	1.42	1.38
22	a	2251	OMG	C5-C6	2.56	1.53	1.44
1	A	1518	MA6	C8-N9	-2.54	1.33	1.37
55	V	10	2MG	C5-C6	2.53	1.53	1.44
55	V	49	5MC	O2-C2	-2.49	1.19	1.23
1	A	1518	MA6	C4-N9	-2.48	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	10	2MG	O6-C6	-2.47	1.18	1.23
22	a	1835	2MG	C4-N9	-2.46	1.31	1.38
22	a	2605	PSU	C6-C5	2.46	1.38	1.35
1	A	1516	2MG	C4-N9	-2.45	1.31	1.38
55	V	37	12A	CC-N6	2.43	1.42	1.37
55	V	10	2MG	C6-N1	2.43	1.43	1.38
1	A	527	G7M	C6-N1	2.40	1.43	1.38
22	a	1618	6MZ	C8-N9	-2.38	1.33	1.37
1	A	1207	2MG	C4-N9	-2.38	1.31	1.38
22	a	1915	3TD	O2-C2	-2.36	1.18	1.23
22	a	1835	2MG	C5-C6	2.35	1.53	1.44
55	V	6	2MG	C5-C6	2.33	1.53	1.44
22	a	2251	OMG	C8-N9	-2.31	1.32	1.37
1	A	1516	2MG	C5-C6	2.31	1.53	1.44
22	a	747	5MU	O4-C4	-2.30	1.19	1.23
22	a	2552	OMU	C4-N3	2.29	1.42	1.38
54	Z	55	5MU	O4-C4	-2.28	1.19	1.23
55	V	54	2MU	C6-C5	2.28	1.38	1.34
22	a	746	PSU	C6-C5	2.27	1.38	1.35
22	a	2445	2MG	C5-C6	2.26	1.52	1.44
22	a	1915	3TD	C4-N3	2.26	1.45	1.40
1	A	516	PSU	C4-C5	-2.24	1.37	1.44
1	A	966	2MG	C5-C6	2.24	1.52	1.44
22	a	2069	G7M	C2-N1	2.23	1.43	1.37
1	A	1207	2MG	C5-C6	2.22	1.52	1.44
22	a	1915	3TD	O4-C4	-2.21	1.18	1.23
22	a	2503	2MA	C8-N9	-2.21	1.33	1.37
22	a	2580	PSU	O4'-C1'	-2.19	1.40	1.43
22	a	2069	G7M	C4-N9	-2.18	1.32	1.38
22	a	2503	2MA	C5-C4	-2.16	1.35	1.39
55	V	54	2MU	C2-N3	-2.16	1.34	1.38
55	V	54	2MU	C4-C5	2.14	1.48	1.44
54	Z	55	5MU	O2-C2	-2.14	1.19	1.23
22	a	2251	OMG	C4-N9	-2.13	1.32	1.38
22	a	2457	PSU	O4'-C1'	-2.13	1.40	1.43
22	a	746	PSU	C4-C5	-2.11	1.38	1.44
22	a	1917	PSU	O4'-C1'	-2.09	1.40	1.43
1	A	516	PSU	O4'-C1'	-2.08	1.40	1.43
55	V	49	5MC	CM5-C5	2.07	1.55	1.50
22	a	1917	PSU	C4-C5	-2.06	1.38	1.44
22	a	2498	OMC	C5-C4	2.05	1.47	1.42
55	V	6	2MG	C4-N9	-2.04	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	746	PSU	O4'-C1'	-2.02	1.41	1.43
22	a	2503	2MA	CM2-C2	2.00	1.55	1.49

