



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 11:44 am BST

PDB ID : 5LZB / pdb_00005lzb
EMDB ID : EMD-4122
Title : Structure of SelB-Sec-tRNA^{Sec} bound to the 70S ribosome in the initial binding state (IB)
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : 2016-09-29
Resolution : 5.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

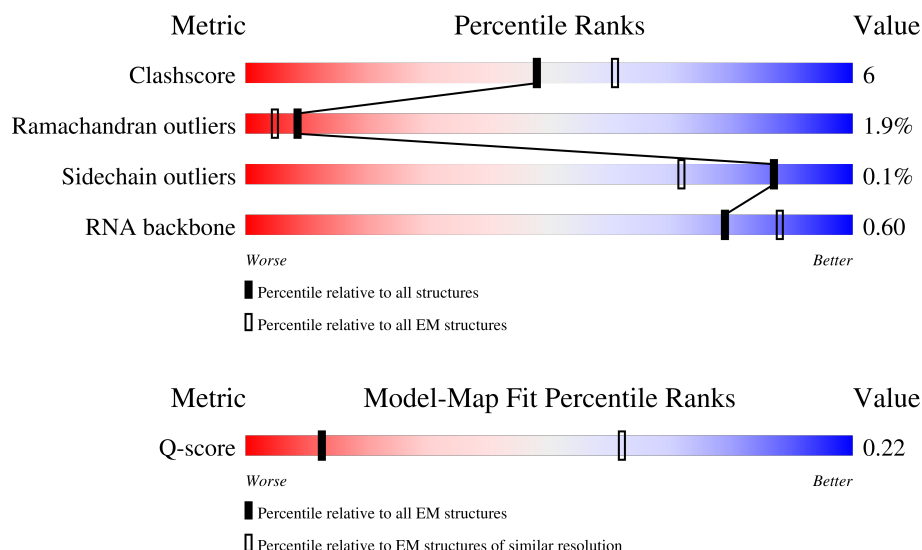
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.30 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	625 (4.80 - 5.80)

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	1539	
2	b	218	

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Mol	Chain	Length	Quality of chain
3	c	206	
4	d	205	
5	e	157	
6	f	100	
7	g	151	
8	h	129	
9	i	127	
10	j	98	
11	k	116	
12	l	123	
13	m	114	
14	n	100	
15	o	88	
16	p	82	
17	q	80	
18	r	65	
19	s	79	
20	t	85	
21	u	65	
22	v	77	
23	x	48	
24	y	95	
25	z	614	
26	A	2903	
27	B	120	

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Mol	Chain	Length	Quality of chain
28	C	271	
29	D	209	
30	E	201	
31	F	177	
32	G	176	
33	I	141	
34	H	149	
35	J	142	
36	K	122	
37	L	143	
38	M	136	
39	N	120	
40	O	116	
41	P	114	
42	Q	117	
43	R	103	
44	S	110	
45	T	93	
46	U	102	
47	V	94	
48	W	75	
49	X	77	
50	Y	63	
51	Z	58	
52	0	56	

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Mol	Chain	Length	Quality of chain
53	1	50	
54	2	46	
55	3	64	
56	4	38	
57	6	66	
58	w	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
26	G7M	A	2069	X	-	-	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 152991 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- 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
			1625	1028	305	289	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	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	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
			787	493	150	143	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- 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
			955	590	196	165	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	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
			794	495	164	132	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	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called fMet-tRNA^{fMet}.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called Sec-tRNA^{Sec}.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	95	Total	C	N	O	P	0	0
			2031	907	357	672	95		

- Molecule 25 is a protein called Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	614	Total	C	N	O	S	1	0
			4863	3049	904	893	17		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2903	Total	C	N	O	P	0	0
			62335	27815	11467	20150	2903		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
46	U	102	Total	C	N	O	0	0
			780	492	146	142		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

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

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

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

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

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

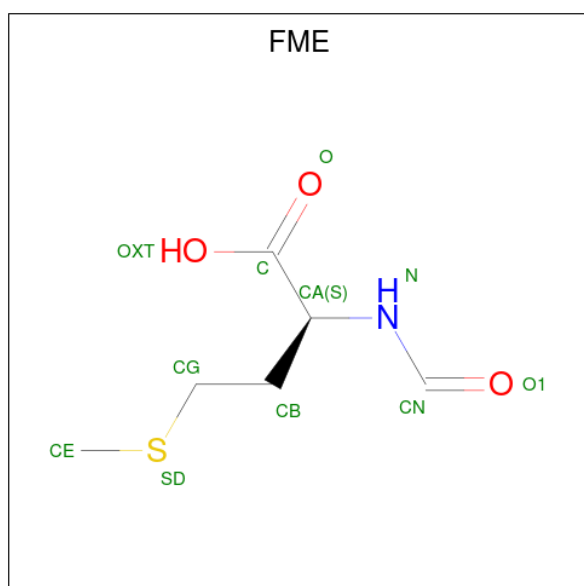
- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 58 is a RNA chain called CCA 3' end of E-site tRNA^{Sec} (low occupancy).

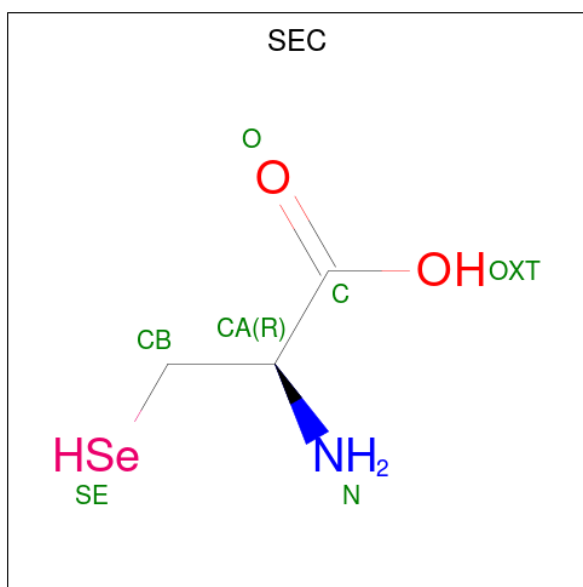
Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



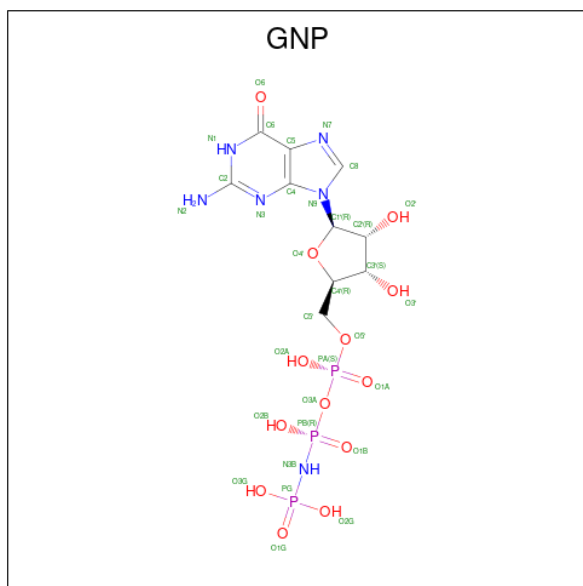
Mol	Chain	Residues	Atoms					AltConf
59	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is SELENOCYSTEINE (CCD ID: SEC) (formula: C₃H₇NO₂Se).



Mol	Chain	Residues	Atoms					AltConf
60	y	1	Total	C	N	O	Se	0
			6	3	1	1	1	

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms		AltConf
62	z	1	Total	Mg	0
			1	1	

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
63	4	1	Total	Zn	0
			1	1	
63	6	1	Total	Zn	0
			1	1	

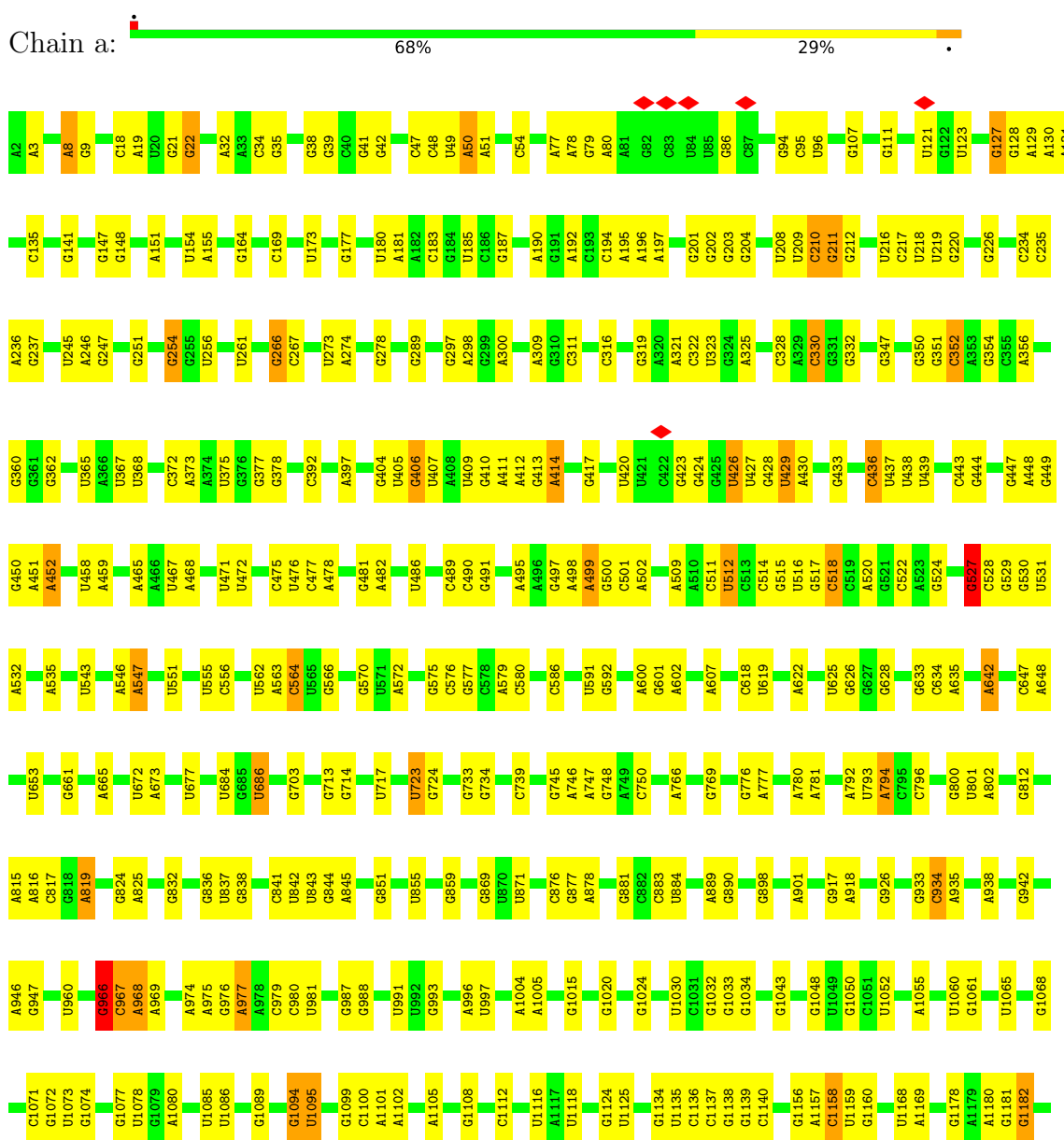
- Molecule 64 is water.

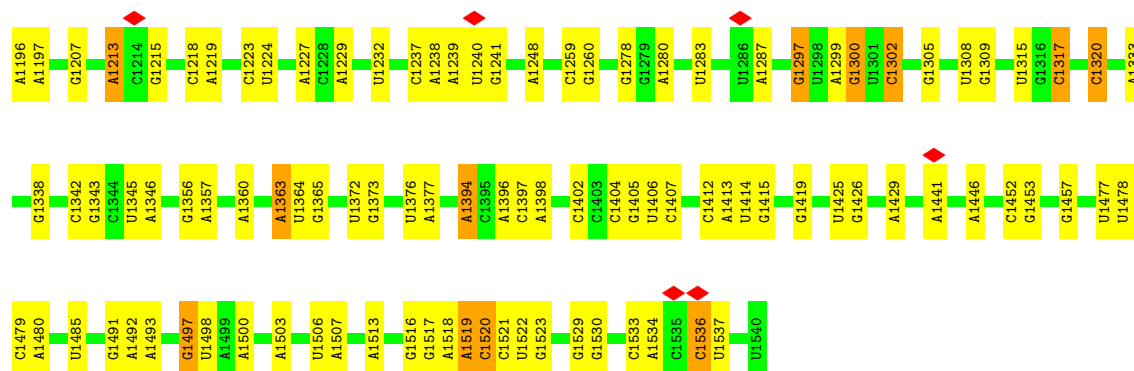
Mol	Chain	Residues	Atoms		AltConf
64	z	2	Total	O	0
			2	2	

3 Residue-property plots

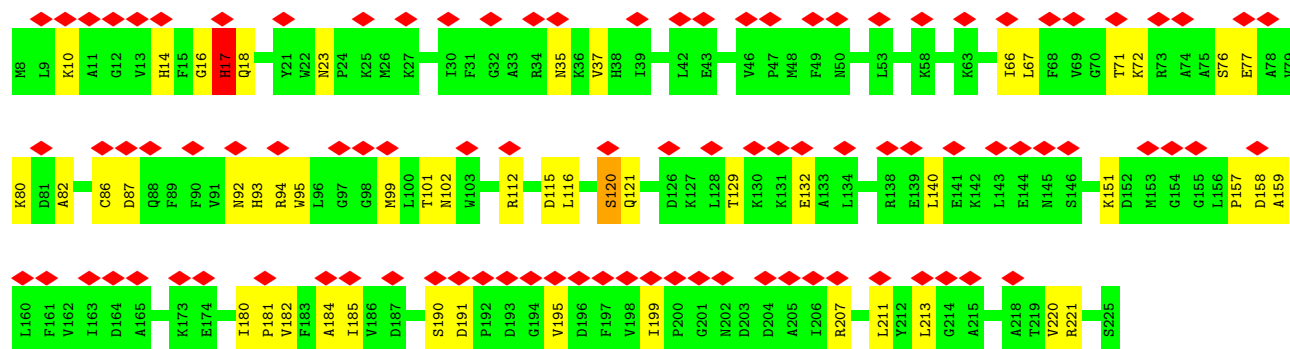
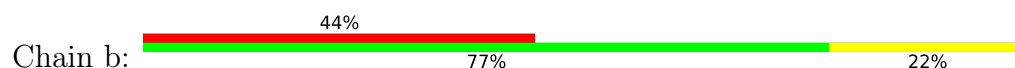
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

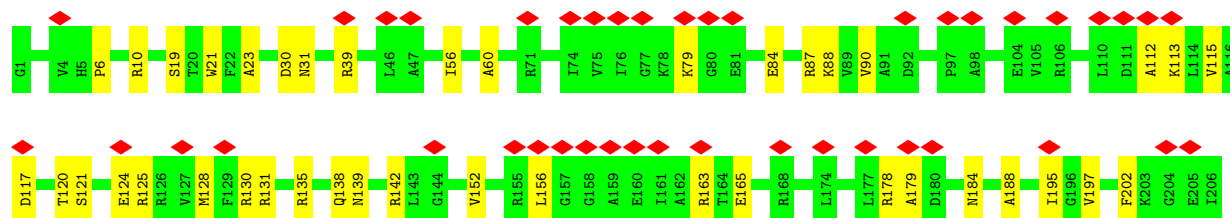
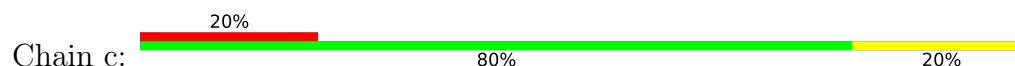




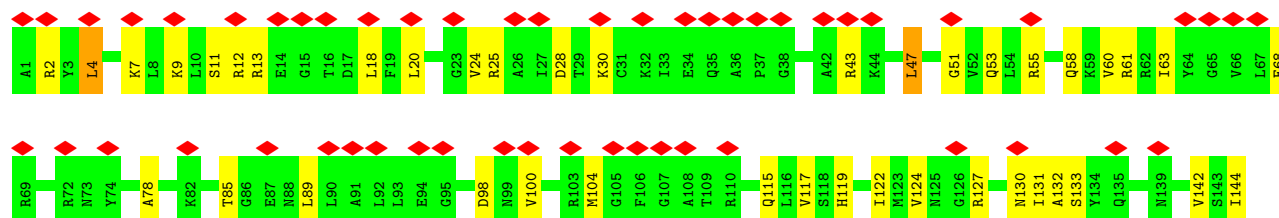
• Molecule 2: 30S ribosomal protein S2

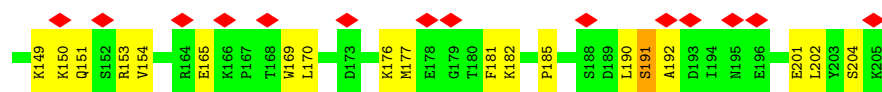


• Molecule 3: 30S ribosomal protein S3

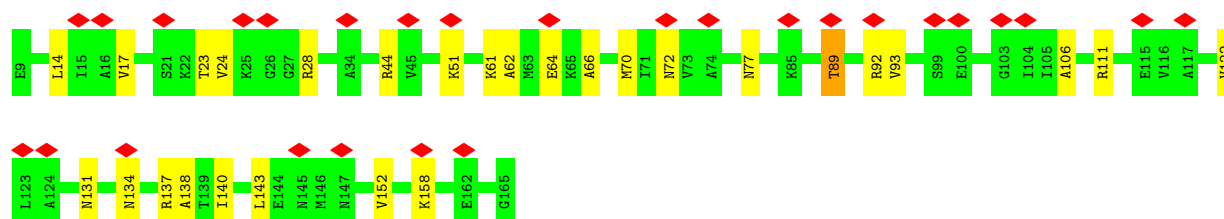
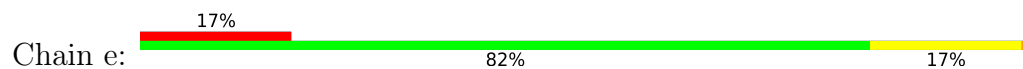


• Molecule 4: 30S ribosomal protein S4

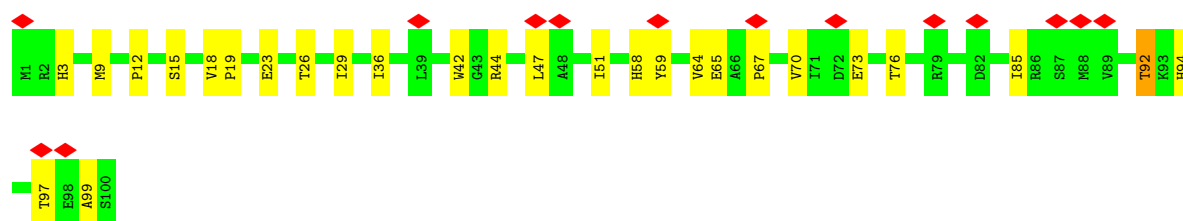




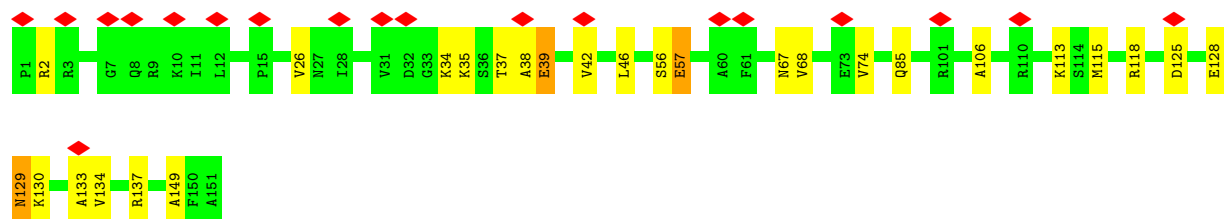
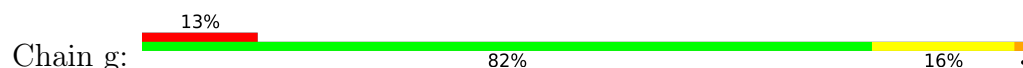
• Molecule 5: 30S ribosomal protein S5



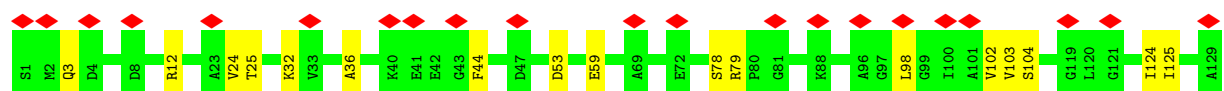
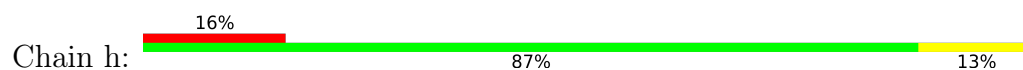
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

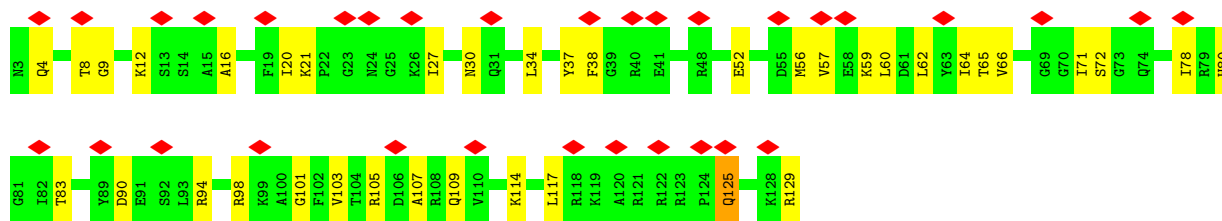


• Molecule 8: 30S ribosomal protein S8

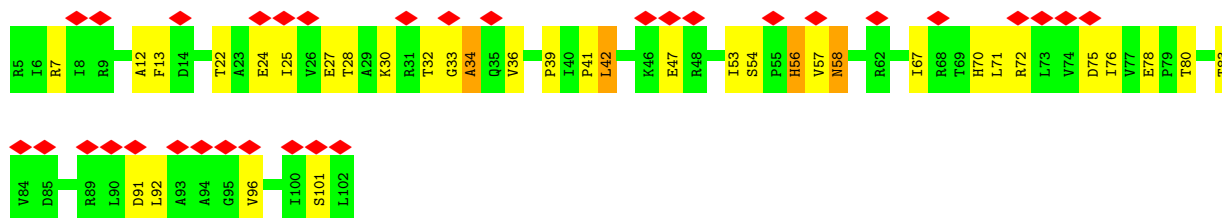


• Molecule 9: 30S ribosomal protein S9

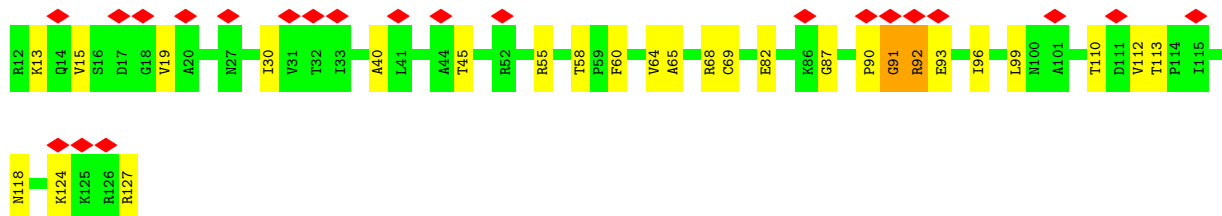
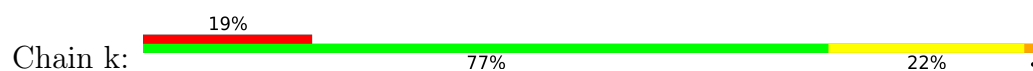




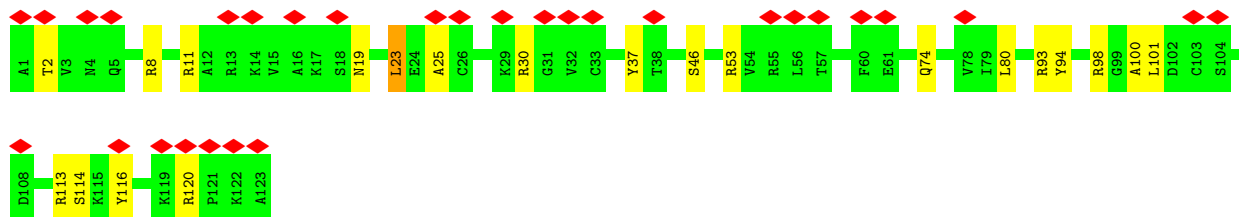
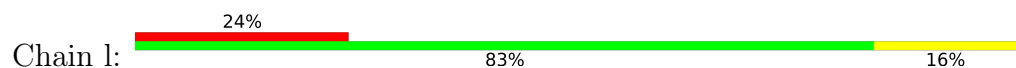
• Molecule 10: 30S ribosomal protein S10



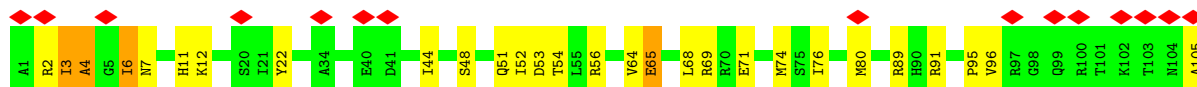
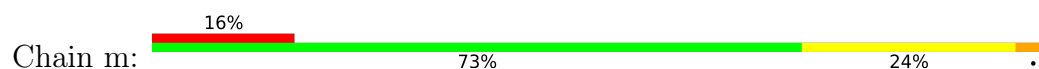
• Molecule 11: 30S ribosomal protein S11

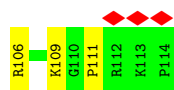


• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13

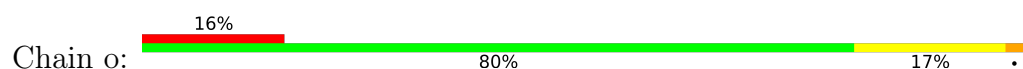




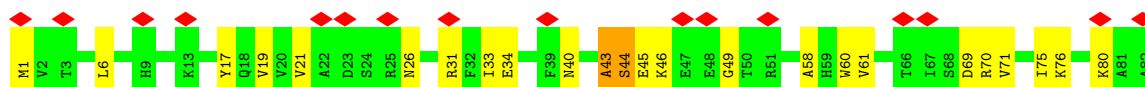
- Molecule 14: 30S ribosomal protein S14



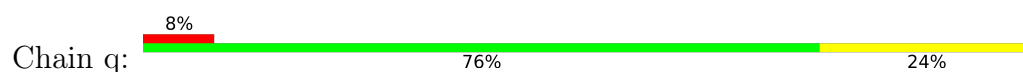
- Molecule 15: 30S ribosomal protein S15



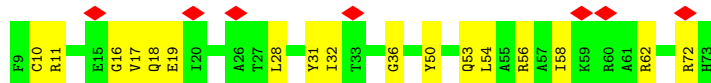
- Molecule 16: 30S ribosomal protein S16



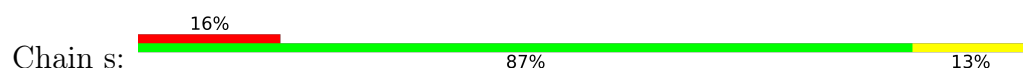
- Molecule 17: 30S ribosomal protein S17

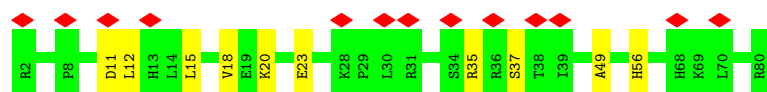


- Molecule 18: 30S ribosomal protein S18

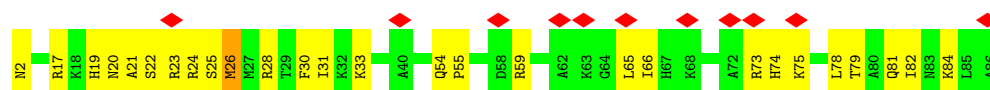


- Molecule 19: 30S ribosomal protein S19

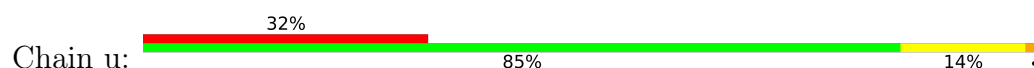




- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



- Molecule 22: fMet-tRNAfMet



- Molecule 23: SECIS mRNA

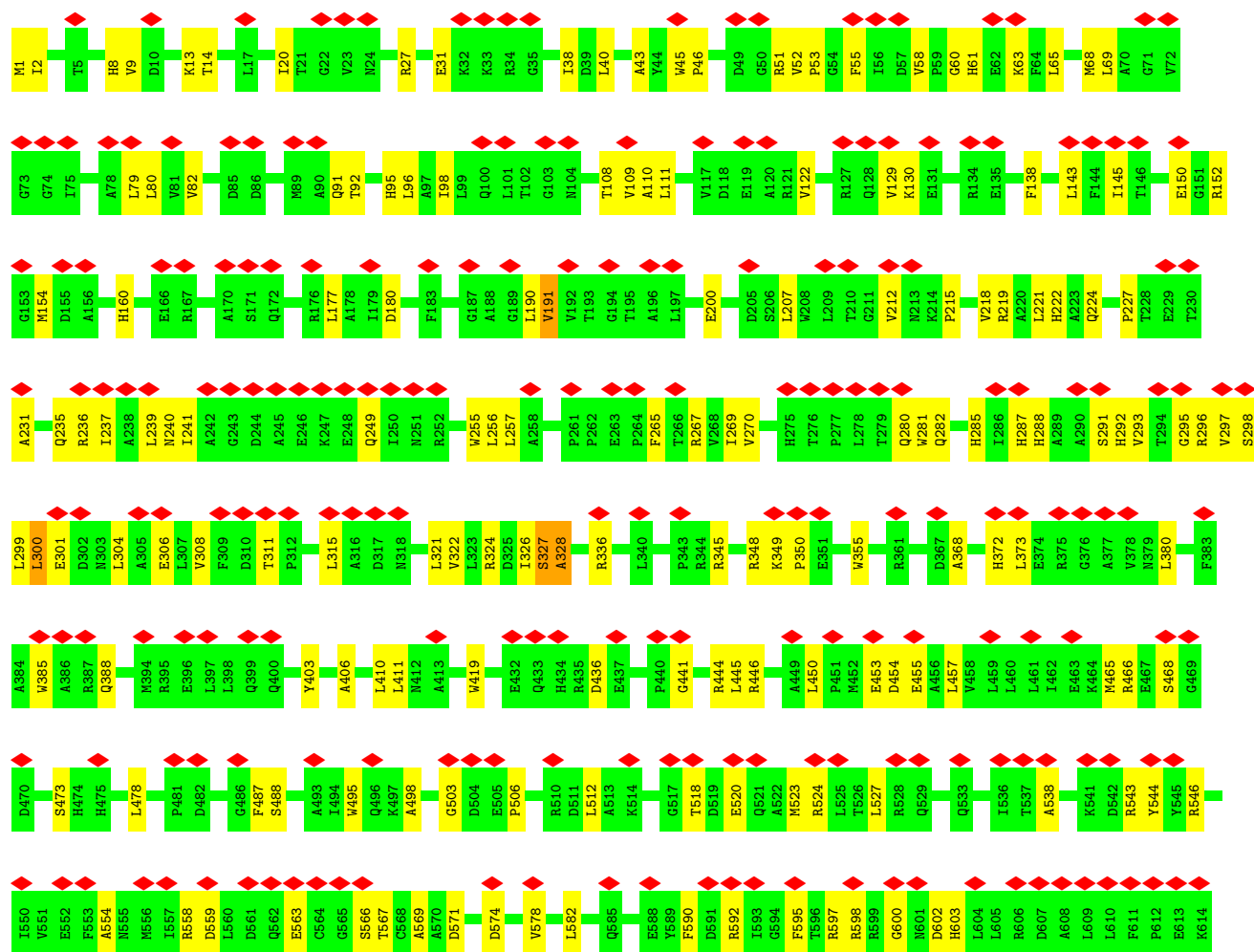


- Molecule 24: Sec-tRNA^{Sec}

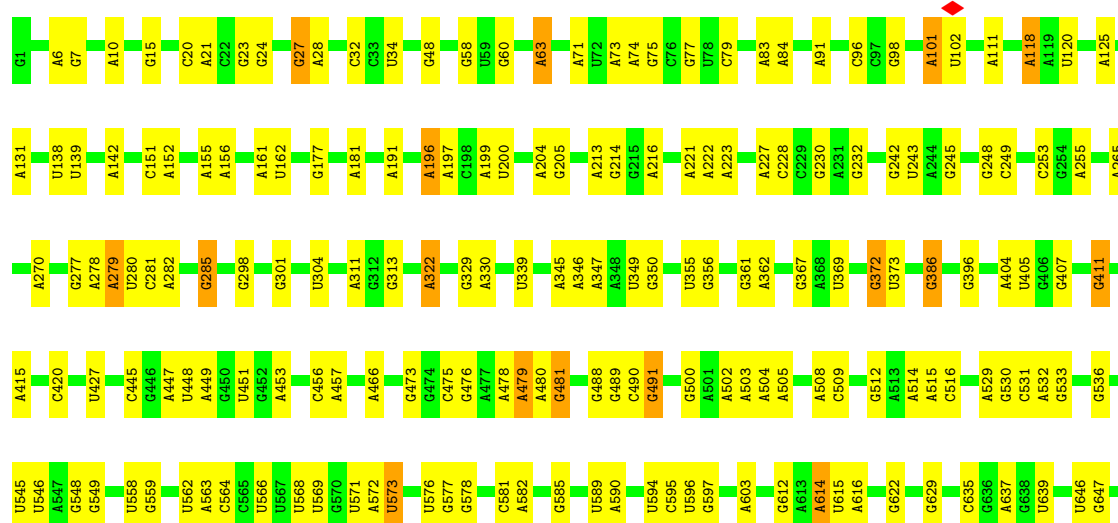


- Molecule 25: Selenocysteine-specific elongation factor

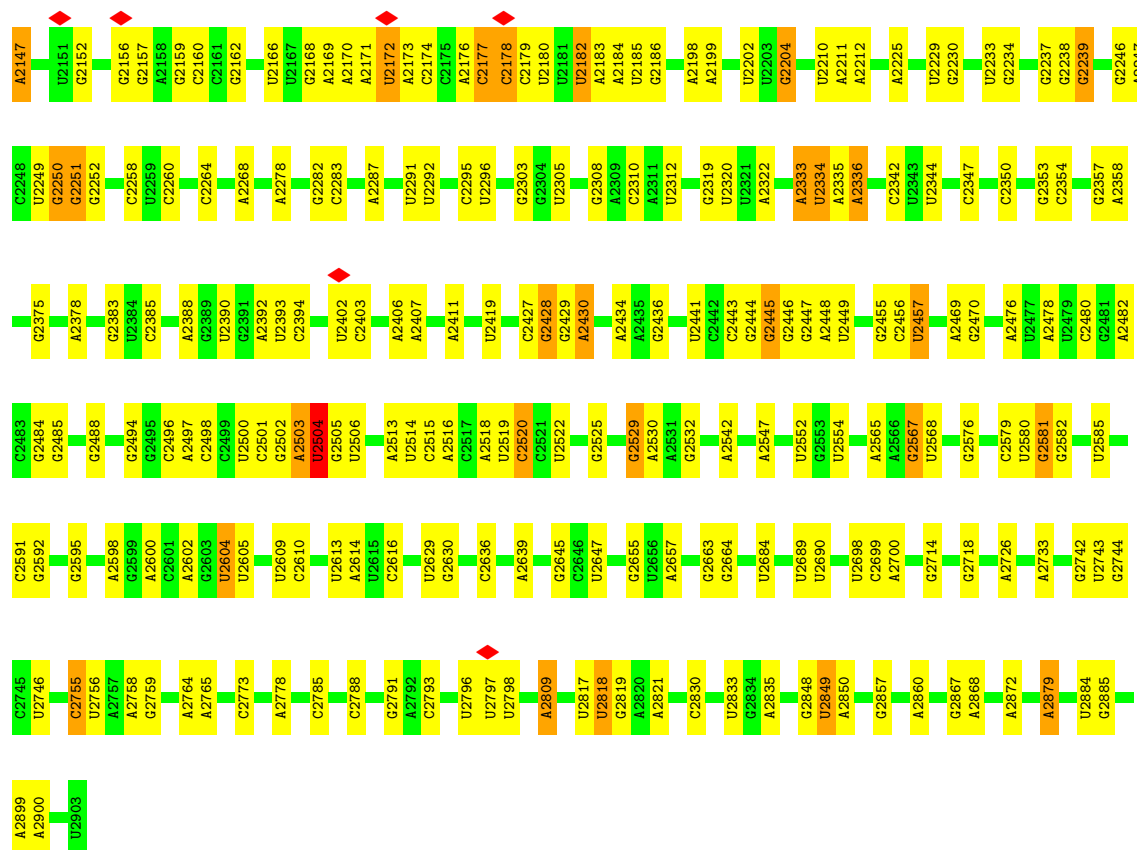




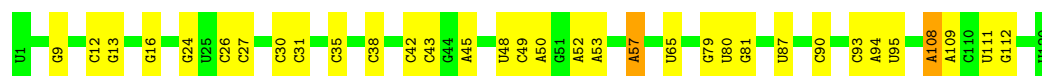
• Molecule 26: 23S ribosomal RNA



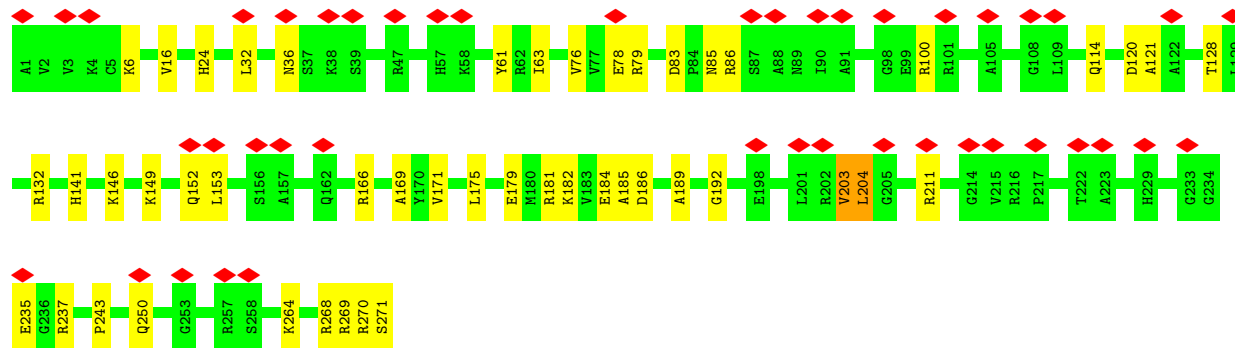
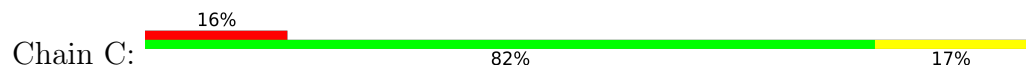




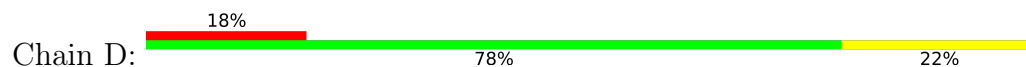
• Molecule 27: 5S ribosomal RNA

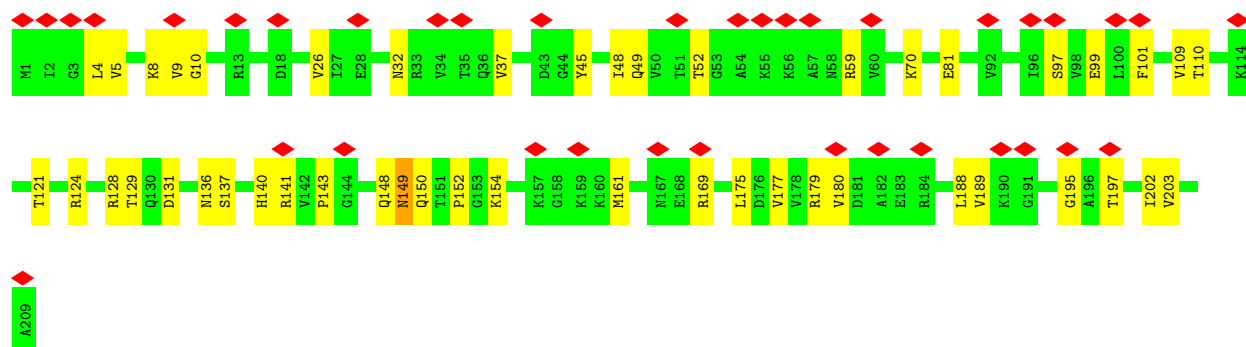


• Molecule 28: 50S ribosomal protein L2

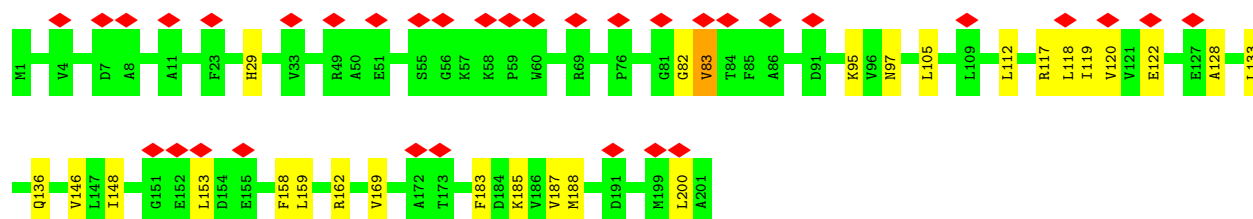
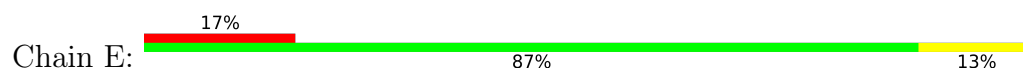