All (292) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Z	55	5MU	C5-C4-N3	12.66	126.12	115.31
22	a	1939	5MU	C5-C4-N3	12.27	125.78	115.31
22	a	747	5MU	C5-C4-N3	11.84	125.42	115.31
22	a	1939	5MU	C5-C6-N1	-10.40	112.64	123.34
54	Z	55	5MU	C5-C6-N1	-10.27	112.77	123.34
22	a	747	5MU	C5-C6-N1	-9.59	113.47	123.34
22	a	2503	2MA	C5-C4-N3	-8.69	117.41	127.19
54	Z	8	4SU	C4-N3-C2	-7.81	119.75	127.34
22	a	1835	2MG	C2-N3-C4	6.89	120.58	112.04
55	V	6	2MG	C2-N3-C4	6.65	120.28	112.04
55	V	10	2MG	C2-N3-C4	6.59	120.20	112.04
1	A	966	2MG	C2-N3-C4	6.58	120.20	112.04
22	a	2503	2MA	N3-C4-N9	6.46	135.96	126.99
1	A	1516	2MG	C2-N3-C4	6.40	119.97	112.04
1	A	1518	MA6	N1-C2-N3	-6.32	118.72	128.60
22	a	2445	2MG	C2-N3-C4	6.23	119.77	112.04
54	Z	55	5MU	O4-C4-C5	-6.14	117.79	124.90
22	a	2503	2MA	C4-N9-C1'	-6.14	111.97	126.59
22	a	2251	OMG	C5-C4-N3	-6.04	118.66	128.46
22	a	2503	2MA	C1'-N9-C8	5.85	140.33	127.14
22	a	2030	6MZ	N1-C2-N3	-5.76	119.59	128.60
1	A	1207	2MG	C2-N3-C4	5.73	119.15	112.04
22	a	2552	OMU	C4-N3-C2	-5.68	119.09	126.58
22	a	2457	PSU	N1-C2-N3	5.60	121.47	115.13
1	A	966	2MG	C5-C4-N3	-5.53	119.50	128.46
22	a	1618	6MZ	N1-C2-N3	-5.49	120.02	128.60
55	V	6	2MG	C5-C4-N3	-5.48	119.57	128.46
1	A	1519	MA6	N1-C2-N3	-5.46	120.07	128.60
22	a	1917	PSU	N1-C2-N3	5.35	121.19	115.13
55	V	55	PSU	N1-C2-N3	5.34	121.18	115.13
54	Z	8	4SU	C5-C4-N3	5.28	119.59	114.69
22	a	2580	PSU	N1-C2-N3	5.28	121.11	115.13
22	a	2605	PSU	C4-N3-C2	-5.26	118.76	126.34
54	Z	55	5MU	C4-N3-C2	-5.26	120.54	127.35
22	a	2605	PSU	N1-C2-N3	5.24	121.07	115.13
22	a	1618	6MZ	C9-N6-C6	-5.24	118.36	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	V	10	2MG	C5-C4-N3	-5.22	119.99	128.46
22	a	1915	3TD	N1-C2-N3	5.21	120.25	116.14
22	a	1939	5MU	O4-C4-C5	-5.20	118.87	124.90
22	a	1917	PSU	C4-N3-C2	-5.19	118.86	126.34
22	a	1939	5MU	C4-N3-C2	-5.19	120.64	127.35
22	a	2604	PSU	N1-C2-N3	5.18	121.00	115.13
22	a	2030	6MZ	C5-C4-N3	-5.16	120.02	126.75
22	a	1835	2MG	C5-C4-N3	-5.09	120.20	128.46
22	a	955	PSU	C4-N3-C2	-5.02	119.10	126.34
22	a	2457	PSU	C4-N3-C2	-5.00	119.14	126.34
22	a	746	PSU	C4-N3-C2	-4.97	119.17	126.34
22	a	955	PSU	N1-C2-N3	4.95	120.74	115.13
22	a	1618	6MZ	C5-C4-N3	-4.93	120.31	126.75
55	V	55	PSU	C4-N3-C2	-4.93	119.24	126.34
22	a	1911	PSU	C4-N3-C2	-4.92	119.26	126.34
22	a	2445	2MG	C5-C4-N3	-4.90	120.51	128.46
54	Z	56	PSU	C4-N3-C2	-4.90	119.28	126.34
22	a	746	PSU	N1-C2-N3	4.88	120.66	115.13
1	A	1498	UR3	C4-N3-C2	-4.87	119.98	124.56
22	a	747	5MU	C5M-C5-C4	4.84	124.09	118.77
22	a	747	5MU	O4-C4-C5	-4.84	119.30	124.90
1	A	1518	MA6	C2-N1-C6	4.84	123.17	111.75
55	V	54	2MU	N3-C2-N1	4.80	121.26	114.89
1	A	1516	2MG	C5-C4-N3	-4.75	120.76	128.46
22	a	2251	OMG	C2-N3-C4	4.74	120.75	112.30
55	V	6	2MG	C2-N1-C6	-4.73	119.03	124.48
55	V	10	2MG	C2-N1-C6	-4.73	119.04	124.48
54	Z	55	5MU	N3-C2-N1	4.68	121.10	114.89
22	a	747	5MU	C4-N3-C2	-4.68	121.30	127.35
1	A	1518	MA6	N9-C8-N7	-4.68	107.52	113.91
1	A	1207	2MG	C5-C4-N3	-4.66	120.90	128.46
55	V	39	PSU	N1-C2-N3	4.65	120.40	115.13
22	a	1939	5MU	N3-C2-N1	4.63	121.03	114.89
55	V	39	PSU	C4-N3-C2	-4.61	119.69	126.34
1	A	1519	MA6	N9-C8-N7	-4.60	107.62	113.91
55	V	46	G7M	C2-N3-C4	4.59	120.47	112.30
22	a	2604	PSU	C4-N3-C2	-4.59	119.73	126.34
55	V	27	PSU	C4-N3-C2	-4.58	119.74	126.34
22	a	1911	PSU	N1-C2-N3	4.57	120.31	115.13
22	a	2030	6MZ	N9-C8-N7	-4.57	107.66	113.91
22	a	747	5MU	N3-C2-N1	4.57	120.95	114.89
1	A	966	2MG	C2-N1-C6	-4.55	119.25	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	MA6	C2-N1-C6	4.53	122.45	111.75
22	a	2069	G7M	C2-N3-C4	4.53	120.37	112.30
1	A	1518	MA6	C5-C4-N3	-4.47	120.92	126.75
22	a	747	5MU	C5M-C5-C6	-4.44	116.92	122.85
22	a	2580	PSU	C4-N3-C2	-4.43	119.96	126.34
1	A	1519	MA6	C5-C4-N3	-4.41	120.99	126.75
54	Z	56	PSU	N1-C2-N3	4.41	120.13	115.13
22	a	2504	PSU	N1-C2-N3	4.39	120.10	115.13
1	A	1516	2MG	C2-N1-C6	-4.38	119.44	124.48
22	a	1939	5MU	C5M-C5-C6	-4.37	117.02	122.85
55	V	37	12A	CA-N-CC	-4.37	114.66	121.94
1	A	516	PSU	C4-N3-C2	-4.36	120.06	126.34
1	A	527	G7M	C5-C4-N3	-4.35	119.80	128.15
22	a	2504	PSU	C4-N3-C2	-4.34	120.09	126.34
1	A	527	G7M	C2-N3-C4	4.34	120.03	112.30
22	a	1835	2MG	C2-N1-C6	-4.32	119.50	124.48
22	a	1618	6MZ	N9-C8-N7	-4.27	108.07	113.91
1	A	1207	2MG	C2-N1-C6	-4.27	119.57	124.48
22	a	2552	OMU	N3-C2-N1	4.27	120.56	114.89
55	V	27	PSU	N1-C2-N3	4.20	119.89	115.13
55	V	54	2MU	C4-N3-C2	-4.20	121.92	127.35
55	V	46	G7M	C5-C4-N3	-4.19	120.11	128.15
22	a	2251	OMG	N9-C4-N3	4.18	134.34	125.94
22	a	1939	5MU	C5M-C5-C4	4.12	123.30	118.77
54	Z	8	4SU	N3-C2-N1	4.08	120.31	114.89
1	A	1519	MA6	C4-C5-C6	4.06	120.43	115.88
22	a	2069	G7M	C5-C6-N1	4.03	120.21	111.79
22	a	2030	6MZ	C9-N6-C6	-4.03	119.40	122.87
22	a	745	1MG	C5-C4-N3	-4.00	121.98	128.46
33	l	81	4D4	NE-CZ-NH2	3.96	127.65	120.70
22	a	2552	OMU	C5-C4-N3	3.95	120.76	114.84
1	A	966	2MG	N9-C4-N3	3.94	133.86	125.94
22	a	2445	2MG	C2-N1-C6	-3.93	119.96	124.48
55	V	46	G7M	C5-C6-N1	3.91	119.96	111.79
55	V	6	2MG	N9-C4-N3	3.91	133.78	125.94
1	A	516	PSU	N1-C2-N3	3.87	119.51	115.13
55	V	54	2MU	C5-C4-N3	3.85	118.59	115.31
22	a	1962	5MC	C5-C6-N1	-3.79	119.44	123.34
22	a	2069	G7M	C5-C4-N3	-3.77	120.92	128.15
22	a	745	1MG	C2-N3-C4	3.76	120.44	111.98
22	a	2445	2MG	N9-C8-N7	-3.72	106.38	113.39
1	A	527	G7M	C5-C6-N1	3.70	119.52	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2030	6MZ	C2-N3-C4	3.69	120.47	111.75
22	a	2030	6MZ	C5-N7-C8	3.66	108.72	103.51
22	a	747	5MU	O2-C2-N1	-3.66	117.92	122.79
1	A	1518	MA6	C4-C5-C6	3.66	119.98	115.88
22	a	2503	2MA	N9-C8-N7	-3.66	108.91	113.91
1	A	1516	2MG	N9-C8-N7	-3.64	106.54	113.39
22	a	2251	OMG	C2-N1-C6	-3.63	118.48	125.10
22	a	1915	3TD	C4-N3-C2	-3.62	120.68	124.61
22	a	1618	6MZ	C4-C5-C6	3.61	119.61	116.81
1	A	1207	2MG	N9-C8-N7	-3.57	106.66	113.39
1	A	1518	MA6	C2-N3-C4	3.52	120.08	111.75
1	A	1518	MA6	C5-N7-C8	3.52	108.52	103.51
1	A	1519	MA6	C5-N7-C8	3.51	108.50	103.51
1	A	967	5MC	C5-C6-N1	-3.49	119.74	123.34
55	V	10	2MG	N9-C4-N3	3.49	132.95	125.94
1	A	1407	5MC	C5-C6-N1	-3.46	119.78	123.34
22	a	2251	OMG	N9-C8-N7	-3.41	106.96	113.39
22	a	2069	G7M	O6-C6-C5	-3.41	120.37	128.06
22	a	1618	6MZ	C2-N3-C4	3.40	119.79	111.75
22	a	1835	2MG	N9-C4-N3	3.39	132.76	125.94
22	a	2030	6MZ	C4-C5-C6	3.38	119.43	116.81
54	Z	8	4SU	C5-C4-S4	-3.37	120.12	124.47
55	V	48	5MC	C5-C6-N1	-3.31	119.93	123.34
55	V	54	2MU	O4-C4-C5	-3.28	121.09	124.90
55	V	10	2MG	N9-C8-N7	-3.28	107.21	113.39
22	a	745	1MG	N9-C8-N7	-3.27	107.24	113.39
55	V	6	2MG	N9-C8-N7	-3.26	107.24	113.39
55	V	46	G7M	C2-N1-C6	-3.26	119.15	125.10
1	A	527	G7M	C2-N1-C6	-3.26	119.15	125.10
54	Z	55	5MU	C5M-C5-C6	-3.24	118.52	122.85
55	V	46	G7M	O6-C6-C5	-3.24	120.76	128.06
22	a	2503	2MA	C6-C5-C4	3.24	121.53	117.18
22	a	1962	5MC	CM5-C5-C6	-3.22	118.54	122.85
1	A	1207	2MG	N9-C4-N3	3.20	132.36	125.94
22	a	2069	G7M	C2-N1-C6	-3.17	119.33	125.10
1	A	527	G7M	O6-C6-C5	-3.15	120.95	128.06
1	A	966	2MG	N9-C8-N7	-3.15	107.46	113.39
1	A	1519	MA6	C2-N3-C4	3.14	119.18	111.75
22	a	2445	2MG	N9-C4-N3	3.12	132.20	125.94
22	a	1618	6MZ	C5-N7-C8	3.09	107.91	103.51
1	A	1519	MA6	C4-C5-N7	-3.07	106.89	110.62
55	V	46	G7M	N9-C4-N3	3.05	132.06	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	V	39	PSU	O2-C2-N1	-3.04	119.44	122.79
22	a	2503	2MA	N3-C2-N1	-3.03	120.15	125.72
22	a	2251	OMG	C5-C6-N1	3.02	120.87	113.19
22	a	745	1MG	C5-C6-N1	3.01	120.73	114.91
22	a	955	PSU	O2-C2-N1	-3.00	119.49	122.79
55	V	54	2MU	C5M-C5-C4	3.00	122.06	118.77
55	V	49	5MC	C5-C6-N1	-2.98	120.27	123.34
22	a	1835	2MG	N9-C8-N7	-2.97	107.80	113.39
22	a	2580	PSU	C6-N1-C2	-2.97	119.65	122.68
1	A	1516	2MG	C5-C6-N1	2.96	120.71	113.19
55	V	6	2MG	C5-C6-N1	2.96	120.71	113.19
22	a	2030	6MZ	N3-C4-N9	2.94	131.93	127.08
55	V	55	PSU	O2-C2-N1	-2.94	119.56	122.79
1	A	1516	2MG	N9-C4-N3	2.91	131.78	125.94
55	V	10	2MG	C5-C6-N1	2.89	120.52	113.19
54	Z	55	5MU	O2-C2-N1	-2.88	118.96	122.79
1	A	527	G7M	N9-C4-N3	2.88	131.72	125.94
1	A	966	2MG	C5-C6-N1	2.86	120.46	113.19
1	A	1518	MA6	C4-C5-N7	-2.86	107.14	110.62
22	a	2503	2MA	C5-N7-C8	2.85	107.56	103.51
22	a	1917	PSU	O2-C2-N1	-2.85	119.65	122.79
22	a	1835	2MG	C5-C6-N1	2.82	120.36	113.19
55	V	37	12A	N6-CC-N	2.82	117.70	113.76
22	a	2604	PSU	C6-N1-C2	-2.80	119.82	122.68
54	Z	55	5MU	C5M-C5-C4	2.79	121.83	118.77
1	A	1207	2MG	O6-C6-C5	-2.78	119.23	126.60
33	l	82	MS6	CE-SD-CG	2.78	109.94	100.40
22	a	2069	G7M	N2-C2-N1	2.77	122.60	116.71
22	a	1618	6MZ	N3-C4-N9	2.73	131.59	127.08
1	A	1207	2MG	C5-C6-N1	2.73	120.12	113.19
1	A	1498	UR3	C6-N1-C2	-2.71	119.36	121.79
22	a	1835	2MG	N1-C2-N3	-2.71	119.76	123.95
55	V	6	2MG	O6-C6-C5	-2.70	119.43	126.60
1	A	1402	4OC	O2-C2-N3	-2.70	117.94	122.33
22	a	2445	2MG	C8-N7-C5	2.70	109.12	104.24
1	A	1519	MA6	C5-C4-N9	2.69	108.92	105.78
55	V	10	2MG	O6-C6-C5	-2.69	119.45	126.60
55	V	55	PSU	C6-N1-C2	-2.67	119.95	122.68
1	A	966	2MG	O6-C6-C5	-2.67	119.52	126.60
22	a	2030	6MZ	C4-C5-N7	-2.66	107.37	110.62
22	a	2503	2MA	CM2-C2-N3	2.65	121.28	117.15
54	Z	56	PSU	O2-C2-N1	-2.64	119.89	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2498	OMC	O2-C2-N3	-2.62	118.07	122.33
55	V	34	70U	C1'-N1-C6	-2.62	116.77	121.12
22	a	2457	PSU	C6-C5-C4	2.61	120.03	118.20
1	A	1516	2MG	N1-C2-N3	-2.60	119.94	123.95
22	a	1917	PSU	C6-N1-C2	-2.59	120.03	122.68
22	a	1835	2MG	O6-C6-C5	-2.59	119.73	126.60
22	a	2251	OMG	C8-N7-C5	2.59	108.92	104.24
22	a	1939	5MU	O2-C2-N1	-2.55	119.40	122.79
1	A	1519	MA6	N1-C6-N6	-2.54	114.31	117.08
22	a	2445	2MG	C5-C6-N1	2.53	119.61	113.19
55	V	54	2MU	C6-N1-C2	-2.53	118.74	121.30
22	a	747	5MU	O4-C4-N3	-2.52	115.28	120.12
1	A	1518	MA6	N1-C6-N6	-2.52	114.33	117.08
22	a	1939	5MU	O4-C4-N3	-2.51	115.31	120.12
22	a	2457	PSU	O2-C2-N1	-2.50	120.04	122.79
55	V	27	PSU	O2-C2-N1	-2.50	120.04	122.79
1	A	1402	4OC	C6-C5-C4	2.49	120.01	116.96
22	a	2457	PSU	C6-N1-C2	-2.48	120.14	122.68
1	A	1516	2MG	C1'-N9-C4	-2.47	119.15	126.50
33	l	81	4D4	O-C-CA	-2.47	118.31	124.78
25	d	150	MEQ	CG-CD-NE2	-2.46	112.88	116.29
55	V	6	2MG	N1-C2-N3	-2.43	120.20	123.95
22	a	746	PSU	C6-N1-C2	-2.43	120.20	122.68
33	l	81	4D4	CB-CA-C	-2.42	107.91	111.77
1	A	1516	2MG	C8-N7-C5	2.41	108.61	104.24
1	A	1518	MA6	C4-N9-C8	2.41	108.34	105.73
12	L	89	D2T	O-C-CA	-2.41	118.47	124.78
1	A	1516	2MG	O6-C6-C5	-2.39	120.26	126.60
55	V	10	2MG	N1-C2-N3	-2.39	120.26	123.95
22	a	2552	OMU	O4-C4-C5	-2.37	121.00	125.16
22	a	2580	PSU	O4'-C1'-C2'	2.37	108.48	105.14
22	a	2251	OMG	O6-C6-C5	-2.36	120.33	126.60
22	a	2605	PSU	C6-C5-C4	2.36	119.84	118.20
1	A	966	2MG	N1-C2-N3	-2.35	120.31	123.95
1	A	1518	MA6	C5-C4-N9	2.32	108.48	105.78
55	V	39	PSU	C6-N1-C2	-2.32	120.31	122.68
55	V	54	2MU	O2-C2-N3	-2.32	117.18	121.50
1	A	1207	2MG	C8-N7-C5	2.32	108.44	104.24
1	A	516	PSU	O4'-C1'-C2'	2.32	108.41	105.14
1	A	1207	2MG	CM2-N2-C2	-2.31	118.76	123.86
22	a	2445	2MG	N1-C2-N3	-2.30	120.39	123.95
55	V	47	H2U	O4-C4-N3	2.29	123.91	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	l	81	4D4	CG-CD-NE	-2.28	105.28	111.87
22	a	2030	6MZ	C4-N9-C8	2.28	108.19	105.73
22	a	2069	G7M	N9-C4-N3	2.27	130.50	125.94
55	V	48	5MC	CM5-C5-C6	-2.26	119.83	122.85
55	V	37	12A	OG1-CB-CA	2.24	113.62	109.13
1	A	516	PSU	O2-C2-N1	-2.24	120.33	122.79
22	a	2580	PSU	O2-C2-N3	-2.22	117.62	121.82
55	V	37	12A	CG2-CB-CA	-2.22	107.80	112.29
22	a	2504	PSU	C6-N1-C2	-2.21	120.42	122.68
22	a	745	1MG	C6-C5-N7	2.20	134.33	129.35
1	A	966	2MG	C8-N7-C5	2.19	108.19	104.24
54	Z	21	H2U	C5-C6-N1	-2.18	104.43	111.61
1	A	1207	2MG	N1-C2-N3	-2.17	120.59	123.95
1	A	1519	MA6	C4-N9-C8	2.16	108.07	105.73
22	a	746	PSU	O2-C2-N1	-2.16	120.41	122.79
55	V	6	2MG	C8-N7-C5	2.15	108.12	104.24
22	a	2069	G7M	CN7-N7-C5	2.15	129.43	126.77
55	V	10	2MG	C8-N7-C5	2.14	108.12	104.24
22	a	2552	OMU	O2-C2-N1	-2.14	119.94	122.79
22	a	1835	2MG	CM2-N2-C2	-2.14	119.14	123.86
22	a	2605	PSU	C5-C6-N1	-2.13	118.91	122.11
22	a	2604	PSU	O2-C2-N1	-2.13	120.45	122.79
1	A	1518	MA6	N3-C4-N9	2.12	130.58	127.08
55	V	55	PSU	C6-C5-C4	2.12	119.68	118.20
22	a	2445	2MG	C4-C5-N7	-2.11	107.38	110.72
22	a	2069	G7M	N9-C8-N7	-2.11	106.99	112.21
54	Z	55	5MU	O4-C4-N3	-2.11	116.08	120.12
33	l	81	4D4	NH1-CZ-NE	-2.11	114.33	119.19
22	a	2605	PSU	O2-C2-N1	-2.11	120.47	122.79
22	a	1915	3TD	O4'-C1'-C2'	2.09	108.09	105.14
55	V	46	G7M	CN7-N7-C5	2.09	129.36	126.77
55	V	49	5MC	CM5-C5-C6	-2.08	120.07	122.85
22	a	1618	6MZ	C4-C5-N7	-2.08	108.09	110.62
55	V	54	2MU	C5M-C5-C6	-2.08	120.07	122.85
55	V	37	12A	C2M-S2-C2	2.06	103.80	102.27
22	a	1917	PSU	C6-C5-C4	2.06	119.64	118.20
22	a	2503	2MA	N6-C6-N1	2.05	119.94	117.03
55	V	46	G7M	N9-C8-N7	-2.04	107.16	112.21
1	A	967	5MC	CM5-C5-C6	-2.04	120.13	122.85
1	A	527	G7M	CN7-N7-C5	2.03	129.29	126.77
55	V	54	2MU	O4'-C1'-N1	2.02	112.99	108.36
1	A	1519	MA6	C5-C6-N6	2.02	128.82	125.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	V	10	2MG	O3'-C3'-C2'	2.02	118.36	111.82
55	V	27	PSU	C6-N1-C2	-2.02	120.62	122.68
55	V	37	12A	O-C-CA	-2.01	114.79	121.70
22	a	2503	2MA	C5-C6-N6	-2.00	119.07	123.43