• Molecule 29: 50S ribosomal protein L3

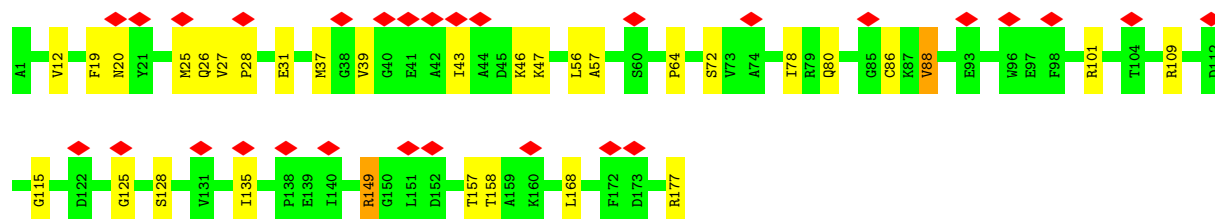
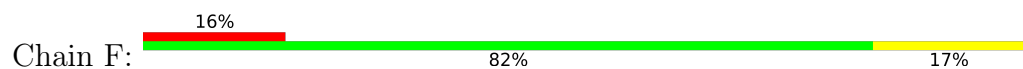




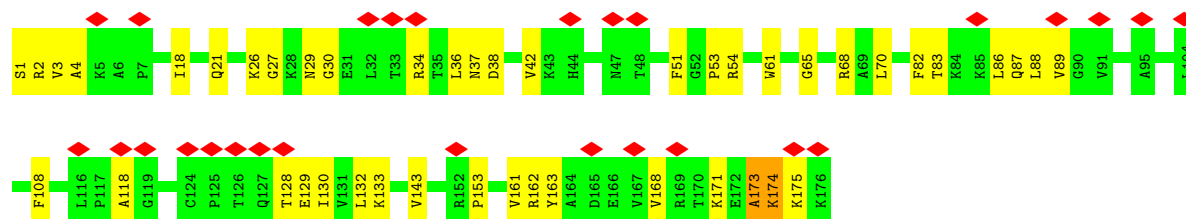
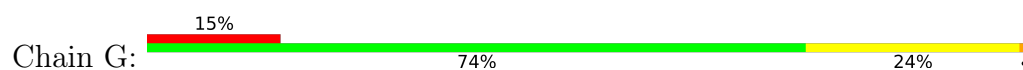
- Molecule 30: 50S ribosomal protein L4



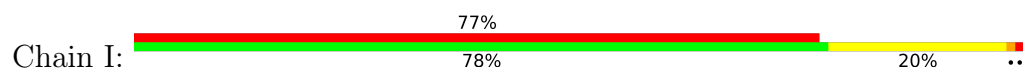
- Molecule 31: 50S ribosomal protein L5

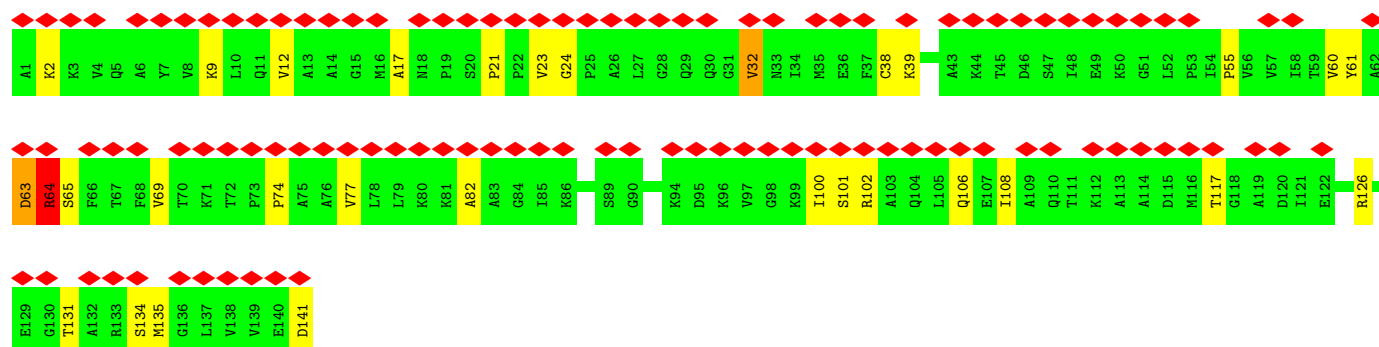


- Molecule 32: 50S ribosomal protein L6

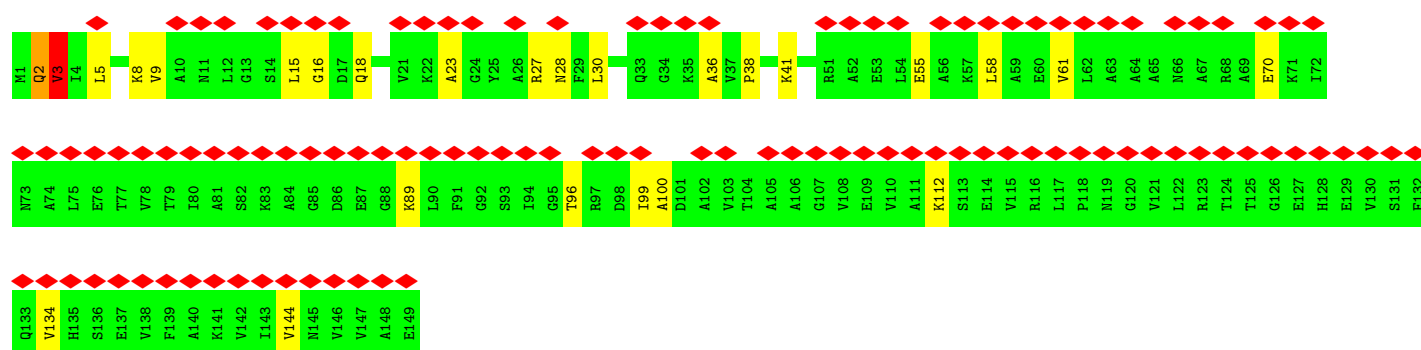
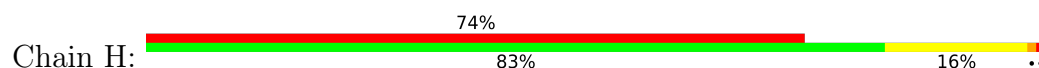


- Molecule 33: 50S ribosomal protein L11

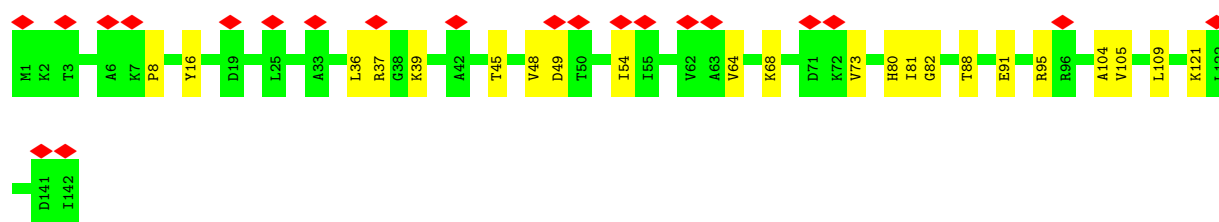
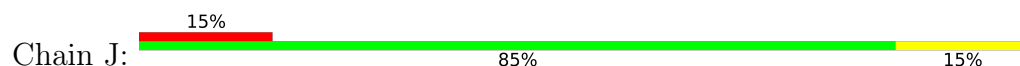




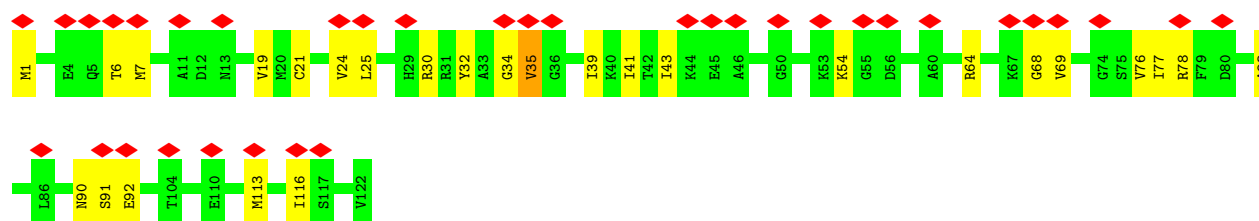
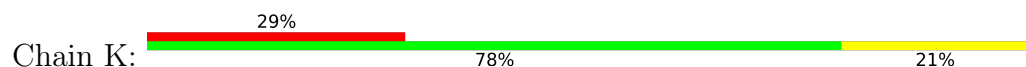
• Molecule 34: 50S ribosomal protein L9



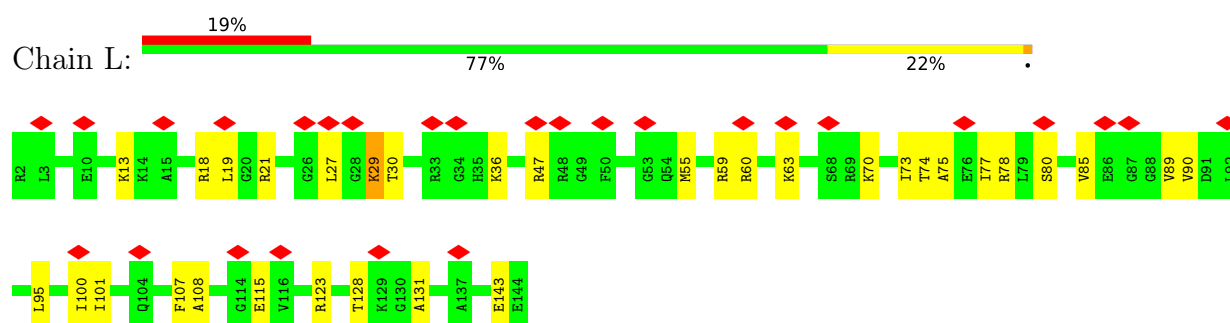
• Molecule 35: 50S ribosomal protein L13



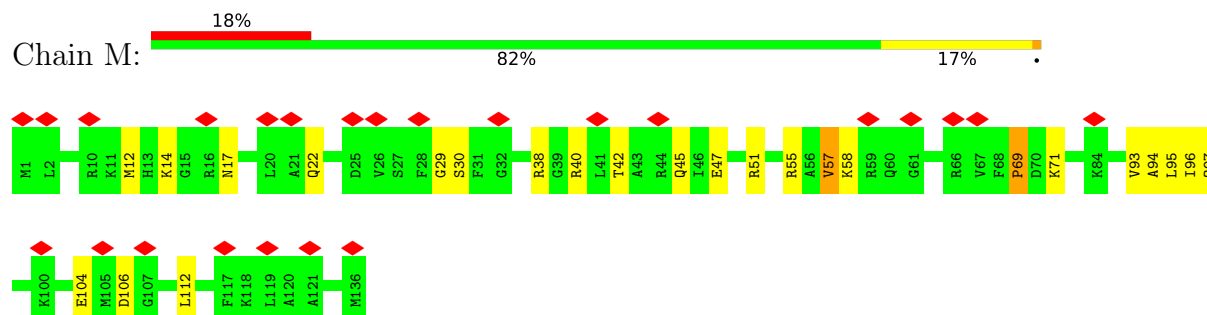
• Molecule 36: 50S ribosomal protein L14



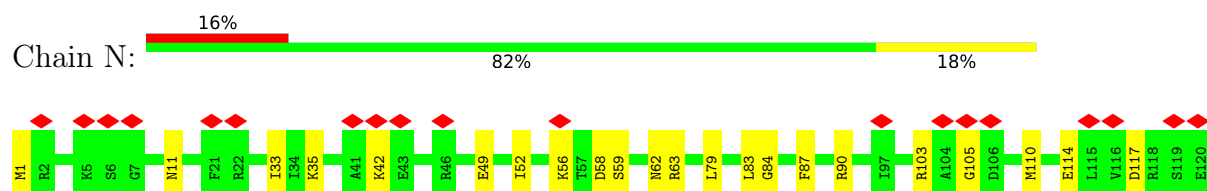
• Molecule 37: 50S ribosomal protein L15



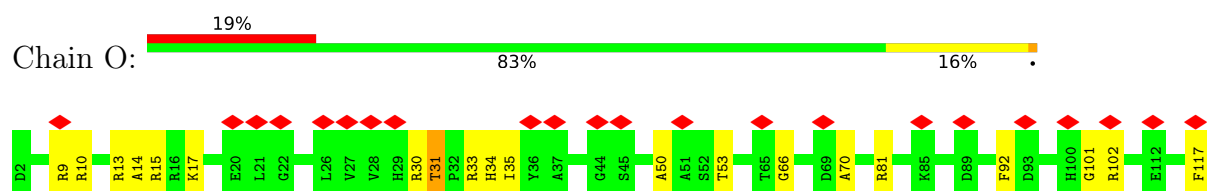
- Molecule 38: 50S ribosomal protein L16



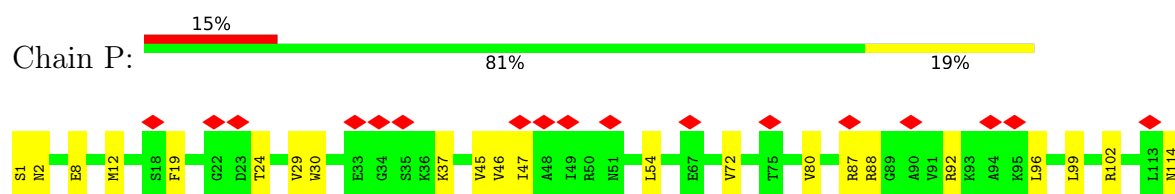
- Molecule 39: 50S ribosomal protein L17



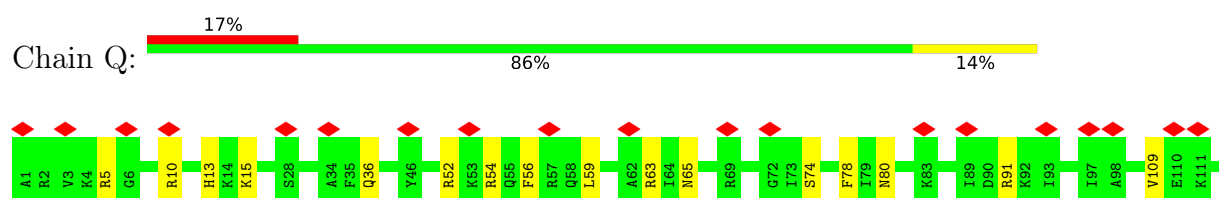
- Molecule 40: 50S ribosomal protein L18



- Molecule 41: 50S ribosomal protein L19

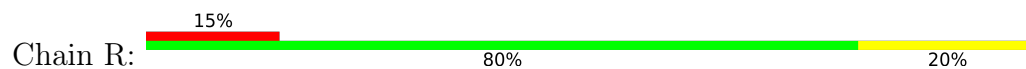


- Molecule 42: 50S ribosomal protein L20

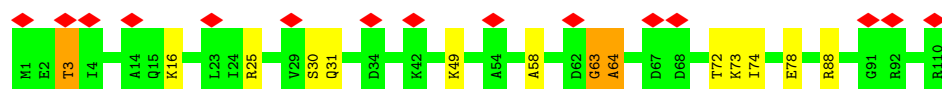
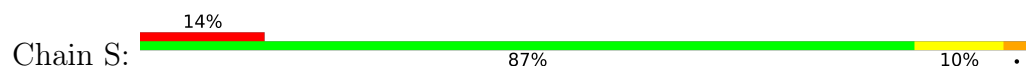




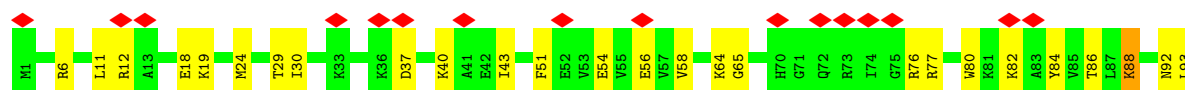
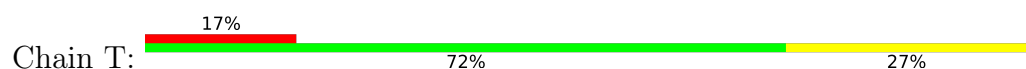
- Molecule 43: 50S ribosomal protein L21



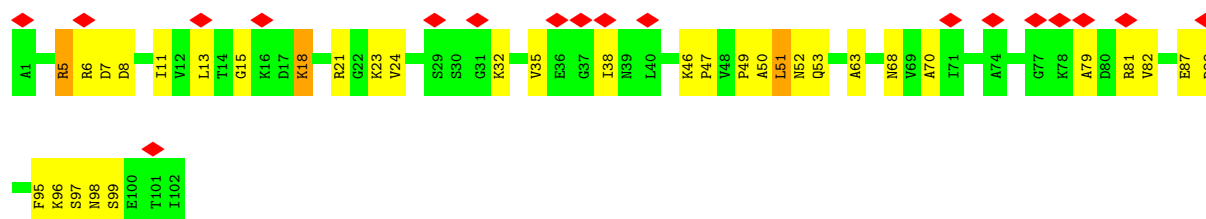
- Molecule 44: 50S ribosomal protein L22



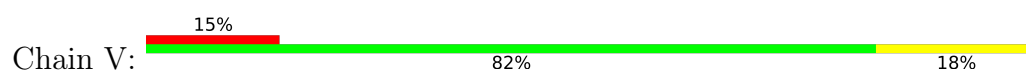
- Molecule 45: 50S ribosomal protein L23



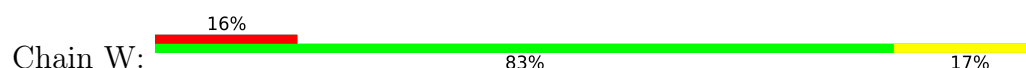
- Molecule 46: 50S ribosomal protein L24

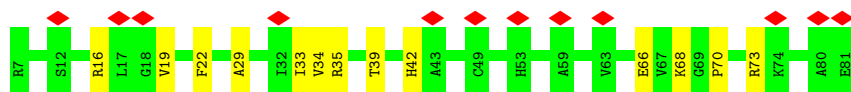


- Molecule 47: 50S ribosomal protein L25

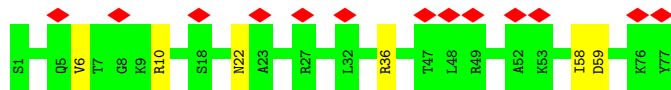


- Molecule 48: 50S ribosomal protein L27

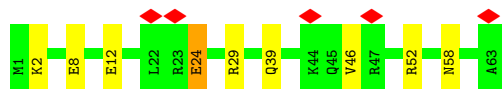
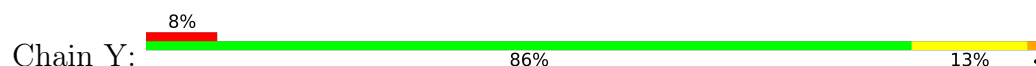




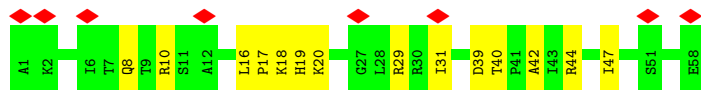
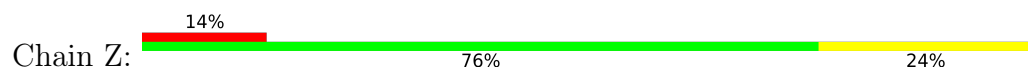
- Molecule 49: 50S ribosomal protein L28