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	d	150	MEQ	C-CA-CB-CG
54	Z	21	H2U	O4'-C1'-N1-C2
54	Z	21	H2U	O4'-C1'-N1-C6
22	a	746	PSU	C2'-C1'-C5-C4
22	a	2030	6MZ	O4'-C4'-C5'-O5'
55	V	6	2MG	C3'-C4'-C5'-O5'
55	V	37	12A	N-CA-CB-OG1
55	V	37	12A	C-CA-CB-OG1
55	V	37	12A	C-CA-CB-CG2
55	V	47	H2U	O4'-C1'-N1-C6
55	V	47	H2U	C2'-C1'-N1-C6
55	V	49	5MC	O4'-C4'-C5'-O5'
55	V	47	H2U	O4'-C1'-N1-C2
55	V	47	H2U	C2'-C1'-N1-C2
1	A	1519	MA6	O4'-C4'-C5'-O5'
55	V	48	5MC	O4'-C4'-C5'-O5'
55	V	48	5MC	C3'-C4'-C5'-O5'
55	V	49	5MC	C3'-C4'-C5'-O5'
55	V	34	70U	C5M-C8-O9-C9
1	A	1519	MA6	C3'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
55	V	6	2MG	O4'-C4'-C5'-O5'
55	V	47	H2U	O4'-C4'-C5'-O5'
55	V	47	H2U	C3'-C4'-C5'-O5'
25	d	150	MEQ	NE2-CD-CG-CB
25	d	150	MEQ	OE1-CD-CG-CB
55	V	37	12A	N-CA-CB-CG2
54	Z	55	5MU	C3'-C4'-C5'-O5'
55	V	37	12A	N1-C2-S2-C2M
55	V	37	12A	N3-C2-S2-C2M
55	V	34	70U	O8-C8-O9-C9
55	V	37	12A	O-C-CA-N
55	V	37	12A	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
54	Z	55	5MU	O4'-C4'-C5'-O5'
55	V	58	1MA	O4'-C4'-C5'-O5'
22	a	1915	3TD	O4'-C4'-C5'-O5'
22	a	1917	PSU	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C10
1	A	966	2MG	C3'-C4'-C5'-O5'
55	V	46	G7M	C3'-C4'-C5'-O5'
55	V	58	1MA	C3'-C4'-C5'-O5'
1	A	966	2MG	O4'-C4'-C5'-O5'
1	A	527	G7M	C4'-C5'-O5'-P
55	V	47	H2U	C4'-C5'-O5'-P
22	a	747	5MU	C3'-C4'-C5'-O5'
54	Z	21	H2U	C2'-C1'-N1-C6
22	a	1915	3TD	C3'-C4'-C5'-O5'
55	V	46	G7M	O4'-C4'-C5'-O5'
22	a	1917	PSU	C3'-C4'-C5'-O5'
22	a	2251	OMG	C1'-C2'-O2'-CM2
12	L	89	D2T	CG-CB-SB-CB1
22	a	746	PSU	O4'-C1'-C5-C6
33	l	82	MS6	CB-CG-SD-CE
22	a	2069	G7M	O4'-C4'-C5'-O5'
22	a	2503	2MA	O4'-C4'-C5'-O5'
22	a	2445	2MG	C3'-C4'-C5'-O5'
22	a	2504	PSU	O4'-C4'-C5'-O5'
22	a	1962	5MC	C2'-C1'-N1-C6
54	Z	21	H2U	C2'-C1'-N1-C2
33	l	81	4D4	O-C-CA-CB
55	V	46	G7M	C4'-C5'-O5'-P
25	d	150	MEQ	N-CA-CB-CG

There are no ring outliers.

12 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519	MA6	1	0
54	Z	21	H2U	1	0
22	a	2552	OMU	1	0
54	Z	56	PSU	1	0
22	a	747	5MU	1	0
1	A	1516	2MG	1	0
55	V	47	H2U	1	0
55	V	10	2MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	V	34	70U	1	0
22	a	2251	OMG	1	0
22	a	2030	6MZ	2	0
12	L	89	D2T	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 445 ligands modelled in this entry, 445 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

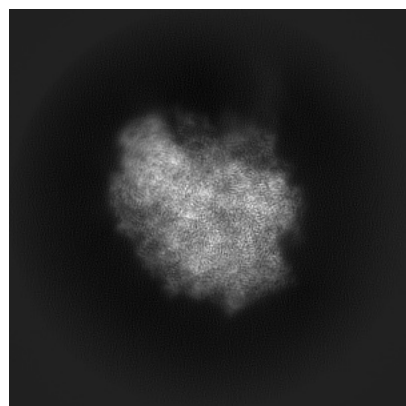
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61709. These allow visual inspection of the internal detail of the map and identification of artifacts.

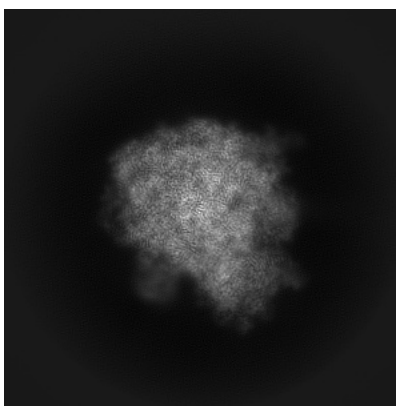
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

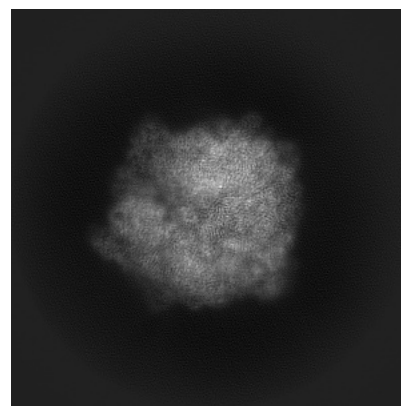
6.1.1 Primary map



X

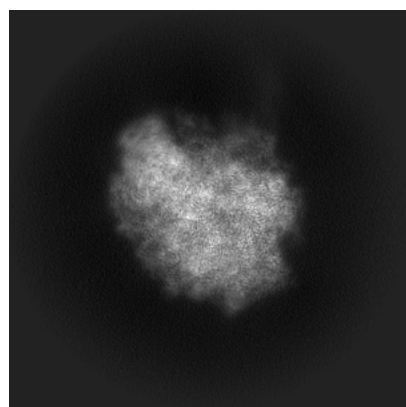


Y

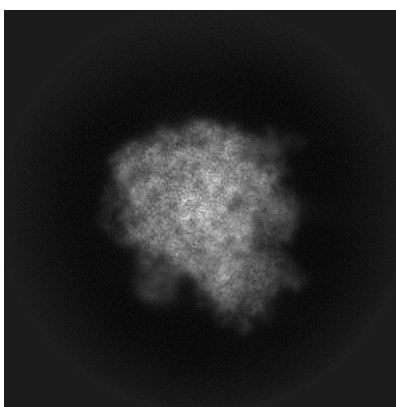


Z

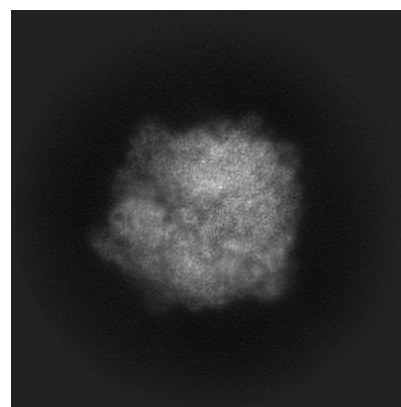
6.1.2 Raw map



X



Y



Z

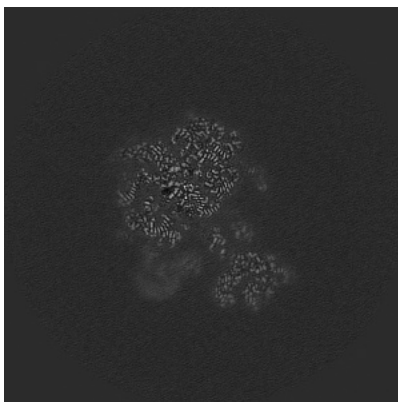
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