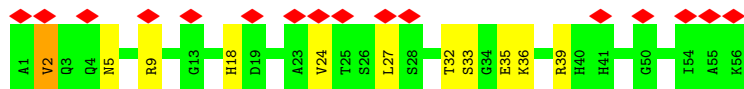
- Molecule 50: 50S ribosomal protein L29



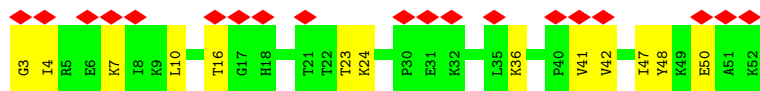
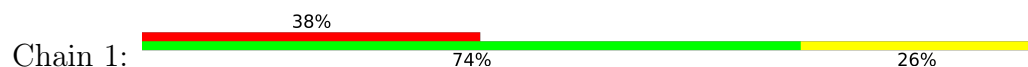
- Molecule 51: 50S ribosomal protein L30



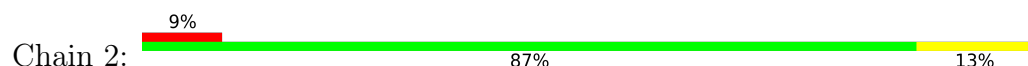
- Molecule 52: 50S ribosomal protein L32



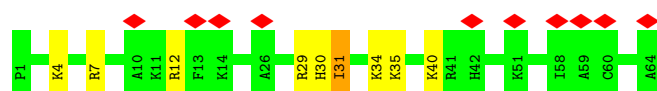
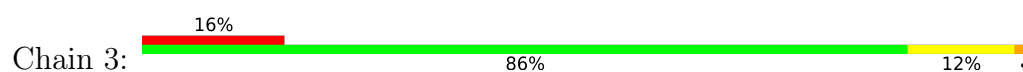
- Molecule 53: 50S ribosomal protein L33



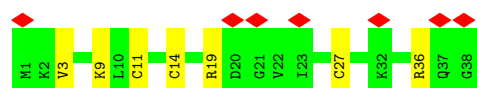
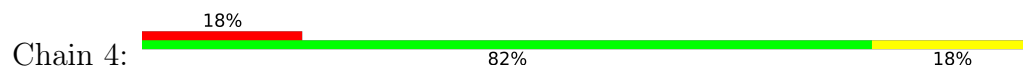
- Molecule 54: 50S ribosomal protein L34



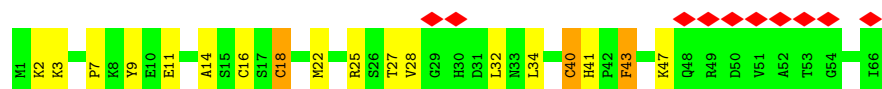
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 57: 50S ribosomal protein L31



- Molecule 58: CCA 3' end of E-site tRNA^{Sec} (low occupancy)



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8002	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.675	Depositor
Minimum map value	-0.887	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.36	Depositor
Map size ($\text{\AA}$)	315.52, 315.52, 315.52	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SEC, 4OC, H2U, 2MG, 6MZ, 5MU, G7M, OMG, PSU, 3TD, MA6, UR3, 2MA, 4SU, 6IA, OMC, MG, FME, ZN, GNP, 5MC, OMU, 1MG

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	0.34	1/36701 (0.0%)	0.47	5/57246 (0.0%)
2	b	0.48	0/1736	1.00	1/2338 (0.0%)
3	c	0.42	0/1652	0.88	2/2225 (0.1%)
4	d	0.51	0/1665	1.03	0/2227
5	e	0.47	0/1170	1.03	1/1573 (0.1%)
6	f	0.52	0/836	1.01	2/1128 (0.2%)
7	g	0.45	0/1196	0.98	3/1602 (0.2%)
8	h	0.44	0/989	0.88	0/1326
9	i	0.50	0/1034	1.04	0/1375
10	j	0.48	0/797	1.06	3/1077 (0.3%)
11	k	0.52	0/886	1.11	3/1195 (0.3%)
12	l	0.42	0/969	0.92	0/1300
13	m	0.46	0/893	1.04	4/1193 (0.3%)
14	n	0.48	0/806	1.01	4/1074 (0.4%)
15	o	0.46	0/722	0.96	4/964 (0.4%)
16	p	0.50	0/659	0.93	0/884
17	q	0.45	0/658	1.06	3/881 (0.3%)
18	r	0.38	0/512	0.86	0/689
19	s	0.39	0/653	0.81	0/877
20	t	0.53	0/671	1.07	0/888
21	u	0.46	0/501	1.04	1/668 (0.1%)
22	v	0.34	0/1745	0.45	0/2716
23	x	0.53	0/1145	1.14	10/1781 (0.6%)
24	y	0.49	0/2168	0.81	2/3375 (0.1%)
25	z	0.49	0/4963	1.01	2/6727 (0.0%)
26	A	0.33	1/69240 (0.0%)	0.46	7/108014 (0.0%)
27	B	0.32	0/2873	0.43	0/4478
28	C	0.39	0/2122	0.87	3/2852 (0.1%)
29	D	0.44	0/1586	0.88	0/2134
30	E	0.44	0/1571	0.85	2/2113 (0.1%)
31	F	0.51	0/1435	1.00	4/1926 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	G	0.46	0/1343	0.95	2/1816 (0.1%)
33	I	0.47	0/1046	1.08	5/1410 (0.4%)
34	H	0.42	0/1122	0.88	0/1515
35	J	0.40	0/1152	0.85	0/1551
36	K	0.42	0/948	0.88	0/1268
37	L	0.41	0/1054	0.92	0/1403
38	M	0.42	0/1093	0.86	0/1460
39	N	0.44	0/974	0.85	0/1301
40	O	0.46	0/902	0.87	1/1209 (0.1%)
41	P	0.39	0/929	0.84	0/1242
42	Q	0.42	0/960	0.73	0/1278
43	R	0.42	0/829	0.92	0/1107
44	S	0.42	0/864	0.89	3/1156 (0.3%)
45	T	0.43	0/745	0.83	0/994
46	U	0.41	0/788	1.05	4/1051 (0.4%)
47	V	0.43	0/766	0.80	0/1025
48	W	0.38	0/582	0.81	0/769
49	X	0.35	0/635	0.78	0/848
50	Y	0.52	0/510	1.05	0/677
51	Z	0.43	0/453	0.84	0/605
52	0	0.43	0/450	0.96	3/599 (0.5%)
53	1	0.38	0/417	0.88	2/554 (0.4%)
54	2	0.42	0/380	0.90	0/498
55	3	0.43	0/513	0.74	0/676
56	4	0.44	0/303	0.99	0/397
57	6	0.51	0/532	1.15	5/709 (0.7%)
58	w	0.17	0/68	0.34	0/103
All	All	0.38	2/164912 (0.0%)	0.65	91/246067 (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
1	a	2	0
2	b	0	2
5	e	0	1
10	j	0	2
11	k	0	1
12	l	0	2
13	m	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	o	0	1
18	r	0	2
25	z	0	3
26	A	2	0
28	C	0	1
33	I	0	2
34	H	0	3
36	K	0	1
38	M	0	1
44	S	0	1
46	U	0	2
55	3	0	1
All	All	4	28

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	527	G7M	O3'-P	6.65	1.62	1.56
26	A	2069	G7M	O3'-P	6.13	1.62	1.56

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	z	328	ALA	N-CA-C	-10.27	88.92	110.80
33	I	64	ARG	CA-CB-CG	8.12	130.35	114.10
23	x	126	G	C2'-C3'-O3'	-8.04	97.44	109.50
1	a	516	PSU	O3'-P-O5'	-7.81	92.28	104.00
1	a	450	G	O5'-P-OP1	7.70	131.09	108.00
30	E	82	GLY	N-CA-C	7.42	130.76	113.18
57	6	18	CYS	CA-CB-SG	-7.39	97.40	114.40
32	G	173	ALA	CA-C-N	7.39	135.65	121.54
32	G	173	ALA	C-N-CA	7.39	135.65	121.54
44	S	64	ALA	N-CA-C	-7.30	95.25	110.80
1	a	452	A	O5'-P-OP1	-7.05	86.83	108.00
33	I	32	VAL	CG1-CB-CG2	-6.93	95.56	110.80
46	U	51	LEU	CA-CB-CG	6.86	140.32	116.30
26	A	2069	G7M	P-O3'-C3'	6.77	127.82	119.70
33	I	64	ARG	N-CA-CB	-6.74	99.10	110.49
23	x	125	G	N9-C1'-C2'	-6.62	102.07	112.00
23	x	125	G	C4'-C3'-O3'	6.61	122.91	113.00
10	j	91	ASP	CA-C-N	6.60	134.14	121.54
10	j	91	ASP	C-N-CA	6.60	134.14	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	527	G7M	P-O3'-C3'	6.57	127.58	119.70
2	b	17	HIS	N-CA-C	6.56	124.77	110.80
46	U	87	GLU	N-CA-C	-6.42	100.12	110.32
26	A	1042	G	P-O3'-C3'	6.39	129.78	120.20
23	x	127	U	P-O3'-C3'	6.31	129.67	120.20
46	U	5	ARG	CA-C-N	6.22	133.43	121.54
46	U	5	ARG	C-N-CA	6.22	133.43	121.54
23	x	103	G	O3'-P-O5'	6.18	113.26	104.00
57	6	40	CYS	N-CA-CB	6.17	120.92	110.49
17	q	15	LYS	CA-C-N	6.14	133.27	121.54
17	q	15	LYS	C-N-CA	6.14	133.27	121.54
44	S	63	GLY	N-CA-C	6.14	123.07	113.86
6	f	97	THR	CA-C-N	5.95	132.91	121.54
6	f	97	THR	C-N-CA	5.95	132.91	121.54
28	C	203	VAL	CA-C-N	5.94	132.88	121.54
28	C	203	VAL	C-N-CA	5.94	132.88	121.54
14	n	33	VAL	CA-C-N	5.92	132.85	121.54
14	n	33	VAL	C-N-CA	5.92	132.85	121.54
23	x	126	G	O5'-C5'-C4'	5.87	120.51	111.70
26	A	2146	C	O5'-P-OP1	5.78	125.33	108.00
23	x	129	U	C5'-C4'-C3'	5.75	124.62	116.00
26	A	1186	G	O5'-P-OP2	5.74	125.20	108.00
40	O	31	THR	CB-CA-C	5.72	119.10	109.32
7	g	128	GLU	CA-C-N	5.70	132.42	121.54
7	g	128	GLU	C-N-CA	5.70	132.42	121.54
52	0	24	VAL	CA-C-N	5.67	132.38	121.54
52	0	24	VAL	C-N-CA	5.67	132.38	121.54
15	o	86	LEU	CA-C-N	5.66	132.34	121.54
15	o	86	LEU	C-N-CA	5.66	132.34	121.54
13	m	111	PRO	N-CA-C	-5.62	101.70	111.32
26	A	1026	G	O5'-P-OP1	-5.54	91.37	108.00
25	z	328	ALA	N-CA-CB	5.52	119.82	110.49
1	a	1302	C	OP1-P-O3'	-5.52	91.45	108.00
5	e	89	THR	N-CA-CB	-5.51	101.18	110.49
13	m	65	GLU	N-CA-C	5.51	122.53	110.80
26	A	1086	A	C4'-C3'-O3'	-5.49	104.76	113.00
11	k	112	VAL	CA-CB-CG1	5.48	119.71	110.40
14	n	36	SER	N-CA-C	5.46	122.44	110.80
33	I	63	ASP	CA-C-N	5.45	131.96	121.54
33	I	63	ASP	C-N-CA	5.45	131.96	121.54
31	F	149	ARG	N-CA-C	5.44	122.39	110.80
10	j	39	PRO	N-CA-C	-5.43	102.75	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	S	64	ALA	N-CA-CB	5.40	119.62	110.49
30	E	82	GLY	CA-C-O	-5.34	111.28	120.57
17	q	74	LEU	N-CA-C	5.33	118.24	109.72
24	y	55	PSU	P-O3'-C3'	5.32	128.19	120.20
24	y	56	C	OP2-P-O3'	-5.29	92.11	108.00
53	1	3	GLY	CA-C-N	5.29	131.49	121.97
53	1	3	GLY	C-N-CA	5.29	131.49	121.97
7	g	39	GLU	CA-CB-CG	5.28	124.66	114.10
13	m	64	VAL	CA-C-N	5.27	131.61	121.54
13	m	64	VAL	C-N-CA	5.27	131.61	121.54
52	0	2	VAL	N-CA-CB	-5.24	102.58	111.23
23	x	126	G	P-O3'-C3'	5.24	128.06	120.20
57	6	40	CYS	CB-CA-C	-5.24	100.00	110.42
23	x	132	A	P-O5'-C5'	5.17	128.66	120.90
26	A	2146	C	OP1-P-O3'	-5.16	92.52	108.00
3	c	125	ARG	CA-C-N	5.16	129.66	122.08
3	c	125	ARG	C-N-CA	5.16	129.66	122.08
23	x	127	U	C2'-C3'-O3'	5.15	117.23	109.50
57	6	3	LYS	CA-C-N	5.15	131.38	121.54
57	6	3	LYS	C-N-CA	5.15	131.38	121.54
31	F	19	PHE	CA-C-N	5.13	131.33	121.54
31	F	19	PHE	C-N-CA	5.13	131.33	121.54
31	F	88	VAL	CG1-CB-CG2	-5.13	99.52	110.80
11	k	90	PRO	CA-C-N	5.12	131.45	121.41
11	k	90	PRO	C-N-CA	5.12	131.45	121.41
15	o	45	HIS	CA-C-N	5.12	131.32	121.54
15	o	45	HIS	C-N-CA	5.12	131.32	121.54
21	u	15	LEU	CA-CB-CG	5.12	134.23	116.30
14	n	37	ASP	N-CA-C	-5.03	100.81	110.56
28	C	204	LEU	N-CA-C	5.03	121.50	110.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3',C4'
26	A	2069	G7M	C3',C4'

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
55	3	30	HIS	Peptide
28	C	120	ASP	Peptide

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Mol	Chain	Res	Type	Group
34	H	2	GLN	Peptide
34	H	8	LYS	Peptide,Mainchain
33	I	23	VAL	Peptide
33	I	63	ASP	Peptide
36	K	34	GLY	Peptide
38	M	57	VAL	Mainchain
44	S	63	GLY	Peptide
46	U	5	ARG	Peptide
46	U	50	ALA	Peptide
2	b	16	GLY	Peptide
2	b	17	HIS	Mainchain
5	e	92	ARG	Peptide
10	j	33	GLY	Peptide
10	j	56	HIS	Peptide
11	k	91	GLY	Peptide
12	l	100	ALA	Peptide
12	l	74	GLN	Peptide
13	m	3	ILE	Peptide
13	m	4	ALA	Mainchain
15	o	87	ARG	Mainchain
18	r	10	CYS	Peptide
18	r	16	GLY	Peptide
25	z	190	LEU	Peptide
25	z	300	LEU	Peptide
25	z	327	SER	Mainchain