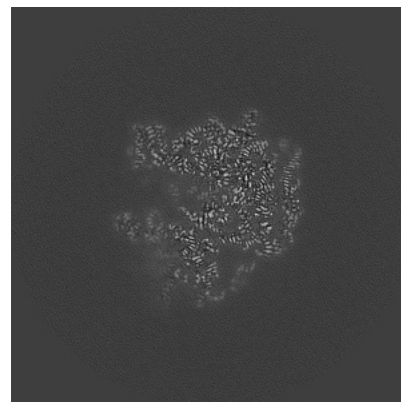
6.2.1 Primary map



X Index: 265

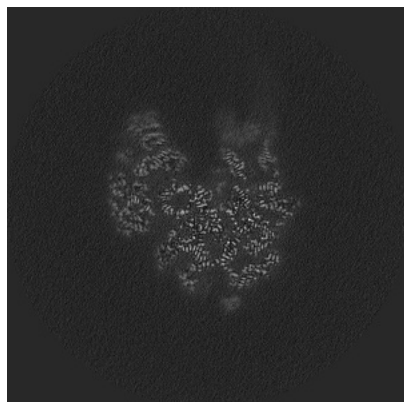


Y Index: 265

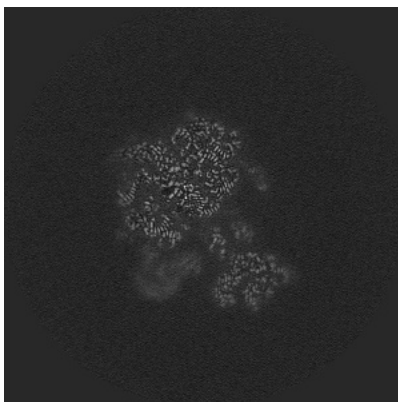


Z Index: 265

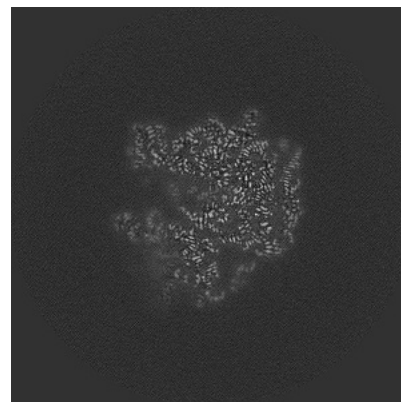
6.2.2 Raw map



X Index: 265



Y Index: 265

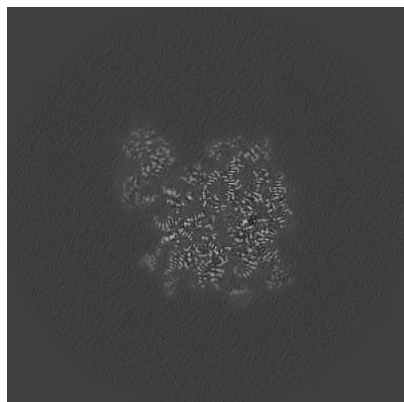


Z Index: 265

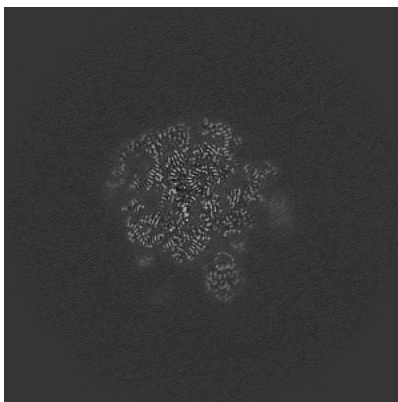
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

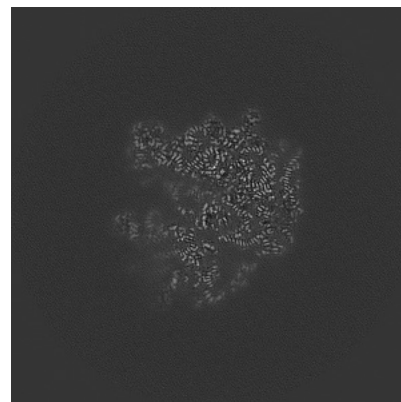
6.3.1 Primary map



X Index: 298

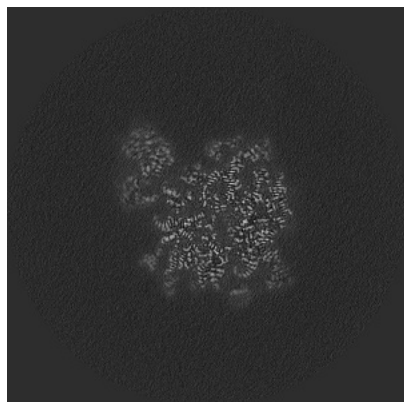


Y Index: 316

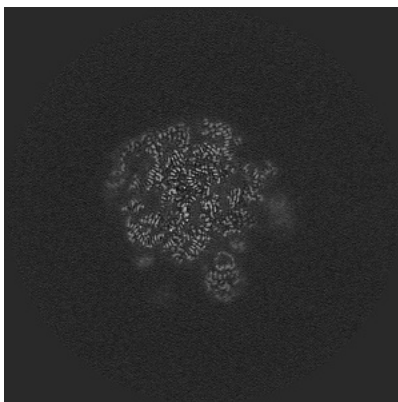


Z Index: 267

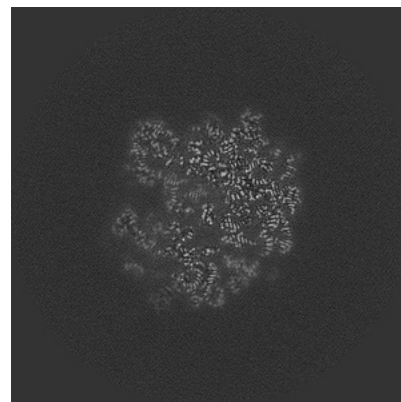
6.3.2 Raw map



X Index: 298



Y Index: 316

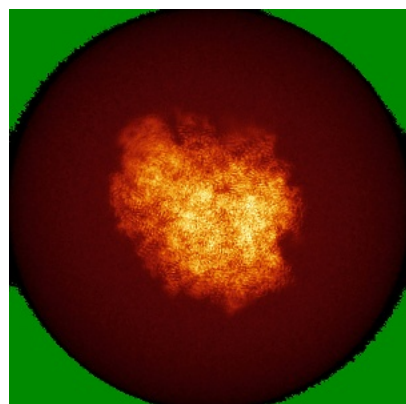


Z Index: 273

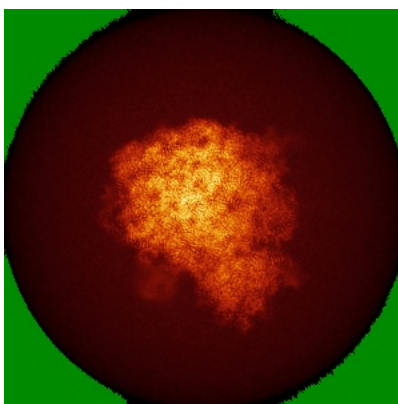
The images above show the largest variance slices of the map in three orthogonal directions.

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

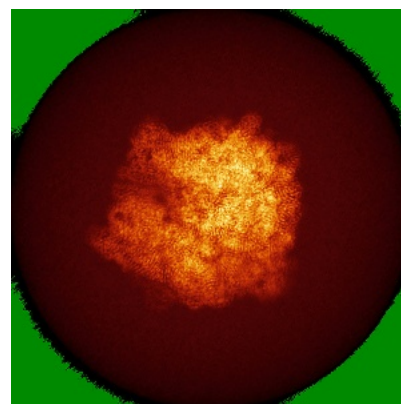
6.4.1 Primary map



X

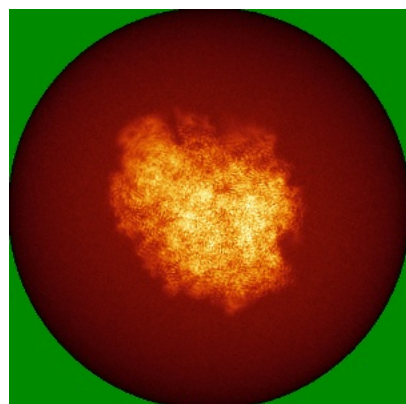


Y

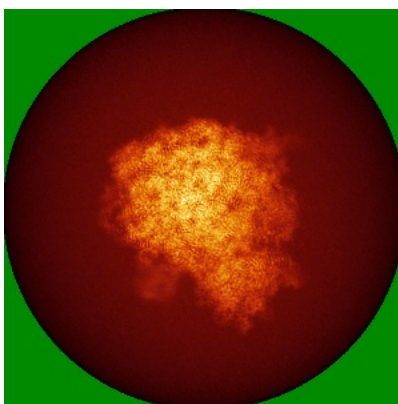


Z

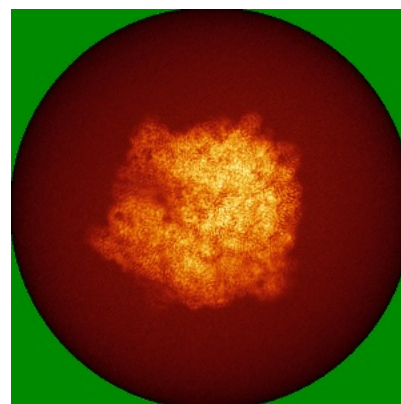
6.4.2 Raw map



X



Y

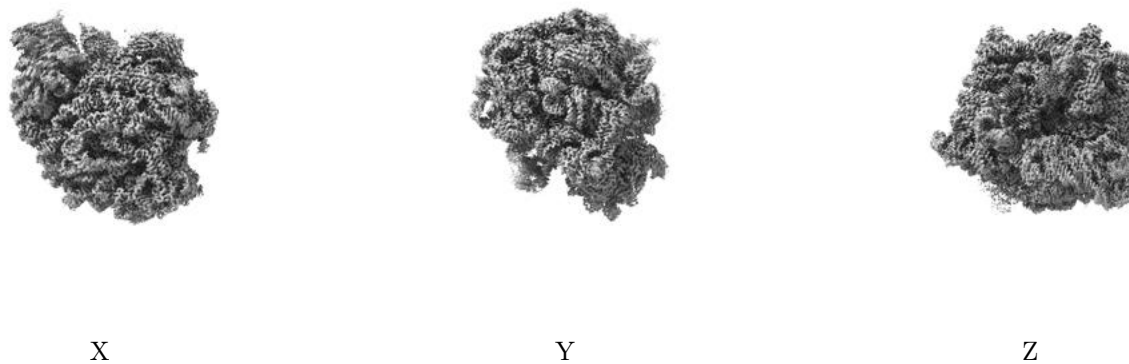


Z

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.