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	33029	0	16643	240	0
2	b	1705	0	1732	30	0
3	c	1625	0	1699	25	0
4	d	1643	0	1710	44	0
5	e	1157	0	1199	14	0
6	f	818	0	808	14	0
7	g	1182	0	1240	20	0
8	h	979	0	1034	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	i	1022	0	1070	22	0
10	j	787	0	828	18	0
11	k	870	0	878	20	0
12	l	955	0	1019	13	0
13	m	884	0	944	21	0
14	n	794	0	836	18	0
15	o	714	0	737	13	0
16	p	649	0	666	15	0
17	q	649	0	691	10	0
18	r	505	0	502	9	0
19	s	638	0	665	6	0
20	t	665	0	714	21	0
21	u	496	0	486	4	0
22	v	1642	0	839	6	0
23	x	1025	0	518	9	0
24	y	2031	0	1039	44	0
25	z	4863	0	4837	115	0
26	A	62335	0	31375	420	0
27	B	2570	0	1301	21	0
28	C	2083	0	2157	30	0
29	D	1565	0	1616	31	0
30	E	1552	0	1619	15	0
31	F	1411	0	1447	21	0
32	G	1323	0	1374	29	0
33	I	1032	0	1088	17	0
34	H	1111	0	1148	13	0
35	J	1129	0	1162	12	0
36	K	939	0	1012	16	0
37	L	1045	0	1117	22	0
38	M	1074	0	1157	17	0
39	N	961	0	1000	15	0
40	O	892	0	923	14	0
41	P	917	0	965	14	0
42	Q	947	0	1022	14	0
43	R	816	0	839	12	0
44	S	857	0	922	9	0
45	T	739	0	807	17	0
46	U	780	0	834	15	0
47	V	753	0	780	13	0
48	W	575	0	592	9	0
49	X	625	0	655	6	0
50	Y	509	0	543	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Z	449	0	491	10	0
52	0	444	0	461	7	0
53	1	410	0	440	7	0
54	2	377	0	418	4	0
55	3	504	0	574	7	0
56	4	302	0	340	6	0
57	6	523	0	521	10	0
58	w	62	0	34	0	0
59	v	10	0	10	0	0
60	y	6	0	3	2	0
61	z	32	0	13	3	0
62	z	1	0	0	0	0
63	4	1	0	0	0	0
63	6	1	0	0	0	0
64	z	2	0	0	2	0
All	All	152991	0	104094	1391	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 (1391) 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)
26:A:279:A:N6	26:A:361:G:N3	2.04	1.05
26:A:2166:U:O2	26:A:2170:A:N6	2.08	0.85
13:m:91:ARG:HH22	26:A:887:U:H5'	1.48	0.77
1:a:414:A:N3	25:z:444:ARG:NH1	2.32	0.77
4:d:117:VAL:HG12	4:d:122:ILE:HG13	1.68	0.76
24:y:5:G:N2	24:y:68:C:O2	2.17	0.76
25:z:597:ARG:O	25:z:603:HIS:HA	1.87	0.75
36:K:35:VAL:HG21	36:K:69:VAL:HG12	1.69	0.74
2:b:86:CYS:SG	2:b:221:ARG:NH1	2.61	0.73
26:A:1072:C:OP1	26:A:1077:A:N6	2.23	0.72
1:a:1086:U:H3	1:a:1099:G:H22	1.34	0.72
11:k:87:GLY:H	11:k:113:THR:HG22	1.54	0.72
3:c:179:ALA:HB1	3:c:202:PHE:HE1	1.56	0.71
25:z:454:ASP:HB2	25:z:457:LEU:HD13	1.71	0.71
11:k:45:THR:O	11:k:68:ARG:NH2	2.23	0.70
47:V:32:GLY:O	47:V:93:ARG:NH2	2.24	0.70
39:N:35:LYS:NZ	39:N:110:MET:SD	2.64	0.70
1:a:180:U:O2	1:a:195:A:N7	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:y:16:C:N4	24:y:59:C:O2	2.23	0.70
4:d:124:VAL:HG12	4:d:142:VAL:HG23	1.72	0.69
1:a:527:G7M:O2'	1:a:535:A:N1	2.23	0.69
15:o:87:ARG:O	15:o:88:ARG:NH1	2.25	0.68
4:d:149:LYS:NZ	4:d:176:LYS:O	2.27	0.68
32:G:88:LEU:HG	32:G:161:VAL:HG22	1.74	0.68
8:h:103:VAL:HG12	8:h:124:ILE:HA	1.75	0.68
26:A:1250:G:N7	37:L:18:ARG:NH2	2.40	0.68
25:z:27:ARG:NH2	25:z:40:LEU:O	2.26	0.68
7:g:115:MET:SD	7:g:118:ARG:NH1	2.68	0.67
1:a:677:U:H3	1:a:713:G:H22	1.43	0.67
6:f:29:ILE:HD13	6:f:64:VAL:HG21	1.76	0.67
4:d:100:VAL:HG12	4:d:104:MET:HE2	1.77	0.67
1:a:375:U:OP1	16:p:70:ARG:NH1	2.28	0.66
24:y:20:G:O6	24:y:48:G:C2	2.48	0.66
26:A:585:G:N7	42:Q:5:ARG:NH1	2.43	0.66
1:a:979:C:OP1	1:a:1223:C:N4	2.29	0.66
25:z:281:TRP:N	25:z:297:VAL:O	2.29	0.66
26:A:2296:U:OP2	40:O:9:ARG:NH2	2.28	0.66
1:a:261:U:OP2	20:t:73:ARG:NH2	2.29	0.65
14:n:3:GLN:HA	14:n:6:LYS:HG2	1.77	0.65
15:o:88:ARG:NH2	26:A:714:U:OP2	2.30	0.65
18:r:36:GLY:O	18:r:62:ARG:NH2	2.29	0.65
25:z:380:LEU:HD21	25:z:410:LEU:HD13	1.77	0.65
1:a:1239:A:N6	1:a:1299:A:C2	2.65	0.65
25:z:8:HIS:O	25:z:13:LYS:NZ	2.30	0.65
25:z:406:ALA:HB3	25:z:457:LEU:HD12	1.79	0.65
7:g:149:ALA:HB3	11:k:55:ARG:HH11	1.61	0.65
26:A:1311:G:H21	26:A:1603:A:H62	1.43	0.65
1:a:437:U:O2	1:a:495:A:N7	2.30	0.64
43:R:48:LYS:NZ	43:R:49:ILE:O	2.30	0.64
57:6:28:VAL:HG11	57:6:32:LEU:HD23	1.79	0.64
1:a:1060:U:O2'	10:j:58:ASN:ND2	2.30	0.64
29:D:128:ARG:NH1	29:D:129:THR:O	2.30	0.64
33:I:32:VAL:HG23	33:I:60:VAL:HG13	1.79	0.64
24:y:20:G:N7	24:y:48:G:O6	2.31	0.64
26:A:956:G:N7	38:M:14:LYS:NZ	2.43	0.64
28:C:181:ARG:NH1	28:C:182:LYS:O	2.31	0.64
7:g:26:VAL:HG22	7:g:42:VAL:HG21	1.79	0.64
10:j:47:GLU:HB2	10:j:67:ILE:HB	1.80	0.64
26:A:994:C:OP1	42:Q:52:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1457:G:O2'	20:t:26:MET:SD	2.55	0.64
2:b:87:ASP:OD1	2:b:221:ARG:NH1	2.31	0.64
24:y:20:G:N7	24:y:48:G:C6	2.65	0.64
26:A:2848:G:O2'	26:A:2867:G:N2	2.31	0.64
26:A:850:U:OP1	51:Z:18:LYS:NZ	2.31	0.63
25:z:219:ARG:N	25:z:240:ASN:O	2.29	0.63
26:A:1454:C:OP1	39:N:63:ARG:NH2	2.31	0.63
9:i:114:LYS:HB2	9:i:117:LEU:HD11	1.80	0.63
1:a:50:A:O2'	1:a:360:G:N2	2.31	0.63
4:d:58:GLN:OE1	4:d:61:ARG:NH2	2.32	0.63
7:g:125:ASP:HB3	7:g:130:LYS:HB2	1.79	0.63
26:A:910:A:N3	26:A:2264:C:O2'	2.29	0.63
26:A:2743:U:OP2	26:A:2755:C:N4	2.32	0.63
26:A:2250:G:O2'	26:A:2496:C:OP1	2.16	0.63
4:d:144:ILE:HG12	4:d:177:MET:HE2	1.81	0.63
26:A:475:C:O2	26:A:479:A:N6	2.31	0.63
27:B:30:C:H1'	27:B:57:A:H61	1.64	0.63
40:O:50:ALA:O	40:O:81:ARG:NH2	2.32	0.63
1:a:977:A:N6	1:a:1224:U:O4'	2.31	0.62
2:b:82:ALA:HB2	2:b:213:LEU:HD13	1.81	0.62
24:y:30:G:OP2	24:y:32:C:N4	2.32	0.62
26:A:764:A:N3	28:C:211:ARG:NH1	2.47	0.62
6:f:3:HIS:ND1	6:f:65:GLU:OE2	2.33	0.62
27:B:48:U:OP1	40:O:30:ARG:NH2	2.31	0.62
1:a:780:A:N6	1:a:801:U:OP2	2.32	0.62
1:a:1394:A:N6	1:a:1500:A:O2'	2.33	0.62
3:c:39:ARG:HH21	3:c:56:ILE:HG12	1.63	0.62
24:y:47(F):C:O2	24:y:47(H):A:O2'	2.18	0.62
1:a:107:G:OP1	1:a:325:A:N6	2.33	0.62
1:a:1158:C:O2	1:a:1181:G:N2	2.31	0.62
31:F:31:GLU:OE2	31:F:158:THR:OG1	2.18	0.62
24:y:47(A):G:HO2'	25:z:281:TRP:NE1	1.98	0.62
31:F:101:ARG:NH1	57:6:9:TYR:OH	2.33	0.62
1:a:427:U:OP1	4:d:12:ARG:NH2	2.34	0.61
25:z:108:THR:OG1	25:z:160:HIS:NE2	2.31	0.61
1:a:405:U:OP2	4:d:2:ARG:NH1	2.31	0.61
26:A:516:C:OP1	52:0:9:ARG:NH1	2.33	0.61
29:D:37:VAL:HA	29:D:48:ILE:HG22	1.83	0.61
26:A:24:G:N2	44:S:78:GLU:OE2	2.34	0.61
26:A:961:C:OP1	26:A:2456:C:O2'	2.19	0.61
23:x:117:C:H3'	23:x:118:G:H8	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:97:SER:OG	29:D:99:GLU:OE1	2.18	0.61
1:a:717:U:O3'	11:k:118:ASN:ND2	2.34	0.61
26:A:545:U:O2	26:A:548:G:O6	2.19	0.61
26:A:2830:C:OP2	29:D:59:ARG:NH2	2.34	0.61
33:I:17:ALA:HB1	33:I:38:CYS:HA	1.81	0.61
11:k:58:THR:HG22	11:k:60:PHE:H	1.66	0.61
26:A:200:U:O2	26:A:386:G:N2	2.32	0.61
26:A:245:G:N7	55:3:7:ARG:NH2	2.48	0.61
35:J:105:VAL:HG12	35:J:109:LEU:HD23	1.83	0.61
1:a:766:A:OP2	1:a:812:G:N2	2.33	0.61
1:a:1095:U:OP1	1:a:1108:G:N2	2.28	0.61
31:F:177:ARG:O	57:6:47:LYS:NZ	2.33	0.61
43:R:69:GLY:O	43:R:90:ARG:NE	2.29	0.61
1:a:1178:G:N7	9:i:98:ARG:NH1	2.48	0.60
25:z:45:TRP:HB3	25:z:53:PRO:HG2	1.81	0.60
26:A:453:A:N3	26:A:457:A:O2'	2.34	0.60
26:A:1056:G:O2'	26:A:1103:A:N6	2.34	0.60
26:A:2334:U:O2'	40:O:13:ARG:NH2	2.34	0.60
6:f:3:HIS:HB2	6:f:92:THR:HA	1.83	0.60
1:a:512:U:OP1	4:d:43:ARG:NH1	2.34	0.60
26:A:908:C:OP2	38:M:22:GLN:NE2	2.34	0.60
26:A:1737:G:OP2	26:A:1737:G:N2	2.34	0.60
41:P:8:GLU:HG2	41:P:54:LEU:HD23	1.84	0.60
26:A:750:A:OP1	26:A:1615:C:N4	2.35	0.60
1:a:181:A:H61	1:a:194:C:H3'	1.67	0.60
1:a:686:U:O2'	1:a:703:G:N2	2.34	0.60
24:y:58:A:O2'	24:y:60:U:OP2	2.19	0.60
25:z:281:TRP:HA	25:z:297:VAL:O	2.01	0.60
32:G:21:GLN:NE2	32:G:37:ASN:O	2.35	0.60
28:C:182:LYS:NZ	28:C:264:LYS:O	2.34	0.60
1:a:501:C:OP1	12:l:120:ARG:NH2	2.35	0.60
14:n:85:GLU:OE2	14:n:89:ARG:NH1	2.35	0.60
26:A:877:A:O2'	26:A:900:A:N6	2.31	0.60
12:l:19:ASN:O	12:l:93:ARG:NH2	2.35	0.60
26:A:1753:G:N2	26:A:1756:G:OP2	2.34	0.60
24:y:10:C:O4'	24:y:44:U:O2'	2.20	0.59
1:a:373:A:O2'	1:a:451:A:N6	2.33	0.59
24:y:9:U:O4'	24:y:47(Q):G:N2	2.35	0.59
26:A:1000:A:OP2	26:A:1154:G:N1	2.32	0.59
25:z:31:GLU:HB3	25:z:38:ILE:HG22	1.84	0.59
25:z:82:VAL:O	25:z:111:LEU:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:771:G:OP2	54:2:11:LYS:NZ	2.35	0.59
26:A:959:A:N3	26:A:2457:PSU:O2'	2.32	0.59
26:A:2746:U:N3	26:A:2756:U:O4	2.34	0.59
26:A:1528:A:OP2	26:A:1543:G:N2	2.34	0.59
1:a:1320:C:O2	19:s:35:ARG:NH2	2.36	0.59
26:A:837:C:N3	26:A:941:A:N6	2.50	0.59
32:G:53:PRO:HG3	32:G:61:TRP:CE2	2.37	0.59
1:a:877:G:O2'	8:h:79:ARG:NH2	2.36	0.59
57:6:14:ALA:HB3	57:6:22:MET:HB2	1.84	0.59
53:1:16:THR:HG21	53:1:41:VAL:HG11	1.83	0.59
26:A:2303:G:HO2'	31:F:128:SER:HG	1.49	0.59
26:A:1997:C:OP2	29:D:128:ARG:NH1	2.35	0.59
26:A:2344:U:OP1	53:1:36:LYS:NZ	2.35	0.59
26:A:2576:G:O2'	26:A:2579:C:OP2	2.21	0.59
36:K:69:VAL:O	36:K:76:VAL:HA	2.03	0.59
1:a:297:G:N2	1:a:300:A:OP2	2.35	0.58
2:b:35:ASN:HB3	2:b:37:VAL:HG12	1.84	0.58
26:A:612:G:OP2	26:A:614:A:N6	2.36	0.58
26:A:1084:A:H2'	26:A:1085:A:C8	2.37	0.58
26:A:1392:A:N6	45:T:18:GLU:OE1	2.35	0.58
26:A:1666:G:HO2'	36:K:6:THR:HG1	1.51	0.58
2:b:116:LEU:HG	2:b:140:LEU:HD12	1.85	0.58
8:h:24:VAL:O	8:h:59:GLU:HA	2.03	0.58
25:z:98:ILE:HG23	25:z:322:VAL:HG11	1.85	0.58
26:A:2394:C:OP1	55:3:29:ARG:NH1	2.36	0.58
4:d:30:LYS:HE3	25:z:592:ARG:HB2	1.84	0.58
9:i:90:ASP:O	9:i:94:ARG:HB2	2.03	0.58
14:n:89:ARG:NE	14:n:91:GLU:OE2	2.37	0.58
26:A:807:U:O2'	26:A:2060:A:N1	2.37	0.58
43:R:63:VAL:HG12	43:R:96:VAL:HG12	1.85	0.58
17:q:29:LYS:HA	17:q:36:PHE:HA	1.85	0.58
26:A:2353:G:O2'	48:W:29:ALA:O	2.20	0.58
27:B:57:A:N3	31:F:26:GLN:NE2	2.52	0.58
25:z:218:VAL:HA	25:z:241:ILE:HG22	1.85	0.58
25:z:281:TRP:CA	25:z:297:VAL:O	2.52	0.58
32:G:4:ALA:HA	32:G:68:ARG:HE	1.67	0.58
1:a:351:G:OP1	20:t:2:ASN:ND2	2.37	0.58
1:a:723:U:O2	1:a:855:U:O2'	2.22	0.58
24:y:10:C:H2'	24:y:11:G:H8	1.67	0.58
2:b:71:THR:O	2:b:76:SER:OG	2.18	0.58
26:A:684:G:O2'	26:A:788:A:N7	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:61:TYR:HA	28:C:85:ASN:HD21	1.67	0.58
28:C:83:ASP:OD2	28:C:86:ARG:NH1	2.36	0.58
5:e:152:VAL:HG11	8:h:98:LEU:HD21	1.85	0.58
24:y:47(A):G:O2'	25:z:281:TRP:NE1	2.37	0.58
1:a:1297:G:O2'	7:g:113:LYS:NZ	2.36	0.57
26:A:1127:A:N7	26:A:2488:G:O2'	2.35	0.57
26:A:2742:G:OP1	56:4:36:ARG:NH1	2.37	0.57
9:i:27:ILE:HD12	9:i:34:LEU:HD13	1.86	0.57
26:A:956:G:N2	26:A:960:A:OP2	2.35	0.57
26:A:2520:C:O2'	26:A:2565:A:O2'	2.21	0.57
1:a:323:U:OP1	20:t:24:ARG:NH2	2.37	0.57
13:m:2:ARG:NH2	31:F:109:ARG:O	2.37	0.57
25:z:512:LEU:HB3	25:z:523:MET:HE2	1.85	0.57
25:z:523:MET:HE3	25:z:527:LEU:HD11	1.87	0.57
26:A:1288:G:OP2	26:A:1288:G:N2	2.32	0.57
51:Z:8:GLN:NE2	51:Z:10:ARG:O	2.36	0.57
26:A:63:A:O2'	45:T:77:ARG:NE	2.36	0.57
40:O:14:ALA:HA	40:O:17:LYS:HE3	1.87	0.57
1:a:148:G:O2'	1:a:1446:A:N3	2.34	0.57
24:y:65:U:O2'	25:z:326:ILE:O	2.19	0.57
26:A:1992:G:O2'	26:A:1997:C:N4	2.37	0.57
28:C:78:GLU:OE2	28:C:100:ARG:NH1	2.38	0.57
43:R:58:VAL:H	43:R:102:SER:HB2	1.70	0.57
9:i:37:TYR:HD2	9:i:38:PHE:HD1	1.52	0.57
26:A:298:G:O2'	26:A:322:A:N1	2.38	0.57
26:A:660:C:O2'	37:L:13:LYS:NZ	2.38	0.57
26:A:1068:G:N3	26:A:1095:A:O2'	2.37	0.57
3:c:131:ARG:NH2	23:x:114:C:O2'	2.37	0.57
14:n:32:ASP:O	14:n:40:ARG:NH2	2.37	0.57
25:z:221:LEU:HD13	25:z:231:ALA:HB2	1.86	0.57
26:A:2406:A:OP2	26:A:2411:A:N6	2.38	0.57
32:G:38:ASP:O	32:G:54:ARG:NH1	2.36	0.57
5:e:106:ALA:O	5:e:111:ARG:NH2	2.38	0.57
22:v:74:C:H42	26:A:2252:G:H1	1.50	0.57
35:J:49:ASP:OD1	35:J:121:LYS:NZ	2.38	0.57
15:o:84:LEU:HD23	15:o:86:LEU:HD23	1.86	0.57
26:A:1365:A:O2'	49:X:10:ARG:NH2	2.37	0.57
26:A:2051:A:N6	26:A:2614:A:O2'	2.38	0.57
1:a:977:A:OP1	14:n:60:ARG:NH2	2.37	0.56
26:A:1156:A:OP1	42:Q:54:ARG:NH1	2.38	0.56
26:A:2835:A:N6	26:A:2879:A:O4'	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:243:PRO:O	28:C:250:GLN:NE2	2.38	0.56
34:H:2:GLN:NE2	34:H:18:GLN:OE1	2.38	0.56
1:a:1005:A:N6	1:a:1024:G:O2'	2.38	0.56
26:A:536:G:H4'	42:Q:56:PHE:HZ	1.70	0.56
26:A:2788:C:O2'	26:A:2809:A:N3	2.32	0.56
41:P:47:ILE:HA	41:P:96:LEU:HD12	1.87	0.56
18:r:32:ILE:HD11	18:r:58:ILE:HD12	1.87	0.56
26:A:279:A:H61	26:A:361:G:H1'	1.69	0.56
26:A:301:G:OP2	46:U:81:ARG:NH1	2.38	0.56
26:A:545:U:O2	26:A:548:G:C6	2.59	0.56
45:T:80:TRP:HZ3	45:T:82:LYS:HB3	1.70	0.56
26:A:196:A:OP2	37:L:47:ARG:NH1	2.39	0.56
46:U:49:PRO:O	46:U:53:GLN:NE2	2.38	0.56
1:a:563:A:O2'	1:a:566:G:O3'	2.23	0.56
25:z:79:LEU:HD11	25:z:110:ALA:HB2	1.88	0.56
1:a:254:G:O2'	17:q:17:GLU:O	2.23	0.56