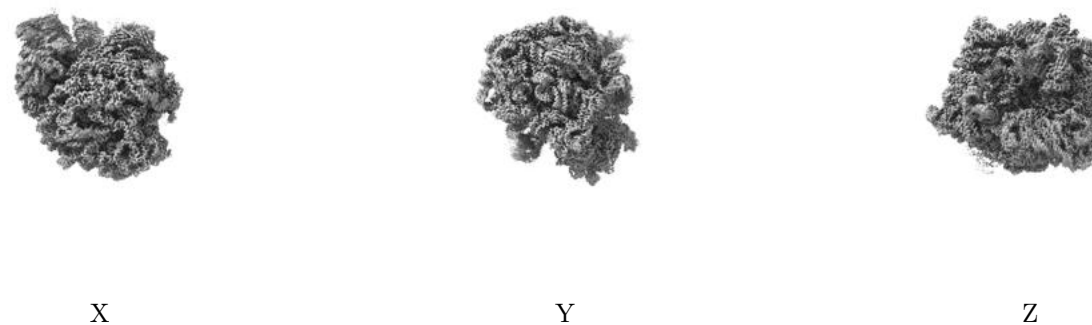
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0169. 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.

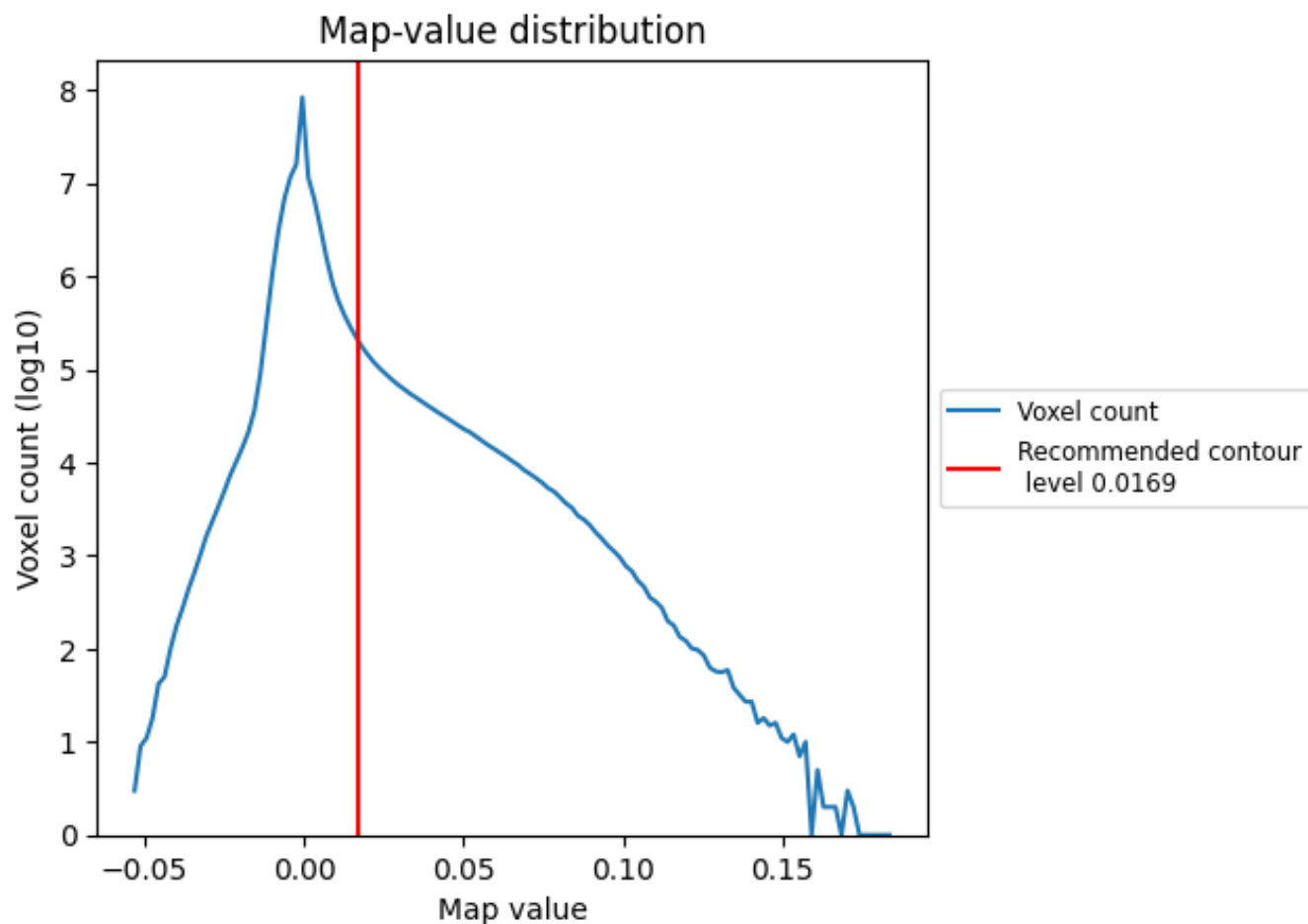
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

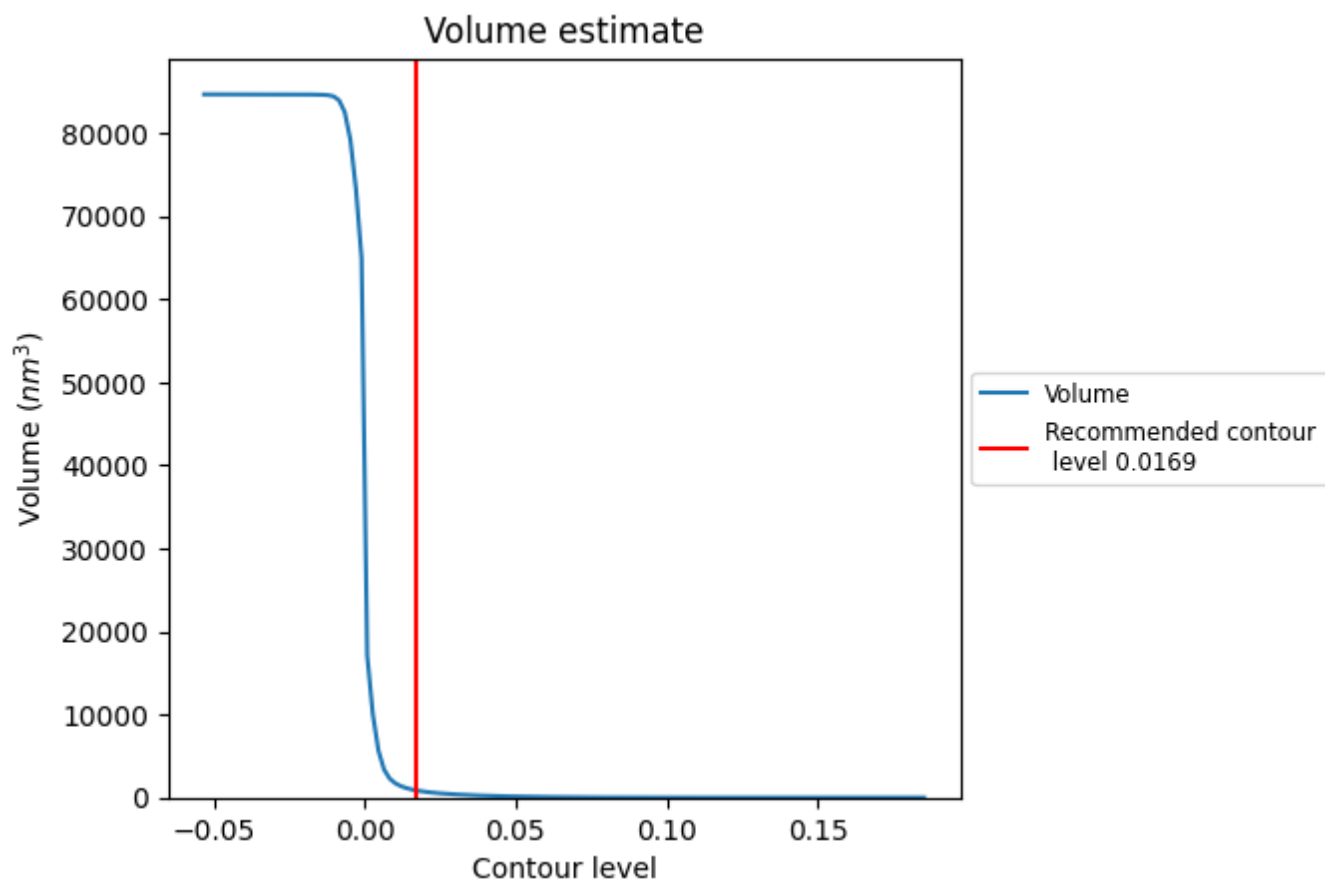
This section contains the results of statistical analysis of the map.

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.

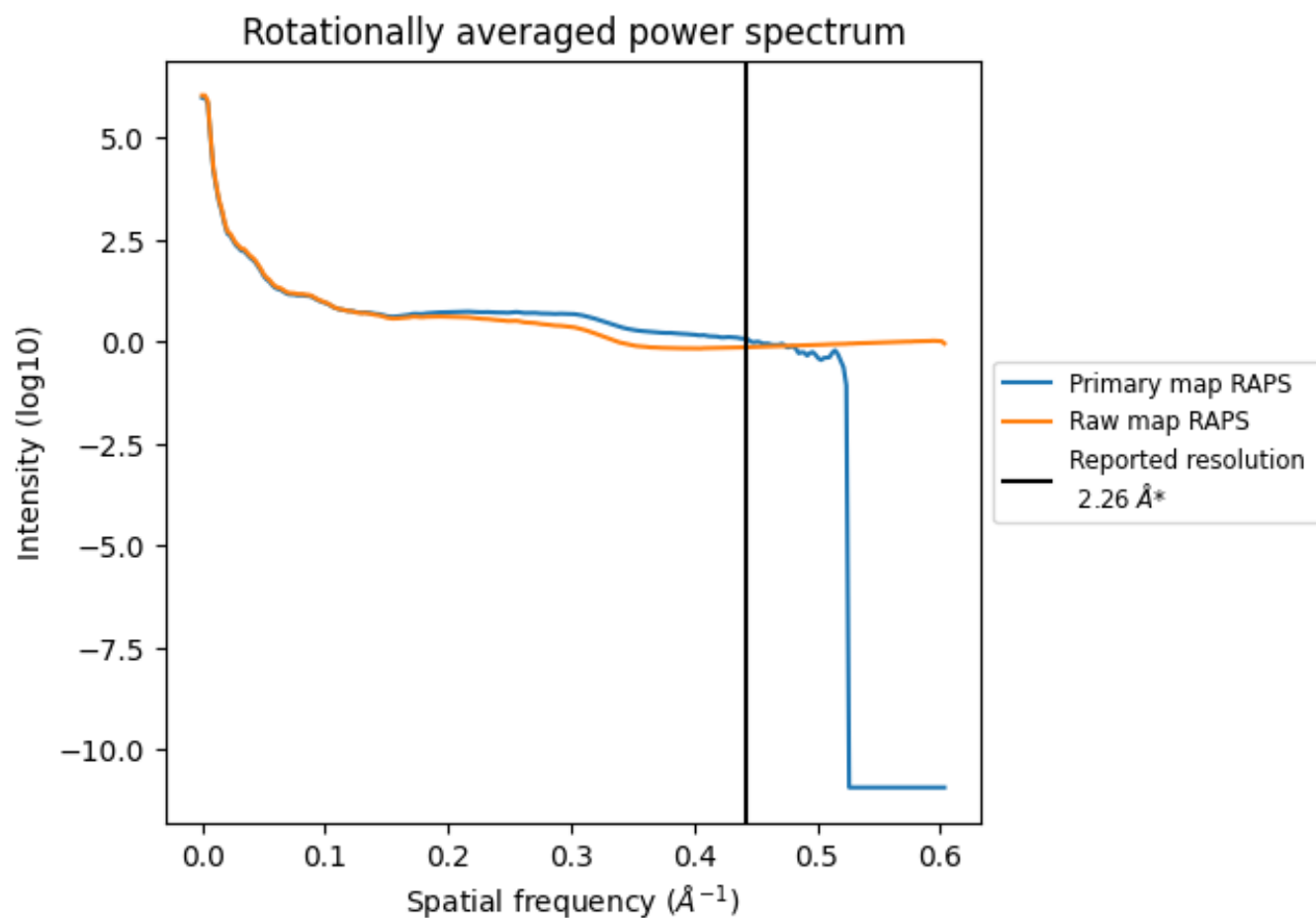
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 879 nm^3 ; this corresponds to an approximate mass of 794 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 ⓘ

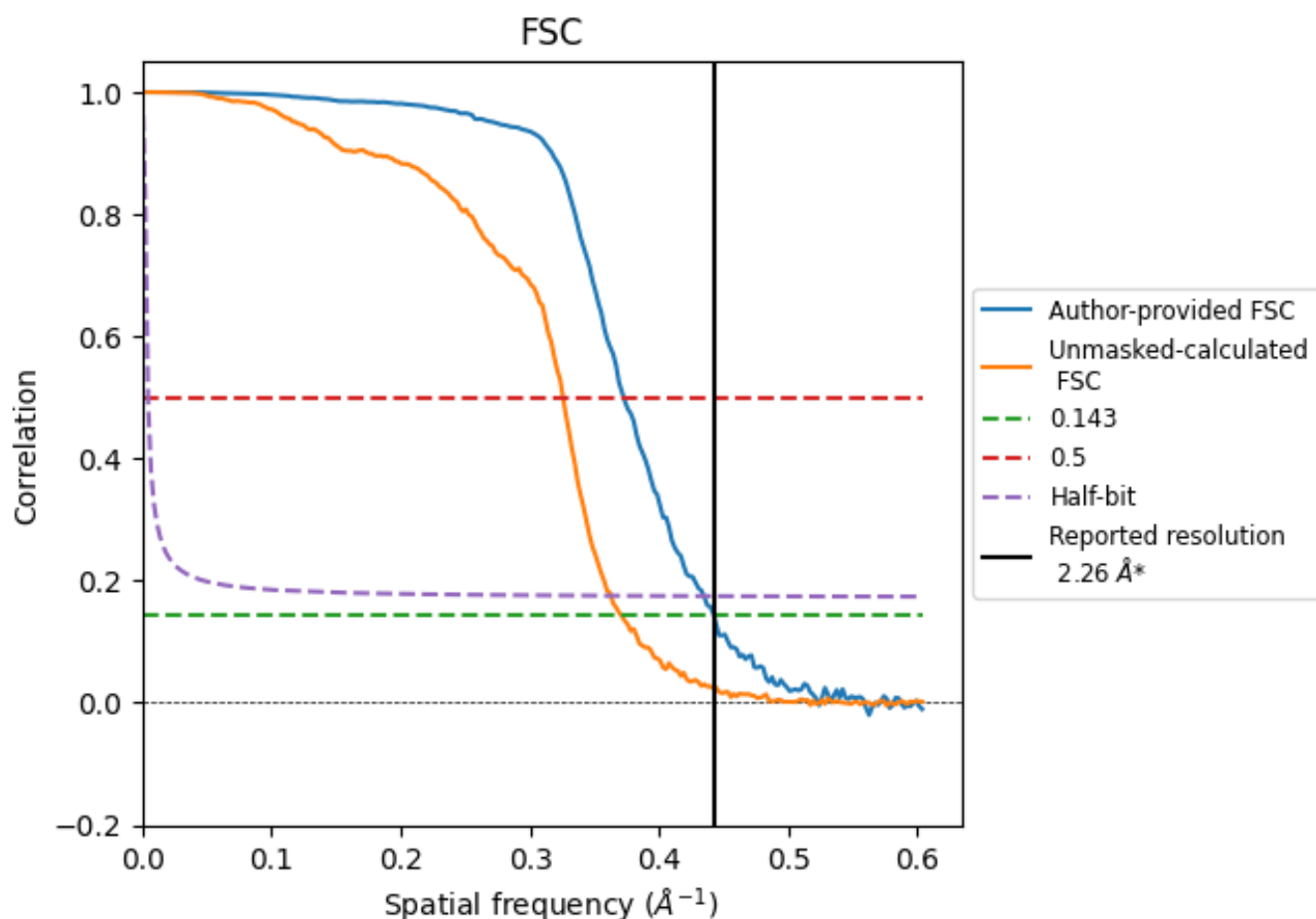


*Reported resolution corresponds to spatial frequency of 0.442 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.442 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

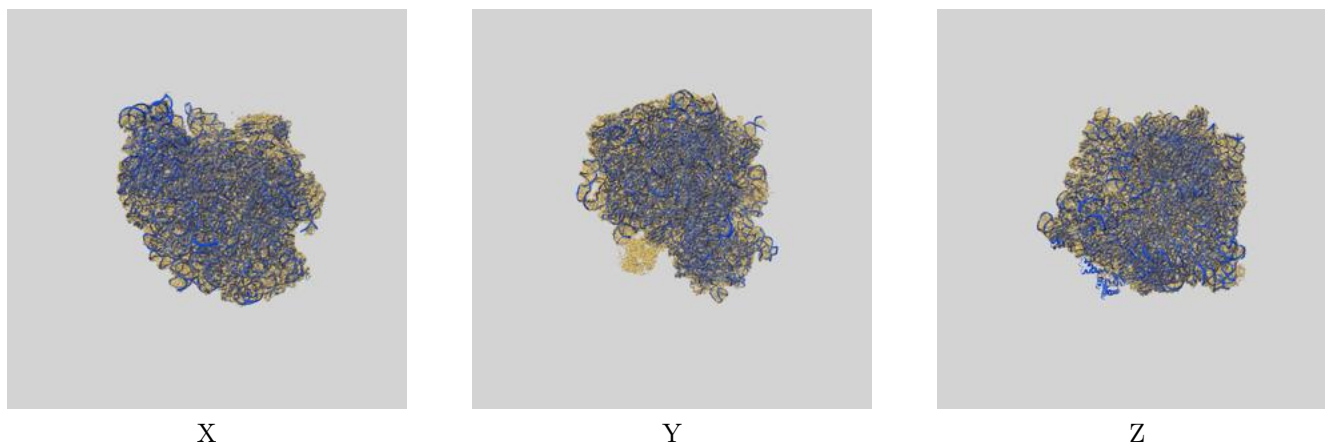
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.26	-	-
Author-provided FSC curve	2.26	2.68	2.30
Unmasked-calculated*	2.70	3.07	2.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.70 differs from the reported value 2.26 by more than 10 %