1:a:1077:G:N2	1:a:1080:A:OP2	2.33	0.56
26:A:2320:U:O2'	26:A:2333:A:N6	2.39	0.56
36:K:76:VAL:H	41:P:72:VAL:HG22	1.70	0.56
1:a:413:G:O3'	1:a:428:G:N2	2.38	0.56
26:A:1315:C:O2'	26:A:1392:A:N3	2.36	0.56
26:A:2522:U:O2'	26:A:2647:U:OP1	2.23	0.56
1:a:859:G:OP2	1:a:869:G:N1	2.33	0.56
6:f:42:TRP:HB2	6:f:59:TYR:HB2	1.88	0.56
24:y:7:C:O2'	24:y:49:G:O4'	2.23	0.56
29:D:8:LYS:NZ	29:D:195:GLY:O	2.35	0.56
29:D:32:ASN:OD1	29:D:52:THR:OG1	2.21	0.56
38:M:17:ASN:O	38:M:38:ARG:NH1	2.38	0.56
53:1:36:LYS:HB3	53:1:47:ILE:HD13	1.88	0.56
1:a:881:G:OP2	12:l:8:ARG:NH2	2.37	0.56
25:z:295:GLY:HA3	25:z:308:VAL:O	2.06	0.56
26:A:221:A:N1	26:A:265:A:O2'	2.35	0.56
5:e:14:LEU:HD21	5:e:17:VAL:HG23	1.88	0.56
16:p:6:LEU:HD22	16:p:17:TYR:HB3	1.87	0.56
35:J:73:VAL:HG12	35:J:88:THR:HG22	1.88	0.56
36:K:21:CYS:HA	36:K:41:ILE:HG22	1.88	0.56
11:k:110:THR:OG1	18:r:72:ARG:NH2	2.39	0.55
26:A:79:C:O2'	26:A:346:A:N3	2.38	0.55
26:A:1088:A:N6	33:I:134:SER:OG	2.39	0.55
26:A:1378:A:O2'	26:A:1380:G:OP2	2.23	0.55
1:a:1363:A:O2'	1:a:1365:G:N7	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:129:ARG:NH1	22:v:33:U:OP2	2.33	0.55
13:m:91:ARG:NH1	26:A:887:U:OP2	2.39	0.55
25:z:191:VAL:HA	25:z:240:ASN:HA	1.88	0.55
43:R:6:GLN:HE22	43:R:39:LEU:HD11	1.70	0.55
26:A:1807:G:N2	26:A:1810:A:OP2	2.38	0.55
51:Z:40:THR:HG22	51:Z:42:ALA:H	1.71	0.55
25:z:207:LEU:O	25:z:215:PRO:HA	2.07	0.55
28:C:132:ARG:NH1	28:C:186:ASP:OD1	2.35	0.55
8:h:12:ARG:NH1	8:h:25:THR:O	2.39	0.55
21:u:22:CYS:SG	21:u:23:GLU:N	2.79	0.55
25:z:538:ALA:HA	25:z:543:ARG:O	2.06	0.55
32:G:88:LEU:N	32:G:128:THR:O	2.33	0.55
40:O:53:THR:HG21	40:O:70:ALA:HB1	1.87	0.55
1:a:246:A:N1	1:a:278:G:O2'	2.38	0.55
25:z:446:ARG:HE	25:z:455:GLU:HA	1.70	0.55
26:A:1071:G:H1'	26:A:1089:A:H2'	1.88	0.55
31:F:56:LEU:HD22	31:F:64:PRO:HG3	1.88	0.55
1:a:417:G:O6	1:a:426:U:C4	2.59	0.55
2:b:71:THR:OG1	2:b:72:LYS:N	2.38	0.55
20:t:22:SER:O	20:t:25:SER:OG	2.24	0.55
26:A:491:G:O6	44:S:49:LYS:NZ	2.34	0.55
26:A:1437:C:HO2'	26:A:1516:G:HO2'	1.54	0.55
26:A:2419:U:OP1	55:3:40:LYS:NZ	2.40	0.55
28:C:32:LEU:HD13	28:C:63:ILE:HB	1.89	0.55
1:a:417:G:N1	1:a:426:U:N3	2.55	0.55
1:a:1073:U:O2	2:b:102:ASN:ND2	2.40	0.55
25:z:300:LEU:O	25:z:304:LEU:HB3	2.07	0.55
39:N:58:ASP:OD1	39:N:63:ARG:NE	2.38	0.55
3:c:6:PRO:O	3:c:10:ARG:NH1	2.40	0.55
49:X:6:VAL:HG21	49:X:58:ILE:HD11	1.89	0.55
4:d:98:ASP:HB3	4:d:132:ALA:HB1	1.89	0.55
13:m:91:ARG:NH2	26:A:888:C:O4'	2.40	0.55
26:A:298:G:N1	26:A:339:U:OP2	2.39	0.55
26:A:1153:C:OP1	42:Q:91:ARG:NH2	2.39	0.55
36:K:25:LEU:O	36:K:30:ARG:NH1	2.39	0.55
1:a:111:G:H1	1:a:330:C:H41	1.55	0.54
30:E:117:ARG:NH2	30:E:183:PHE:O	2.40	0.54
32:G:1:SER:OG	32:G:2:ARG:N	2.40	0.54
26:A:1869:G:N2	26:A:1872:A:OP2	2.40	0.54
1:a:1356:G:H2'	1:a:1357:A:C8	2.42	0.54
5:e:28:ARG:HH11	23:x:109:C:H41	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:z:130:LYS:HE3	25:z:143:LEU:HD22	1.89	0.54
1:a:619:U:O3'	4:d:127:ARG:NH2	2.40	0.54
25:z:222:HIS:HA	25:z:227:PRO:HA	1.90	0.54
26:A:743:A:O2'	26:A:1659:G:OP1	2.24	0.54
26:A:2172:U:OP1	26:A:2174:C:N4	2.39	0.54
32:G:26:LYS:NZ	32:G:27:GLY:O	2.38	0.54
33:I:64:ARG:NH1	33:I:65:SER:OG	2.40	0.54
45:T:40:LYS:HA	45:T:43:ILE:HG12	1.88	0.54
25:z:285:HIS:NE2	25:z:326:ILE:O	2.41	0.54
26:A:197:A:N6	26:A:2430:A:O2'	2.41	0.54
26:A:2469:A:O4'	38:M:55:ARG:NH1	2.40	0.54
28:C:16:VAL:HG12	28:C:203:VAL:HG22	1.90	0.54
1:a:1356:G:H2'	1:a:1357:A:H8	1.73	0.54
25:z:567:THR:HB	25:z:603:HIS:H	1.73	0.54
26:A:270:A:N1	26:A:369:U:O2'	2.40	0.54
1:a:981:U:O2'	14:n:60:ARG:NH1	2.40	0.54
1:a:1536:C:N4	23:x:94:U:O4	2.41	0.54
26:A:635:C:O2'	26:A:639:U:OP1	2.26	0.54
26:A:1798:U:OP2	28:C:270:ARG:NH2	2.41	0.54
9:i:59:LYS:HG3	9:i:60:LEU:HG	1.89	0.54
11:k:96:ILE:HD12	11:k:99:LEU:HD12	1.90	0.54
10:j:78:GLU:OE1	10:j:80:THR:OG1	2.25	0.54
26:A:27:G:O2'	26:A:512:G:N2	2.41	0.54
26:A:2530:A:N7	32:G:171:LYS:NZ	2.51	0.54
26:A:2636:C:O2'	29:D:45:TYR:OH	2.25	0.54
35:J:36:LEU:HD11	35:J:54:ILE:HG12	1.88	0.54
40:O:66:GLY:O	40:O:102:ARG:NH2	2.41	0.54
4:d:9:LYS:HA	4:d:12:ARG:HG2	1.90	0.54
29:D:131:ASP:O	29:D:136:ASN:ND2	2.41	0.54
47:V:47:VAL:HA	47:V:50:MET:HE2	1.89	0.54
18:r:50:TYR:O	18:r:54:LEU:HB2	2.08	0.53
26:A:2532:G:O2'	26:A:2657:A:N1	2.41	0.53
32:G:82:PHE:O	32:G:133:LYS:HA	2.08	0.53
12:l:19:ASN:OD1	12:l:93:ARG:NH2	2.41	0.53
25:z:270:VAL:HA	25:z:336:ARG:O	2.07	0.53
26:A:111:A:O2'	50:Y:58:ASN:ND2	2.35	0.53
35:J:16:TYR:HB2	35:J:54:ILE:HG22	1.89	0.53
7:g:149:ALA:HB1	11:k:58:THR:HG21	1.91	0.53
25:z:46:PRO:HA	25:z:52:VAL:HG22	1.90	0.53
26:A:2336:A:H61	48:W:39:THR:HG21	1.74	0.53
26:A:910:A:H62	38:M:12:MET:HA	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2136:G:N2	26:A:2156:G:O2'	2.42	0.53
30:E:105:LEU:HD11	30:E:200:LEU:HD21	1.90	0.53
1:a:792:A:O2'	1:a:794:A:N7	2.40	0.53
4:d:85:THR:O	4:d:89:LEU:CB	2.56	0.53
8:h:78:SER:OG	8:h:124:ILE:O	2.21	0.53
25:z:503:GLY:HA2	25:z:546:ARG:HD2	1.89	0.53
27:B:27:C:OP1	40:O:34:HIS:NE2	2.41	0.53
40:O:92:PHE:HB2	40:O:117:PHE:HD2	1.72	0.53
1:a:127:G:O2'	17:q:5:ARG:NH2	2.41	0.53
20:t:21:ALA:HA	20:t:24:ARG:HG2	1.91	0.53
26:A:415:A:O2'	26:A:1866:A:OP1	2.25	0.53
26:A:2107:G:N2	26:A:2182:U:O2'	2.41	0.53
26:A:2773:C:OP1	29:D:169:ARG:NH2	2.41	0.53
30:E:120:VAL:HG12	30:E:188:MET:HB2	1.91	0.53
1:a:739:C:HO2'	15:o:41:HIS:HD1	1.57	0.53
13:m:22:TYR:HB3	13:m:65:GLU:HG2	1.90	0.53
35:J:80:HIS:O	35:J:82:GLY:N	2.41	0.53
27:B:79:G:O6	47:V:14:LYS:NZ	2.32	0.53
10:j:13:PHE:O	10:j:70:HIS:ND1	2.38	0.53
23:x:126:G:H21	25:z:598:ARG:CZ	2.22	0.53
26:A:304:U:H3	26:A:313:G:H1	1.54	0.53
26:A:1682:G:OP2	26:A:1699:G:N2	2.42	0.53
26:A:1796:U:H2'	26:A:1797:G:H8	1.72	0.53
1:a:966:2MG:H3'	1:a:967:5MC:HM53	1.91	0.53
9:i:20:ILE:HG22	9:i:62:LEU:HG	1.91	0.53
26:A:571:U:O2'	26:A:573:U:OP2	2.27	0.53
26:A:1223:G:N2	26:A:1226:A:OP2	2.33	0.53
26:A:1942:C:OP2	26:A:1943:U:O2'	2.26	0.53
34:H:27:ARG:NH2	49:X:59:ASP:OD2	2.42	0.53
26:A:1802:A:H2'	26:A:1803:A:C8	2.44	0.52
1:a:933:G:N7	7:g:2:ARG:NH1	2.57	0.52
3:c:84:GLU:OE2	3:c:88:LYS:NZ	2.42	0.52
25:z:40:LEU:HG	25:z:58:VAL:HG12	1.90	0.52
26:A:1138:G:O2'	35:J:104:ALA:O	2.28	0.52
32:G:29:ASN:OD1	32:G:30:GLY:N	2.40	0.52
1:a:1015:G:N2	1:a:1218:C:O2	2.42	0.52
10:j:7:ARG:O	10:j:101:SER:OG	2.22	0.52
13:m:48:SER:OG	13:m:51:GLN:OE1	2.26	0.52
26:A:1065:U:O2	26:A:1066:U:O2'	2.22	0.52
26:A:2144:G:O2'	26:A:2147:A:N6	2.42	0.52
31:F:37:MET:HG3	31:F:56:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:34:C:H2'	1:a:35:G:H8	1.73	0.52
7:g:74:VAL:HG22	7:g:85:GLN:HB3	1.90	0.52
10:j:53:ILE:O	14:n:84:ARG:NH1	2.42	0.52
26:A:2140:G:N2	26:A:2152:G:N7	2.58	0.52
29:D:109:VAL:HG12	29:D:203:VAL:HG12	1.90	0.52
1:a:1157:A:OP1	1:a:1158:C:N4	2.43	0.52
26:A:349:U:H2'	26:A:350:G:H8	1.75	0.52
26:A:489:G:N2	26:A:1321:A:OP1	2.42	0.52
26:A:1614:A:N6	44:S:88:ARG:H	2.08	0.52
30:E:159:LEU:HA	30:E:162:ARG:HE	1.74	0.52
1:a:256:U:OP1	17:q:18:LYS:NZ	2.42	0.52
1:a:424:G:OP1	25:z:524:ARG:NH2	2.42	0.52
26:A:1998:A:OP2	29:D:141:ARG:NH1	2.40	0.52
26:A:2755:C:OP1	56:4:19:ARG:NH2	2.42	0.52
27:B:31:C:O2'	27:B:53:A:N1	2.36	0.52
51:Z:16:LEU:HD12	51:Z:17:PRO:HD2	1.91	0.52
1:a:1342:C:H2'	1:a:1343:G:C8	2.45	0.52
7:g:35:LYS:O	7:g:39:GLU:CB	2.58	0.52
26:A:253:C:OP2	55:3:4:LYS:NZ	2.36	0.52
27:B:95:U:OP2	47:V:19:ARG:NH2	2.43	0.52
32:G:87:GLN:HA	32:G:129:GLU:HA	1.90	0.52
17:q:46:HIS:HB2	17:q:70:LYS:HD3	1.91	0.52
26:A:1437:C:O2'	26:A:1516:G:O2'	2.25	0.52
31:F:46:LYS:HB2	31:F:47:LYS:HD2	1.91	0.52
38:M:47:GLU:OE1	38:M:51:ARG:NH1	2.43	0.52
44:S:25:ARG:NH2	44:S:74:ILE:O	2.41	0.52
1:a:1124:G:N2	1:a:1125:U:O4	2.43	0.52
14:n:39:ASP:O	14:n:43:ALA:HB2	2.10	0.52
26:A:1601:G:OP1	45:T:64:LYS:NZ	2.43	0.52
38:M:40:ARG:HG2	38:M:95:LEU:HA	1.91	0.52
7:g:34:LYS:HB3	7:g:37:THR:HG22	1.92	0.52
26:A:1496:A:N3	26:A:1577:C:O2'	2.39	0.52
26:A:2785:C:O3'	29:D:70:LYS:NZ	2.41	0.52
29:D:148:GLN:HB2	29:D:152:PRO:HG2	1.92	0.52
1:a:135:C:C2	16:p:1:MET:HE3	2.45	0.51
4:d:53:GLN:HG3	4:d:202:LEU:HD13	1.91	0.51
44:S:3:THR:HG21	44:S:58:ALA:HB2	1.90	0.51
48:W:66:GLU:HB3	48:W:68:LYS:HG2	1.91	0.51
3:c:163:ARG:NE	3:c:165:GLU:OE2	2.41	0.51
14:n:25:GLU:HA	14:n:28:ALA:HB3	1.92	0.51
24:y:52:G:H2'	24:y:53:G:C8	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:z:282:GLN:O	25:z:296:ARG:HA	2.10	0.51
26:A:566:U:H5''	37:L:29:LYS:HE3	1.92	0.51
1:a:8:A:N6	4:d:201:GLU:O	2.44	0.51
1:a:187:G:N2	1:a:190:A:OP2	2.37	0.51
5:e:61:LYS:HA	5:e:64:GLU:HG2	1.91	0.51
10:j:30:LYS:HA	10:j:34:ALA:HB2	1.92	0.51
26:A:84:A:N1	26:A:98:G:O2'	2.43	0.51
26:A:2817:U:OP1	39:N:42:LYS:NZ	2.39	0.51
28:C:153:LEU:HD23	28:C:175:LEU:HD21	1.92	0.51
1:a:219:U:H2'	1:a:220:G:H8	1.75	0.51
1:a:837:U:H2'	1:a:838:G:H8	1.75	0.51
1:a:1239:A:O2'	1:a:1297:G:N2	2.43	0.51
9:i:4:GLN:HE22	9:i:21:LYS:HE2	1.76	0.51
28:C:128:THR:HA	28:C:189:ALA:O	2.11	0.51
1:a:1522:U:OP1	11:k:127:ARG:NH2	2.43	0.51
7:g:35:LYS:O	7:g:39:GLU:HB2	2.10	0.51
20:t:81:GLN:HA	20:t:84:LYS:HG2	1.92	0.51
25:z:368:ALA:O	25:z:372:HIS:ND1	2.33	0.51
26:A:834:G:HO2'	26:A:2358:A:HO2'	1.48	0.51
26:A:1071:G:N3	26:A:1089:A:O2'	2.36	0.51
46:U:8:ASP:H	46:U:24:VAL:HG22	1.74	0.51
48:W:16:ARG:O	48:W:35:ARG:NH1	2.44	0.51
1:a:968:A:O2'	1:a:1061:G:O2'	2.27	0.51
2:b:184:ALA:HB3	2:b:195:VAL:HG21	1.93	0.51
3:c:188:ALA:HB3	3:c:195:ILE:HG23	1.93	0.51
5:e:62:ALA:O	5:e:66:ALA:HB2	2.10	0.51
26:A:77:G:OP1	50:Y:52:ARG:NH2	2.41	0.51
26:A:2202:U:O2'	26:A:2204:G:OP1	2.24	0.51
3:c:128:MET:HE3	3:c:131:ARG:H	1.76	0.51
10:j:54:SER:OG	10:j:56:HIS:O	2.29	0.51
26:A:1019:U:OP1	26:A:1035:U:O2'	2.21	0.51
45:T:19:LYS:NZ	45:T:84:TYR:OH	2.40	0.51
1:a:946:A:O2'	1:a:1333:A:N3	2.39	0.51
13:m:76:ILE:O	13:m:80:MET:HB2	2.10	0.51
26:A:2233:U:H2'	26:A:2234:G:C8	2.46	0.51
26:A:2857:G:N2	26:A:2860:A:OP2	2.36	0.51
33:I:74:PRO:HG2	33:I:77:VAL:HG22	1.93	0.51
44:S:30:SER:OG	44:S:31:GLN:OE1	2.29	0.51
15:o:58:MET:HA	15:o:61:GLN:HG2	1.93	0.51
25:z:9:VAL:HG21	25:z:61[A]:HIS:CE1	2.46	0.51
25:z:43:ALA:HB3	25:z:55:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:L:77:ILE:HD13	37:L:101:ILE:HD11	1.93	0.51
46:U:13:LEU:N	46:U:68:ASN:O	2.32	0.51
1:a:522:C:OP1	12:l:116:TYR:OH	2.27	0.51
1:a:499:A:O4'	1:a:547:A:N6	2.44	0.50
1:a:1239:A:O2'	7:g:113:LYS:O	2.24	0.50
24:y:66:G:H4'	25:z:292:HIS:HE1	1.75	0.50
26:A:28:A:O2'	42:Q:10:ARG:NH2	2.44	0.50
26:A:77:G:H5''	50:Y:2:LYS:HE2	1.94	0.50
38:M:71:LYS:HB3	38:M:93:VAL:O	2.11	0.50
56:4:11:CYS:SG	56:4:14:CYS:N	2.85	0.50
4:d:115:GLN:OE1	4:d:119:HIS:NE2	2.44	0.50
6:f:26:THR:HA	6:f:29:ILE:HD12	1.93	0.50
26:A:1889:A:N3	26:A:2086:U:O2'	2.37	0.50
26:A:2258:C:O2'	26:A:2427:C:OP2	2.22	0.50
26:A:2645:G:OP2	26:A:2645:G:N2	2.43	0.50
31:F:72:SER:OG	31:F:80:GLN:N	2.44	0.50
34:H:3:VAL:HA	34:H:38:PRO:HA	1.93	0.50
37:L:74:THR:HG22	37:L:107:PHE:HB2	1.93	0.50
45:T:65:GLY:O	45:T:76:ARG:NH1	2.43	0.50
53:1:41:VAL:HG13	53:1:42:VAL:HG23	1.93	0.50
7:g:67:ASN:O	7:g:137:ARG:NE	2.44	0.50
26:A:200:U:OP1	49:X:22:ASN:ND2	2.44	0.50
26:A:1961:C:H2'	26:A:1962:5MC:C2	2.46	0.50
26:A:2024:G:O3'	29:D:154:LYS:NZ	2.40	0.50
26:A:2237:G:O2'	26:A:2239:G:N7	2.43	0.50
26:A:2282:G:N2	26:A:2390:U:O2	2.43	0.50
31:F:43:ILE:HG12	31:F:78:ILE:HG22	1.93	0.50
39:N:56:LYS:NZ	39:N:87:PHE:O	2.44	0.50
39:N:103:ARG:HE	39:N:110:MET:HE3	1.76	0.50
53:1:24:LYS:NZ	53:1:50:GLU:OE1	2.42	0.50
1:a:38:G:N2	1:a:397:A:O5'	2.41	0.50
10:j:80:THR:HB	10:j:83:THR:HG23	1.93	0.50
26:A:564:C:O4'	42:Q:36:GLN:NE2	2.44	0.50
26:A:2031:A:N3	26:A:2455:G:O2'	2.41	0.50
25:z:69:LEU:HD13	25:z:287:HIS:HB3	1.93	0.50
26:A:2045:C:O2	52:0:18:HIS:NE2	2.45	0.50
1:a:123:U:OP1	1:a:311:C:O2'	2.30	0.50
13:m:53:ASP:OD1	13:m:56:ARG:NH1	2.44	0.50
26:A:1183:U:O3'	51:Z:29:ARG:NH2	2.44	0.50
1:a:436:C:O2'	4:d:153:ARG:NH2	2.43	0.50
1:a:1218:C:H2'	1:a:1219:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1229:A:O2'	22:v:30:G:OP1	2.29	0.50
2:b:112:ARG:O	2:b:116:LEU:CB	2.60	0.50
25:z:180:ASP:HB3	25:z:236:ARG:HH22	1.76	0.50
26:A:1011:G:OP1	42:Q:74:SER:OG	2.29	0.50
26:A:2199:A:O4'	34:H:28:ASN:ND2	2.44	0.50