9 Map-model fit [i](#)

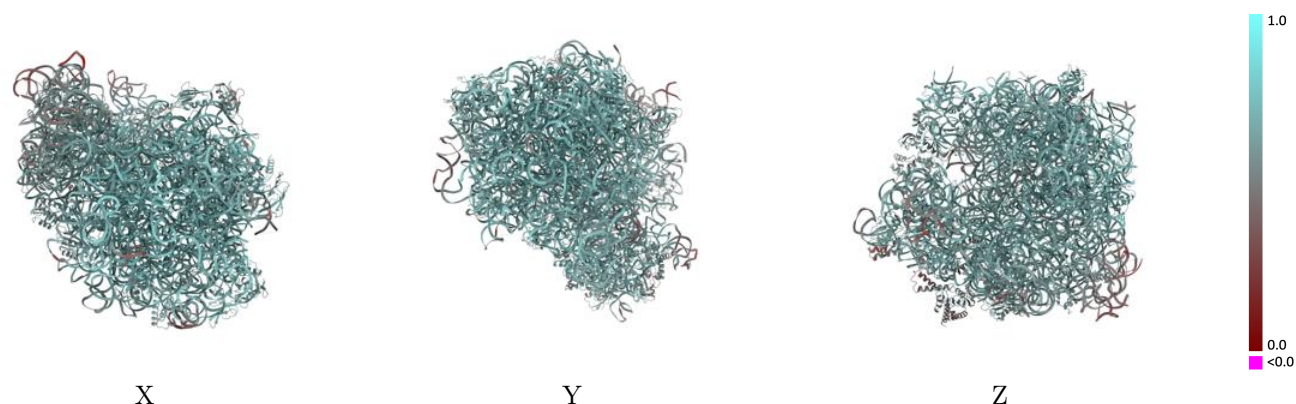
This section contains information regarding the fit between EMDB map EMD-61709 and PDB model 9JPP. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



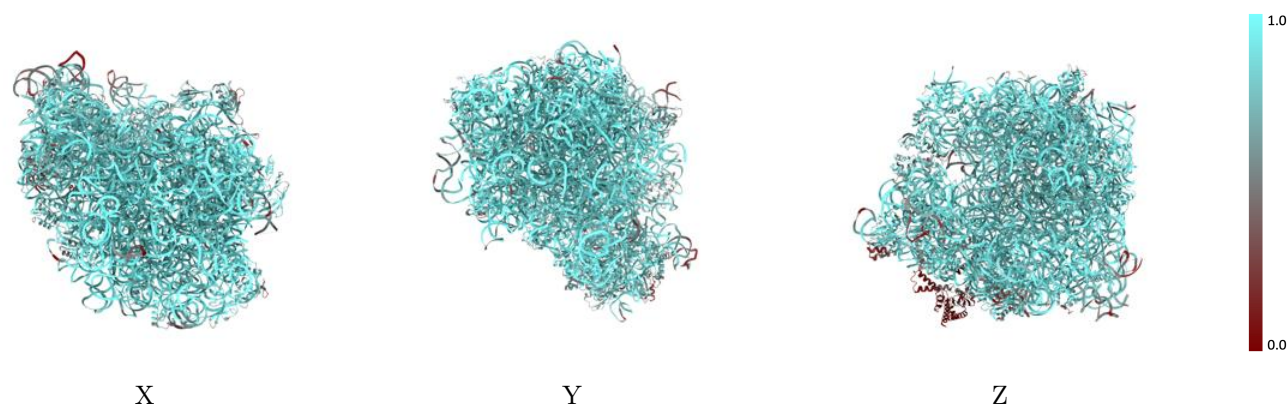
The images above show the 3D surface view of the map at the recommended contour level 0.0169 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



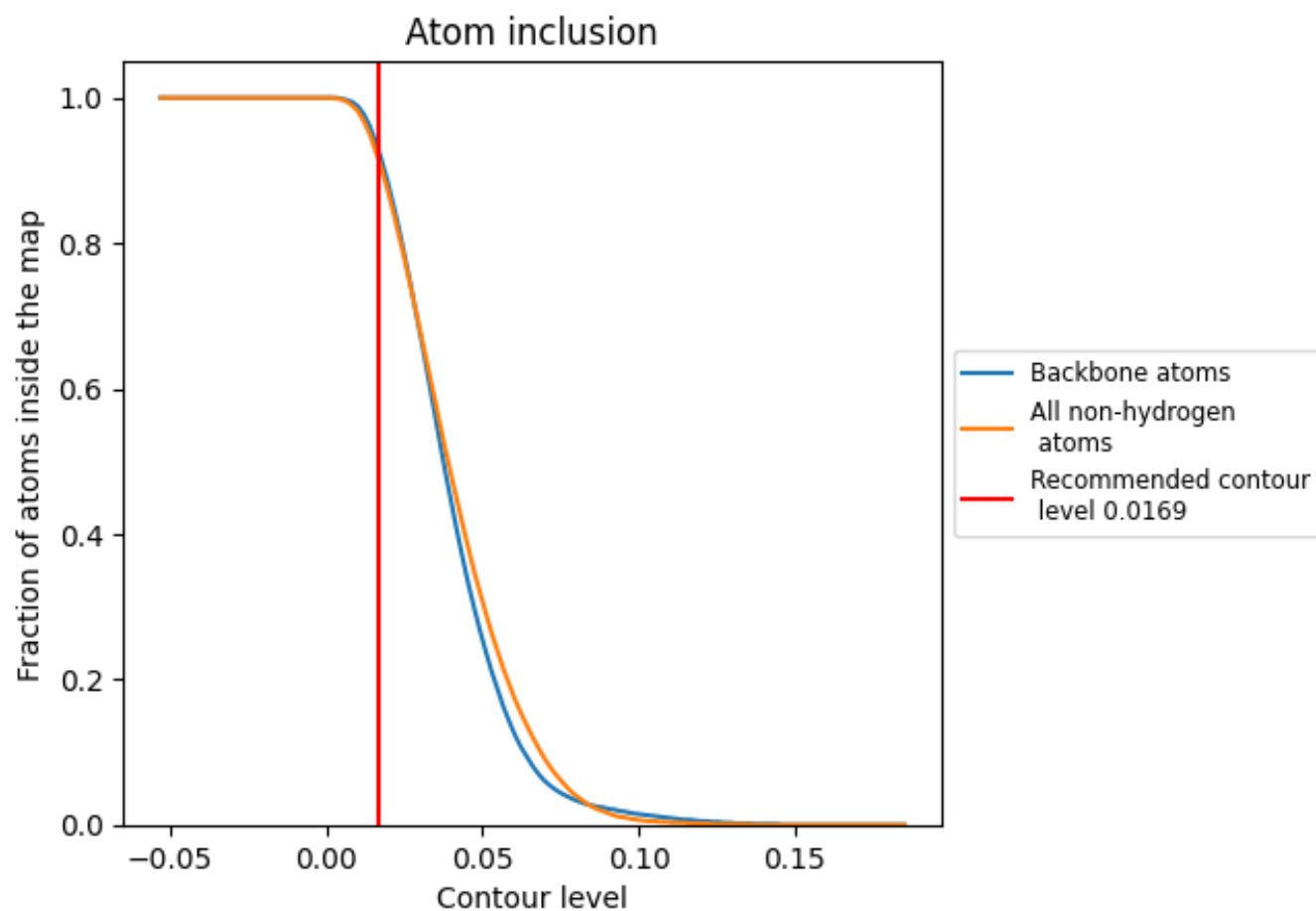
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0169).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.0169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.6550
0	 0.9240	 0.6890
1	 0.9830	 0.7350
2	 0.9780	 0.7220
3	 0.9390	 0.6810
4	 0.7010	 0.5620
A	 0.9270	 0.6270
B	 0.1750	 0.4840
C	 0.8280	 0.6180
D	 0.6300	 0.5290
E	 0.8960	 0.6430
F	 0.7510	 0.5720
G	 0.7840	 0.6010
H	 0.8820	 0.6320
I	 0.8130	 0.6180
J	 0.6520	 0.5580
K	 0.8690	 0.6330
L	 0.8980	 0.6570
M	 0.8150	 0.6170
N	 0.8580	 0.6250
O	 0.8490	 0.6250
P	 0.7460	 0.5530
Q	 0.7730	 0.5790
R	 0.7860	 0.5820
S	 0.8140	 0.6080
T	 0.7560	 0.5540
U	 0.3580	 0.4620
V	 0.9140	 0.6100
X	 0.9620	 0.6550
Z	 0.9250	 0.6230
a	 0.9700	 0.6870
b	 0.9580	 0.6540
c	 0.9710	 0.7150
d	 0.9330	 0.7030
e	 0.8380	 0.6570



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Chain	Atom inclusion	Q-score
f	 0.8220	 0.6140
g	 0.7100	 0.5900
h	 0.4830	 0.5650
i	 0.9410	 0.6930
j	 0.9610	 0.7010
k	 0.9070	 0.6780
l	 0.9530	 0.7030
m	 0.9850	 0.7240
n	 0.8900	 0.6530
o	 0.9080	 0.6840
p	 0.9670	 0.7080
q	 0.8810	 0.6590
r	 0.9340	 0.7030
s	 0.8740	 0.6490
t	 0.8140	 0.6170
u	 0.8460	 0.6460
v	 0.9390	 0.7020
w	 0.9470	 0.6850
x	 0.7970	 0.5910
y	 0.9040	 0.6680
z	 0.9300	 0.6950