29:D:10:GLY:H	29:D:197:THR:HG23	1.76	0.50
29:D:124:ARG:NH2	29:D:161:MET:O	2.41	0.50
46:U:15:GLY:O	46:U:18:LYS:NZ	2.39	0.50
56:4:9:LYS:HG3	56:4:14:CYS:HB2	1.94	0.50
1:a:642:A:N3	8:h:104:SER:OG	2.40	0.50
25:z:60:GLY:N	64:z:801:HOH:O	2.45	0.50
26:A:411:G:OP2	26:A:2406:A:O2'	2.26	0.50
26:A:861:A:N3	27:B:79:G:O2'	2.43	0.50
26:A:1664:A:H61	26:A:1996:C:H42	1.58	0.50
36:K:7:MET:HA	36:K:19:VAL:O	2.12	0.50
41:P:24:THR:HG22	41:P:87:ARG:HB3	1.94	0.50
1:a:745:G:OP1	1:a:851:G:O2'	2.29	0.50
4:d:7:LYS:HB3	4:d:20:LEU:HD13	1.93	0.50
19:s:20:LYS:HA	19:s:23:GLU:HG2	1.94	0.50
26:A:1478:G:H1	26:A:1513:U:H3	1.59	0.50
26:A:2108:A:H2'	26:A:2109:U:C6	2.46	0.50
29:D:4:LEU:HB2	29:D:32:ASN:HD22	1.76	0.50
40:O:35:ILE:HG22	40:O:66:GLY:HA2	1.93	0.50
24:y:72:C:N4	24:y:73:G:O6	2.45	0.49
26:A:581:C:H2'	26:A:582:A:H8	1.77	0.49
38:M:69:PRO:HA	38:M:94:ALA:HB2	1.94	0.49
50:Y:24:GLU:HB3	50:Y:46:VAL:HG21	1.94	0.49
55:3:31:ILE:O	55:3:35:LYS:NZ	2.34	0.49
1:a:377:G:H2'	1:a:378:G:H8	1.77	0.49
25:z:295:GLY:CA	25:z:308:VAL:O	2.60	0.49
25:z:578:VAL:HB	25:z:582:LEU:HD23	1.93	0.49
26:A:882:G:N3	26:A:896:A:N6	2.59	0.49
26:A:1128:G:N3	26:A:2516:A:O2'	2.37	0.49
3:c:19:SER:OG	3:c:39:ARG:NH2	2.41	0.49
6:f:12:PRO:O	6:f:44:ARG:NH2	2.45	0.49
10:j:36:VAL:HG23	10:j:76:ILE:HG22	1.95	0.49
37:L:128:THR:HG23	37:L:131:ALA:H	1.75	0.49
54:2:34:ARG:NE	54:2:42:LEU:O	2.45	0.49
3:c:19:SER:HB3	3:c:21:TRP:HE1	1.77	0.49
3:c:128:MET:HE3	3:c:130:ARG:HB3	1.94	0.49
9:i:30:ASN:OD1	9:i:65:THR:OG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:95:PRO:HG3	13:m:105:ALA:HB1	1.94	0.49
16:p:21:VAL:O	16:p:33:ILE:N	2.43	0.49
25:z:441:GLY:H	25:z:444:ARG:HH21	1.60	0.49
26:A:578:G:OP1	26:A:1255:U:O2'	2.30	0.49
26:A:1326:U:HO2'	26:A:2010:G:HO2'	1.58	0.49
26:A:1493:C:OP1	26:A:1495:A:N6	2.45	0.49
26:A:2600:A:H62	28:C:235:GLU:HG3	1.77	0.49
43:R:68:ARG:NH1	43:R:90:ARG:O	2.45	0.49
1:a:19:A:OP1	5:e:134:ASN:ND2	2.43	0.49
13:m:89:ARG:HB2	13:m:96:VAL:HG12	1.94	0.49
26:A:2178:C:O2'	26:A:2180:U:OP2	2.29	0.49
28:C:141:HIS:ND1	28:C:192:GLY:O	2.40	0.49
29:D:5:VAL:HG22	29:D:202:ILE:HG22	1.94	0.49
47:V:30:ILE:HG12	47:V:91:PHE:HB2	1.95	0.49
1:a:309:A:O2'	1:a:607:A:N1	2.42	0.49
1:a:417:G:O6	1:a:426:U:O4	2.31	0.49
1:a:981:U:O3'	14:n:62:ARG:NH2	2.44	0.49
26:A:1021:A:O2'	26:A:1123:C:OP1	2.28	0.49
26:A:2119:A:H61	26:A:2169:A:N6	2.10	0.49
1:a:520:A:H62	1:a:529:G:H21	1.61	0.49
1:a:1259:C:O2'	1:a:1283:U:O2	2.26	0.49
4:d:85:THR:O	4:d:89:LEU:HB2	2.13	0.49
11:k:19:VAL:HA	11:k:82:GLU:O	2.12	0.49
25:z:14:THR:N	61:z:701:GNP:O1B	2.45	0.49
31:F:25:MET:HG3	31:F:26:GLN:HE21	1.78	0.49
32:G:18:ILE:HD11	32:G:42:VAL:HG13	1.95	0.49
53:1:7:LYS:HA	53:1:23:THR:HA	1.94	0.49
1:a:128:G:H2'	1:a:129:A:C8	2.48	0.49
1:a:413:G:N2	1:a:429:U:OP2	2.46	0.49
24:y:26:G:H1	24:y:44:U:H3	1.60	0.49
24:y:47(A):G:HO2'	25:z:281:TRP:CD1	2.31	0.49
1:a:273:U:O4	1:a:274:A:N6	2.45	0.49
1:a:520:A:H62	1:a:529:G:N2	2.10	0.49
26:A:249:C:OP2	26:A:2394:C:O2'	2.27	0.49
26:A:355:U:H2'	26:A:356:G:H8	1.78	0.49
26:A:478:A:N6	26:A:500:G:O2'	2.46	0.49
26:A:1636:U:H2'	26:A:1637:A:C8	2.48	0.49
29:D:101:PHE:HB2	29:D:180:VAL:HG23	1.94	0.49
1:a:968:A:HO2'	1:a:1061:G:HO2'	1.56	0.49
10:j:80:THR:O	10:j:83:THR:OG1	2.23	0.49
13:m:12:LYS:HZ1	13:m:44:ILE:HG12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:34:GLU:OE2	16:p:60:TRP:NE1	2.46	0.49
25:z:20:ILE:HG12	25:z:154:MET:HE1	1.94	0.49
26:A:688:U:H2'	26:A:689:A:H8	1.78	0.49
30:E:95:LYS:NZ	30:E:97:ASN:OD1	2.46	0.49
30:E:148:ILE:HB	30:E:169:VAL:HG22	1.95	0.49
32:G:132:LEU:HD13	32:G:143:VAL:HG23	1.94	0.49
6:f:23:GLU:HA	6:f:26:THR:HG22	1.95	0.48
26:A:1527:G:N1	26:A:1544:A:OP2	2.38	0.48
26:A:2482:A:H61	38:M:55:ARG:HH12	1.59	0.48
26:A:2655:G:O2'	26:A:2664:G:O6	2.30	0.48
26:A:1085:A:H2'	26:A:1086:A:O4'	2.13	0.48
45:T:12:ARG:HA	50:Y:29:ARG:HH22	1.78	0.48
25:z:348:ARG:HG3	25:z:350:PRO:HD2	1.95	0.48
25:z:466:ARG:HH22	25:z:473:SER:HB3	1.79	0.48
26:A:1011:G:OP2	42:Q:65:ASN:ND2	2.47	0.48
34:H:100:ALA:HB2	34:H:112:LYS:HD3	1.95	0.48
11:k:65:ALA:O	11:k:69:CYS:HB2	2.13	0.48
25:z:465:MET:O	25:z:468:SER:OG	2.28	0.48
37:L:95:LEU:HD22	37:L:100:ILE:HD11	1.95	0.48
38:M:17:ASN:OD1	38:M:97:GLN:NE2	2.46	0.48
1:a:1412:C:H2'	1:a:1413:A:C8	2.49	0.48
1:a:195:A:H2'	1:a:196:A:C4	2.48	0.48
1:a:1116:U:O2'	9:i:109:GLN:NE2	2.46	0.48
3:c:87:ARG:HA	3:c:90:VAL:HG22	1.95	0.48
25:z:590:PHE:HB3	25:z:595:PHE:HB3	1.95	0.48
26:A:1681:G:H21	26:A:1762:A:H3'	1.78	0.48
28:C:132:ARG:O	28:C:166:ARG:NH1	2.41	0.48
31:F:28:PRO:HB2	31:F:168:LEU:HD22	1.96	0.48
32:G:86:LEU:HD22	32:G:130:ILE:HD11	1.95	0.48
38:M:30:SER:N	38:M:106:ASP:OD1	2.45	0.48
4:d:18:LEU:HD23	4:d:20:LEU:HD11	1.95	0.48
18:r:53:GLN:HA	18:r:56:ARG:HG2	1.96	0.48
26:A:2579:C:O3'	29:D:137:SER:OG	2.30	0.48
1:a:1232:U:H3'	9:i:125:GLN:HE21	1.78	0.48
1:a:1297:G:N2	7:g:113:LYS:O	2.47	0.48
1:a:1414:U:H2'	1:a:1415:G:H8	1.77	0.48
2:b:120:SER:OG	2:b:121:GLN:N	2.47	0.48
2:b:158:ASP:OD1	2:b:159:ALA:N	2.47	0.48
34:H:30:LEU:HD23	34:H:36:ALA:HB3	1.96	0.48
37:L:75:ALA:O	37:L:108:ALA:HA	2.14	0.48
1:a:350:G:H2'	1:a:351:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1071:C:H2'	1:a:1072:G:C8	2.49	0.48
3:c:117:ASP:HA	3:c:120:THR:HG22	1.95	0.48
13:m:65:GLU:O	13:m:69:ARG:HG3	2.14	0.48
25:z:566:SER:HG	25:z:602:ASP:CG	2.18	0.48
26:A:488:G:O2'	26:A:491:G:O6	2.32	0.48
26:A:1386:C:H2'	26:A:1387:A:H8	1.79	0.48
26:A:2199:A:OP1	49:X:36:ARG:NH2	2.47	0.48
30:E:112:LEU:HB3	30:E:118:LEU:HB2	1.96	0.48
1:a:1178:G:N2	1:a:1181:G:OP2	2.47	0.48
61:z:701:GNP:O3G	64:z:801:HOH:O	2.20	0.48
26:A:1673:G:N2	26:A:1675:C:O4'	2.47	0.48
1:a:235:C:H2'	1:a:236:A:H8	1.78	0.47
3:c:84:GLU:OE2	3:c:87:ARG:NH2	2.39	0.47
12:l:37:TYR:HE1	12:l:53:ARG:HG2	1.79	0.47
13:m:3:ILE:HD11	13:m:7:ASN:HD22	1.79	0.47
25:z:224:GLN:HE21	25:z:235:GLN:HB2	1.79	0.47
26:A:1259:G:H2'	26:A:1260:A:H8	1.79	0.47
1:a:672:U:H2'	1:a:673:A:H8	1.79	0.47
2:b:87:ASP:H	2:b:221:ARG:HH12	1.61	0.47
26:A:2759:G:H1'	32:G:34:ARG:HH22	1.79	0.47
26:A:2849:U:OP1	41:P:92:ARG:NH2	2.47	0.47
1:a:130:A:OP1	17:q:64:ARG:NH1	2.46	0.47
1:a:717:U:O2'	1:a:734:G:O4'	2.24	0.47
1:a:1156:G:O2'	1:a:1180:A:N1	2.48	0.47
16:p:26:ASN:ND2	16:p:31:ARG:O	2.47	0.47
26:A:196:A:H61	26:A:831:G:H21	1.62	0.47
26:A:1070:A:OP2	26:A:1077:A:N6	2.40	0.47
26:A:1079:C:N3	33:I:131:THR:OG1	2.48	0.47
46:U:46:LYS:HD2	46:U:47:PRO:HD2	1.96	0.47
22:v:50:U:H2'	22:v:51:C:C6	2.48	0.47
26:A:1323:C:N4	26:A:1324:G:O6	2.48	0.47
45:T:51:PHE:O	45:T:92:ASN:ND2	2.47	0.47
9:i:16:ALA:HA	9:i:66:VAL:HG12	1.95	0.47
11:k:127:ARG:HA	21:u:34:ARG:HH21	1.79	0.47
17:q:26:ARG:HH21	17:q:28:VAL:HG11	1.80	0.47
26:A:1312:U:O2'	26:A:1314:C:N4	2.46	0.47
26:A:1818:U:O2'	28:C:152:GLN:O	2.28	0.47
45:T:54:GLU:HG3	45:T:88:LYS:HE2	1.96	0.47
1:a:796:C:OP1	11:k:127:ARG:N	2.41	0.47
2:b:129:THR:HB	2:b:132:GLU:HG2	1.97	0.47
26:A:32:C:N4	26:A:447:A:OP2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1915:3TD:H3'	26:A:1916:A:H8	1.80	0.47
41:P:1:SER:OG	41:P:2:ASN:N	2.48	0.47
48:W:33:ILE:HG22	48:W:34:VAL:HG23	1.96	0.47
2:b:180:ILE:HD12	2:b:181:PRO:HD2	1.97	0.47
7:g:106:ALA:HB2	7:g:133:ALA:HB2	1.97	0.47
13:m:106:ARG:HA	13:m:109:LYS:HB3	1.95	0.47
25:z:571:ASP:HA	25:z:574:ASP:HB2	1.96	0.47
26:A:577:G:H2'	26:A:578:G:C8	2.50	0.47
26:A:1057:A:H2	33:I:117:THR:HG21	1.79	0.47
26:A:1715:G:O2'	26:A:1743:G:O6	2.28	0.47
26:A:1796:U:H2'	26:A:1797:G:C8	2.50	0.47
26:A:1799:G:OP2	26:A:1819:A:N6	2.44	0.47
26:A:1995:U:O2	36:K:32:TYR:OH	2.31	0.47
26:A:2052:A:O2'	29:D:149:ASN:O	2.31	0.47
26:A:2796:U:O2'	26:A:2798:U:OP2	2.33	0.47
35:J:8:PRO:HG3	35:J:48:VAL:HG23	1.96	0.47
12:l:98:ARG:HB2	12:l:116:TYR:HA	1.96	0.47
26:A:1853:A:N3	26:A:2233:U:O2'	2.40	0.47
26:A:2032:G:O2'	29:D:150:GLN:NE2	2.48	0.47
28:C:184:GLU:HG3	28:C:186:ASP:H	1.80	0.47
29:D:4:LEU:HB2	29:D:32:ASN:ND2	2.30	0.47
30:E:112:LEU:O	30:E:118:LEU:N	2.44	0.47
45:T:11:LEU:O	50:Y:29:ARG:NH1	2.38	0.47
46:U:35:VAL:HB	46:U:38:ILE:HG13	1.97	0.47
1:a:54:C:H2'	1:a:352:C:H41	1.79	0.47
1:a:776:G:N2	1:a:802:A:OP2	2.46	0.47
1:a:1425:U:H2'	1:a:1426:G:H8	1.80	0.47
4:d:60:VAL:HA	4:d:63:ILE:HG22	1.97	0.47
25:z:122:VAL:HG13	25:z:145:ILE:HG21	1.95	0.47
26:A:355:U:H2'	26:A:356:G:C8	2.50	0.47
26:A:818:G:H21	26:A:1189:A:H62	1.62	0.47
32:G:88:LEU:HA	32:G:161:VAL:HA	1.96	0.47
1:a:405:U:H3'	4:d:4:LEU:HD21	1.96	0.47
25:z:1:MET:N	25:z:51:ARG:HE	2.12	0.47
26:A:927:A:H2'	26:A:928:A:C8	2.49	0.47
28:C:179:GLU:HG3	28:C:269:ARG:HA	1.97	0.47
45:T:24:MET:HE1	45:T:30:ILE:HA	1.95	0.47
6:f:73:GLU:O	6:f:76:THR:OG1	2.26	0.46
26:A:2899:A:H2'	26:A:2900:A:C8	2.50	0.46
53:1:10:LEU:HG	53:1:48:TYR:HB3	1.97	0.46
1:a:447:G:N1	1:a:486:U:OP1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1308:U:H2'	1:a:1309:G:H8	1.80	0.46
18:r:50:TYR:O	18:r:54:LEU:CB	2.63	0.46
25:z:267:ARG:NH2	25:z:306:GLU:OE2	2.49	0.46
25:z:559:ASP:O	25:z:563:GLU:HB2	2.16	0.46
26:A:572:A:OP2	43:R:80:ARG:NH1	2.46	0.46
26:A:1063:G:O6	26:A:1076:C:O2'	2.20	0.46
26:A:1266:G:O2'	26:A:2012:G:O6	2.32	0.46
26:A:1715:G:H1'	26:A:1716:U:H5	1.81	0.46
30:E:118:LEU:HD11	30:E:188:MET:HG2	1.97	0.46
43:R:38:VAL:HG13	43:R:54:VAL:HG12	1.97	0.46
26:A:558:U:H2'	26:A:559:G:C8	2.51	0.46
36:K:68:GLY:HA2	36:K:77:ILE:O	2.15	0.46
51:Z:17:PRO:HA	51:Z:20:LYS:HG2	1.96	0.46
1:a:216:U:H2'	1:a:217:C:C6	2.50	0.46
1:a:570:G:O3'	1:a:819:A:O2'	2.33	0.46
4:d:131:ILE:HG22	4:d:133:SER:H	1.81	0.46
16:p:44:SER:OG	16:p:45:GLU:N	2.39	0.46
26:A:488:G:N1	26:A:491:G:OP2	2.48	0.46
1:a:750:C:O2'	15:o:20:ASP:OD1	2.34	0.46
16:p:6:LEU:HD23	16:p:19:VAL:HB	1.97	0.46
24:y:65:U:OP2	25:z:63:LYS:NZ	2.48	0.46
60:y:701:SEC:SE	25:z:224:GLN:HA	2.65	0.46
25:z:40:LEU:HD11	25:z:68:MET:HA	1.97	0.46
26:A:2246:G:H2'	26:A:2247:A:H8	1.81	0.46
26:A:2500:U:O2'	26:A:2504:PSU:OP1	2.33	0.46
1:a:147:G:H2'	1:a:148:G:C8	2.51	0.46
1:a:362:G:N2	1:a:365:U:OP2	2.36	0.46
3:c:131:ARG:NH1	23:x:116:U:O3'	2.45	0.46
7:g:68:VAL:HG21	7:g:133:ALA:HB1	1.96	0.46
14:n:9:GLU:HA	14:n:12:ARG:HG2	1.98	0.46
1:a:898:G:N2	1:a:901:A:OP2	2.46	0.46
18:r:19:GLU:OE2	18:r:53:GLN:NE2	2.34	0.46
26:A:265:A:N1	26:A:427:U:O2'	2.40	0.46
26:A:1227:G:OP2	42:Q:15:LYS:NZ	2.43	0.46
1:a:203:G:N2	1:a:204:G:O6	2.47	0.46
1:a:321:A:H2'	1:a:322:C:C6	2.51	0.46
1:a:967:5MC:HM52	1:a:968:A:H62	1.81	0.46
1:a:980:C:H1'	14:n:58:ARG:HE	1.81	0.46
1:a:1074:G:O2'	2:b:101:THR:OG1	2.30	0.46
13:m:71:GLU:HA	13:m:74:MET:HG2	1.96	0.46
26:A:6:A:H2'	26:A:7:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:629:G:N3	26:A:639:U:O2'	2.47	0.46
26:A:1469:A:H2'	26:A:1470:A:H8	1.80	0.46
28:C:169:ALA:O	28:C:185:ALA:N	2.46	0.46
34:H:99:ILE:HD11	34:H:144:VAL:HG21	1.97	0.46
1:a:647:C:H2'	1:a:648:A:H8	1.81	0.46
1:a:1373:G:H5''	7:g:35:LYS:HE2	1.98	0.46
25:z:109:VAL:HG11	25:z:129:VAL:HG11	1.97	0.46
26:A:881:G:N2	26:A:896:A:N7	2.64	0.46
26:A:2022:U:O2	26:A:2616:C:O2'	2.33	0.46
1:a:210:C:O2'	1:a:211:G:N2	2.49	0.46
1:a:452:A:H8	16:p:70:ARG:HH12	1.63	0.46
20:t:20:ASN:OD1	20:t:21:ALA:N	2.49	0.46
25:z:200:GLU:HA	25:z:231:ALA:O	2.16	0.46
26:A:581:C:H2'	26:A:582:A:C8	2.50	0.46
26:A:1615:C:OP2	26:A:1617:C:N4	2.37	0.46
46:U:24:VAL:HA	46:U:35:VAL:HG22	1.97	0.46
46:U:95:PHE:HB2	46:U:99:SER:HA	1.98	0.46
3:c:139:ASN:OD1	3:c:142:ARG:NH2	2.49	0.45
13:m:68:LEU:HA	13:m:71:GLU:HG2	1.98	0.45
24:y:8:G:H21	24:y:48:G:H21	1.64	0.45
25:z:177:LEU:HB3	25:z:256:LEU:HB2	1.98	0.45
26:A:1907:G:O6	26:A:1924:C:N4	2.49	0.45
36:K:1:MET:HA	36:K:32:TYR:HB3	1.98	0.45
10:j:42:LEU:HD22	10:j:71:LEU:HD22	1.98	0.45
24:y:47(B):G:H5'	25:z:281:TRP:CD2	2.51	0.45
26:A:155:A:H2'	26:A:156:A:H8	1.81	0.45
26:A:177:G:OP2	26:A:177:G:N2	2.34	0.45
26:A:279:A:H62	26:A:361:G:N2	2.13	0.45
26:A:516:C:HO2'	26:A:1261:C:HO2'	1.59	0.45
26:A:594:U:H2'	26:A:595:C:C6	2.51	0.45
26:A:1469:A:H2'	26:A:1470:A:C8	2.51	0.45
26:A:2229:U:H2'	26:A:2230:G:H8	1.81	0.45
26:A:2446:G:N7	26:A:2501:C:O2'	2.48	0.45
1:a:1068:G:N7	1:a:1094:G:O2'	2.41	0.45
26:A:200:U:H5'	49:X:22:ASN:HD22	1.81	0.45
26:A:850:U:H5''	51:Z:18:LYS:HG3	1.99	0.45
26:A:993:G:H1'	43:R:91:GLN:HE21	1.81	0.45
29:D:49:GLN:HB3	29:D:81:GLU:HB3	1.99	0.45
43:R:60:LYS:HB2	43:R:99:THR:O	2.16	0.45
1:a:1100:C:O2'	1:a:1102:A:OP1	2.27	0.45
26:A:819:A:OP2	26:A:1187:G:N2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:832:U:H2'	26:A:833:A:C8	2.52	0.45
33:I:38:CYS:SG	33:I:39:LYS:N	2.89	0.45
38:M:17:ASN:ND2	38:M:96:ILE:O	2.44	0.45
51:Z:39:ASP:OD2	51:Z:44:ARG:NH1	2.49	0.45
1:a:417:G:C6	1:a:426:U:N3	2.85	0.45
1:a:423:G:O2'	25:z:520:GLU:OE1	2.32	0.45
1:a:1181:G:O2'	1:a:1182:G:N7	2.47	0.45
25:z:111:LEU:HB2	25:z:145:ILE:HA	1.98	0.45
25:z:150:GLU:OE1	25:z:152:ARG:NH2	2.50	0.45
36:K:24:VAL:HA	36:K:39:ILE:HG22	1.99	0.45
37:L:63:LYS:HA	55:3:12:ARG:HG2	1.97	0.45
1:a:404:G:O2'	1:a:498:A:N1	2.34	0.45
1:a:489:C:H2'	1:a:490:C:H6	1.81	0.45
1:a:555:U:H2'	1:a:556:C:C6	2.52	0.45
1:a:1477:U:H2'	1:a:1478:U:C6	2.52	0.45
7:g:46:LEU:HD21	7:g:57:GLU:HG3	1.97	0.45
17:q:12:VAL:HB	17:q:21:VAL:HG13	1.99	0.45
26:A:546:U:H1'	26:A:548:G:C6	2.51	0.45
26:A:1047:G:N2	26:A:1110:G:O2'	2.48	0.45
26:A:1264:A:N6	26:A:2014:A:OP2	2.46	0.45
26:A:1316:U:H2'	26:A:1317:G:C8	2.52	0.45
26:A:1506:U:H2'	26:A:1507:C:C6	2.52	0.45
26:A:2519:U:O4'	26:A:2542:A:N6	2.50	0.45
31:F:57:ALA:HB2	31:F:64:PRO:HD3	1.99	0.45
1:a:739:C:O2'	15:o:41:HIS:ND1	2.47	0.45
1:a:746:A:H2'	1:a:747:A:C8	2.51	0.45
22:v:1:C:N4	22:v:2:G:O6	2.49	0.45
26:A:971:G:OP1	26:A:989:G:N1	2.43	0.45
27:B:43:C:OP1	57:6:2:LYS:N	2.44	0.45
36:K:64:ARG:HB2	36:K:83:ALA:HB3	1.99	0.45
38:M:42:THR:HA	38:M:93:VAL:HA	1.99	0.45
1:a:266:G:H3'	17:q:68:LYS:HB2	1.98	0.45
2:b:112:ARG:O	2:b:116:LEU:HB2	2.17	0.45
13:m:52:ILE:HG23	13:m:56:ARG:HH12	1.82	0.45
21:u:11:PHE:O	21:u:14:ALA:HB3	2.17	0.45
25:z:80:LEU:HD23	25:z:92:THR:HG23	1.99	0.45
26:A:1769:U:H2'	26:A:1770:G:H8	1.82	0.45
26:A:2250:G:H21	26:A:2497:A:P	2.40	0.45
31:F:64:PRO:HA	31:F:88:VAL:HG23	1.98	0.45
41:P:24:THR:HA	41:P:45:VAL:HA	1.99	0.45
4:d:11:SER:HB2	4:d:20:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:y:19:H2U:H2'	24:y:19:H2U:H61	1.68	0.45
25:z:518:THR:OG1	25:z:523:MET:SD	2.72	0.45
26:A:2140:G:H2'	26:A:2141:G:C8	2.52	0.45
26:A:2375:G:N2	26:A:2378:A:OP2	2.45	0.45
45:T:92:ASN:OD1	45:T:93:LEU:N	2.49	0.45
1:a:35:G:O2'	12:l:114:SER:O	2.34	0.45
1:a:187:G:H5'	20:t:79:THR:HG21	1.99	0.45
25:z:255:TRP:HB3	25:z:257:LEU:HD23	1.99	0.45
25:z:466:ARG:HH12	25:z:478:LEU:HG	1.82	0.45
26:A:1278:C:H2'	26:A:1279:G:H8	1.82	0.45
26:A:1934:C:H2'	26:A:1935:G:C8	2.51	0.45
26:A:1935:G:N2	26:A:1964:G:O4'	2.49	0.45
39:N:49:GLU:HA	39:N:52:ILE:HG22	1.98	0.45
46:U:11:ILE:HG22	46:U:21:ARG:HB3	1.99	0.45
2:b:95:TRP:CZ2	2:b:99:MET:HB2	2.52	0.44
4:d:78:ALA:HB2	4:d:89:LEU:HD13	1.99	0.44
8:h:102:VAL:HG12	8:h:125:ILE:HD12	1.98	0.44
27:B:9:G:OP2	40:O:15:ARG:NH2	2.49	0.44
32:G:3:VAL:HG22	32:G:68:ARG:HH21	1.81	0.44
32:G:153:PRO:HB2	32:G:168:VAL:HG11	1.99	0.44
33:I:102:ARG:NH2	33:I:141:ASP:OD1	2.40	0.44
55:3:31:ILE:HG21	55:3:34:LYS:HD3	1.99	0.44
1:a:514:C:H2'	1:a:515:G:H8	1.83	0.44
1:a:518:C:O2'	1:a:530:G:N2	2.50	0.44
1:a:1078:U:H4'	5:e:137:ARG:HH12	1.82	0.44
2:b:115:ASP:OD1	2:b:116:LEU:N	2.50	0.44
20:t:17:ARG:O	20:t:21:ALA:HB3	2.18	0.44
26:A:2595:G:N2	26:A:2598:A:OP2	2.45	0.44
29:D:121:THR:HG21	29:D:143:PRO:HB3	1.99	0.44
30:E:146:VAL:HG12	30:E:185:LYS:HB2	1.99	0.44
45:T:6:ARG:NH2	45:T:37:ASP:OD2	2.50	0.44
47:V:35:GLU:HB2	47:V:93:ARG:NH2	2.32	0.44
1:a:151:A:OP2	1:a:169:C:N4	2.50	0.44
1:a:967:5MC:H3'	1:a:968:A:C8	2.52	0.44
1:a:1237:C:O2'	1:a:1300:G:N1	2.44	0.44
2:b:23:ASN:ND2	2:b:190:SER:O	2.48	0.44
6:f:15:SER:O	6:f:18:VAL:HG12	2.17	0.44
6:f:36:ILE:HA	6:f:64:VAL:HG23	1.98	0.44
8:h:32:LYS:O	8:h:36:ALA:HB2	2.17	0.44
13:m:51:GLN:O	13:m:54:THR:OG1	2.28	0.44
26:A:281:C:H2'	26:A:282:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:833:A:H2'	26:A:834:G:C8	2.53	0.44
26:A:2291:U:H2'	26:A:2292:U:C6	2.53	0.44
26:A:2581:G:H22	26:A:2610:C:H2'	1.82	0.44
46:U:82:VAL:O	46:U:96:LYS:NZ	2.50	0.44
1:a:217:C:H2'	1:a:218:U:C6	2.52	0.44
1:a:601:G:H2'	1:a:602:A:H8	1.81	0.44
1:a:1497:G:H21	1:a:1519:MA6:H2	1.83	0.44
15:o:55:LEU:HA	15:o:58:MET:HG2	2.00	0.44
25:z:411:LEU:HD21	25:z:419:TRP:CD1	2.52	0.44
26:A:345:A:O2'	26:A:347:A:N6	2.42	0.44
26:A:833:A:H2'	26:A:834:G:H8	1.82	0.44
26:A:848:C:H2'	26:A:849:A:H8	1.82	0.44
26:A:1395:A:O2'	26:A:1397:U:OP2	2.35	0.44
26:A:1432:G:H2'	26:A:1433:A:C8	2.51	0.44
26:A:1704:C:H2'	26:A:1705:A:H8	1.82	0.44
38:M:29:GLY:H	38:M:104:GLU:HG3	1.82	0.44
52:0:33:SER:OG	52:0:35:GLU:OE1	2.28	0.44
25:z:554:ALA:O	25:z:558:ARG:HG3	2.17	0.44
26:A:1003:G:O2'	26:A:1010:A:N1	2.48	0.44
26:A:1023:U:OP2	26:A:1025:G:O2'	2.36	0.44
26:A:1167:C:H2'	26:A:1168:G:C8	2.53	0.44
26:A:1434:A:H2'	26:A:1435:G:C8	2.52	0.44
26:A:1563:U:H2'	26:A:1564:C:C6	2.52	0.44
29:D:179:ARG:HB3	29:D:188:LEU:HB2	2.00	0.44
36:K:43:ILE:HD11	36:K:54:LYS:HA	1.99	0.44
1:a:201:G:H1	1:a:216:U:H3	1.65	0.44
1:a:202:G:O2'	1:a:468:A:N3	2.37	0.44
26:A:516:C:O2'	26:A:1261:C:O2'	2.31	0.44
26:A:918:A:N3	27:B:80:U:O2'	2.46	0.44
26:A:2057:G:H2'	26:A:2058:A:H8	1.81	0.44
26:A:2303:G:O2'	31:F:128:SER:OG	2.23	0.44
26:A:2443:C:H2'	26:A:2444:G:H8	1.83	0.44
35:J:37:ARG:HD3	35:J:39:LYS:HD2	1.98	0.44
50:Y:8:GLU:OE1	50:Y:12:GLU:HB2	2.18	0.44
1:a:745:G:O3'	1:a:836:G:N2	2.49	0.44
9:i:64:ILE:HD12	9:i:78:ILE:HG12	2.00	0.44
19:s:11:ASP:OD1	19:s:37:SER:OG	2.35	0.44
24:y:37:6IA:H163	24:y:37:6IA:H121	1.84	0.44
27:B:12:C:O2'	48:W:70:PRO:O	2.34	0.44
28:C:76:VAL:HG12	28:C:114:GLN:HG3	1.99	0.44
28:C:268:ARG:NH2	28:C:271:SER:OG	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:G:89:VAL:HG21	32:G:162:ARG:NH1	2.33	0.44
39:N:79:LEU:HA	39:N:83:LEU:HB2	1.99	0.44
3:c:112:ALA:HA	3:c:115:VAL:HG22	1.98	0.44
4:d:169:TRP:O	4:d:182:LYS:HB3	2.18	0.44
12:l:30:ARG:HA	12:l:80:LEU:HA	1.99	0.44
24:y:47(A):G:H2'	24:y:47(B):G:C8	2.53	0.44
26:A:514:A:N3	26:A:581:C:O2'	2.49	0.44
26:A:1571:A:H2'	26:A:1572:A:C8	2.53	0.44
1:a:946:A:H2'	1:a:947:G:H8	1.83	0.44
23:x:126:G:N7	25:z:569:ALA:N	2.66	0.44
25:z:27:ARG:N	25:z:31:GLU:OE2	2.41	0.44
25:z:281:TRP:H	25:z:298:SER:HA	1.83	0.44
26:A:151:C:H2'	26:A:152:A:H8	1.82	0.44
33:I:100:ILE:HG22	33:I:101:SER:H	1.82	0.44
36:K:113:MET:HA	36:K:116:ILE:HG22	2.00	0.44
1:a:501:C:H2'	1:a:502:A:C8	2.53	0.43
2:b:182:VAL:HG13	2:b:195:VAL:HG13	2.00	0.43
16:p:43:ALA:O	16:p:46:LYS:NZ	2.49	0.43
22:v:55:PSU:O2'	22:v:57:A:N7	2.40	0.43
24:y:12:U:O4	24:y:23:G:O6	2.36	0.43
24:y:49:G:N2	24:y:65:U:O2	2.49	0.43
26:A:926:G:H2'	26:A:927:A:C8	2.53	0.43
26:A:1311:G:H21	26:A:1603:A:N6	2.13	0.43
34:H:58:LEU:HA	34:H:61:VAL:HG22	1.99	0.43
54:2:25:LYS:O	54:2:28:ARG:N	2.50	0.43
1:a:855:U:OP2	1:a:871:U:N3	2.49	0.43
23:x:126:G:H8	23:x:126:G:OP2	2.01	0.43
25:z:129:VAL:HB	25:z:143:LEU:HD21	2.00	0.43
25:z:288:HIS:HB3	25:z:291:SER:HB3	2.01	0.43
26:A:1167:C:H2'	26:A:1168:G:H8	1.83	0.43
26:A:1802:A:H2'	26:A:1803:A:H8	1.83	0.43
28:C:24:HIS:CG	28:C:79:ARG:HD2	2.52	0.43
31:F:115:GLY:HA3	31:F:177:ARG:HA	2.00	0.43
1:a:217:C:H2'	1:a:218:U:H6	1.84	0.43
3:c:21:TRP:CZ3	3:c:23:ALA:HB2	2.53	0.43
3:c:135:ARG:HD2	3:c:138:GLN:HE21	1.83	0.43
9:i:52:GLU:HB2	9:i:56:MET:HE3	2.00	0.43
10:j:22:THR:HA	10:j:25:ILE:HG22	2.00	0.43
20:t:28:ARG:HA	20:t:31:ILE:HG12	2.00	0.43
24:y:25:G:H2'	24:y:26:G:C8	2.53	0.43
25:z:385:TRP:O	25:z:388:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:161:A:OP2	26:A:162:U:O2'	2.35	0.43
26:A:280:U:H2'	26:A:281:C:C6	2.54	0.43
26:A:1638:C:O2	26:A:2698:U:O2'	2.35	0.43
26:A:1654:A:OP2	39:N:1:MET:N	2.40	0.43
26:A:1667:G:O2'	26:A:1991:U:O4	2.34	0.43
26:A:2176:A:O2'	26:A:2177:C:O5'	2.30	0.43
26:A:2850:A:N7	26:A:2868:A:O2'	2.39	0.43
1:a:410:G:OP2	4:d:25:ARG:NH2	2.51	0.43
1:a:1317:C:O2'	14:n:48:GLN:NE2	2.44	0.43
1:a:1372:U:OP1	9:i:72:SER:OG	2.30	0.43
4:d:185:PRO:HB2	4:d:190:LEU:HD23	2.00	0.43
11:k:96:ILE:HD12	11:k:96:ILE:HA	1.89	0.43
13:m:89:ARG:NE	13:m:95:PRO:O	2.38	0.43
15:o:86:LEU:HD12	15:o:87:ARG:HB2	1.99	0.43
24:y:57:G:H5'	33:I:21:PRO:O	2.18	0.43
25:z:111:LEU:HD12	25:z:145:ILE:HG13	1.99	0.43
25:z:348:ARG:HD2	25:z:349:LYS:H	1.83	0.43
25:z:403:TYR:HB3	25:z:410:LEU:HD23	2.00	0.43
26:A:1013:C:H2'	26:A:1014:A:H8	1.82	0.43
26:A:1114:C:H2'	26:A:1115:G:C8	2.52	0.43
26:A:1229:C:H2'	26:A:1230:A:C8	2.53	0.43
26:A:2885:G:N7	52:0:39:ARG:NH1	2.65	0.43
30:E:119:ILE:O	30:E:187:VAL:HA	2.18	0.43
6:f:47:LEU:HD13	6:f:51:ILE:HD12	2.01	0.43
16:p:40:ASN:HB3	16:p:43:ALA:HB2	2.00	0.43
19:s:12:LEU:HA	19:s:15:LEU:HG	2.00	0.43
26:A:372:G:H1'	26:A:373:U:H5	1.84	0.43
26:A:2249:U:O2'	26:A:2252:G:OP2	2.37	0.43
41:P:30:TRP:HE3	41:P:37:LYS:HG2	1.83	0.43
1:a:586:C:O2	8:h:3:GLN:NE2	2.52	0.43
2:b:67:LEU:HD13	2:b:157:PRO:HG3	2.00	0.43
9:i:27:ILE:HG22	9:i:62:LEU:HB2	2.01	0.43
18:r:28:LEU:HA	18:r:31:TYR:HD2	1.83	0.43
20:t:65:LEU:HD23	20:t:66:ILE:HG23	2.01	0.43
26:A:476:G:O2'	26:A:502:A:N6	2.38	0.43
26:A:1538:G:H2'	26:A:1539:U:C6	2.53	0.43
26:A:1652:A:H62	39:N:11:ASN:HD21	1.66	0.43
26:A:1716:U:H2'	26:A:1717:A:H8	1.83	0.43
26:A:2485:G:OP1	38:M:45:GLN:NE2	2.51	0.43
27:B:80:U:H2'	27:B:81:G:H8	1.83	0.43
35:J:64:VAL:HB	35:J:68:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Q:59:LEU:HD11	42:Q:63:ARG:HH21	1.84	0.43
47:V:4:ILE:HG21	47:V:50:MET:HE1	2.00	0.43
1:a:192:A:N3	20:t:54:GLN:NE2	2.66	0.43
1:a:934:C:N3	1:a:938:A:N1	2.67	0.43
1:a:1095:U:OP2	1:a:1108:G:N1	2.48	0.43
2:b:10:LYS:O	2:b:207:ARG:NH1	2.45	0.43
4:d:24:VAL:HG13	4:d:25:ARG:HG3	2.00	0.43
14:n:39:ASP:O	14:n:43:ALA:CB	2.66	0.43
19:s:49:ALA:HB1	19:s:56:HIS:HB3	2.01	0.43
24:y:5:G:H2'	24:y:5(A):A:H8	1.82	0.43
26:A:721:A:H2'	26:A:722:A:C8	2.54	0.43
26:A:1028:A:H2'	26:A:1029:A:C8	2.54	0.43
26:A:1149:G:H2'	26:A:1150:C:C6	2.54	0.43
26:A:2183:A:H2'	26:A:2184:A:H8	1.82	0.43
26:A:2818:U:H2'	26:A:2819:G:C8	2.54	0.43
27:B:65:U:O4	27:B:108:A:O2'	2.31	0.43
56:4:14:CYS:SG	56:4:27:CYS:HB2	2.59	0.43
1:a:1308:U:H2'	1:a:1309:G:C8	2.54	0.43
24:y:10:C:H2'	24:y:11:G:C8	2.51	0.43
25:z:450:LEU:HD13	25:z:453:GLU:HG3	2.00	0.43
25:z:506:PRO:HB2	25:z:544:TYR:O	2.19	0.43
26:A:96:C:OP1	50:Y:39:GLN:NE2	2.52	0.43
26:A:742:A:H2'	26:A:743:A:C8	2.54	0.43
26:A:796:C:H2'	26:A:797:G:H8	1.84	0.43
26:A:2529:G:H4'	32:G:174:LYS:HD3	2.01	0.43
27:B:52:A:H2'	40:O:33:ARG:HH22	1.82	0.43
29:D:109:VAL:HG22	29:D:175:LEU:HD21	2.00	0.43
34:H:55:GLU:HA	34:H:58:LEU:HG	2.00	0.43
37:L:70:LYS:HG3	37:L:73:ILE:HD11	2.00	0.43
1:a:377:G:H2'	1:a:378:G:C8	2.54	0.43
1:a:672:U:H2'	1:a:673:A:C8	2.54	0.43
1:a:713:G:H2'	1:a:714:G:C8	2.53	0.43
1:a:996:A:H2'	1:a:997:U:C6	2.54	0.43
1:a:1112:C:H1'	3:c:178:ARG:HE	1.84	0.43
1:a:1118:U:H5'	9:i:105:ARG:HE	1.83	0.43
3:c:152:VAL:HG22	3:c:197:VAL:HG23	2.00	0.43
4:d:47:LEU:HD11	4:d:51:GLY:HA3	2.01	0.43
10:j:24:GLU:HA	10:j:27:GLU:HG2	2.00	0.43
24:y:22:G:H2'	24:y:23:G:H8	1.84	0.43
25:z:231:ALA:HB1	25:z:237:ILE:HD13	2.00	0.43
26:A:227:A:O2'	26:A:2407:A:O2'	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:892:A:H2'	26:A:893:C:H6	1.84	0.43
26:A:1081:U:H5'	33:I:126:ARG:HE	1.84	0.43
26:A:1103:A:OP2	26:A:1104:C:N4	2.44	0.43
26:A:1727:C:H2'	26:A:1728:C:C6	2.54	0.43
26:A:2070:A:H2'	26:A:2071:A:H8	1.84	0.43
56:4:3:VAL:HG12	56:4:36:ARG:HD3	2.01	0.43
18:r:54:LEU:O	18:r:58:ILE:HG12	2.19	0.43
20:t:30:PHE:O	20:t:33:LYS:HG2	2.18	0.43
26:A:558:U:H2'	26:A:559:G:H8	1.83	0.43
26:A:1278:C:H2'	26:A:1279:G:C8	2.53	0.43
34:H:23:ALA:HB1	34:H:27:ARG:HH21	1.83	0.43
44:S:72:THR:OG1	44:S:73:LYS:N	2.51	0.43
1:a:471:U:H2'	1:a:472:U:C6	2.54	0.42
1:a:634:C:H2'	1:a:635:A:C8	2.54	0.42
1:a:781:A:OP2	1:a:800:G:N1	2.51	0.42
1:a:824:G:H2'	1:a:825:A:H8	1.84	0.42
2:b:23:ASN:ND2	2:b:191:ASP:OD1	2.52	0.42
26:A:1934:C:H2'	26:A:1935:G:H8	1.84	0.42
30:E:153:LEU:HD12	30:E:158:PHE:HE2	1.83	0.42
45:T:40:LYS:HB2	45:T:58:VAL:HG23	2.01	0.42
47:V:6:ALA:HB3	47:V:65:VAL:HG22	2.01	0.42
47:V:30:ILE:HG13	47:V:40:ILE:HG13	2.00	0.42
14:n:4:SER:OG	14:n:5:MET:N	2.51	0.42
26:A:680:C:H2'	26:A:681:G:C8	2.54	0.42
26:A:1486:U:H2'	26:A:1487:U:C6	2.54	0.42
26:A:2246:G:H2'	26:A:2247:A:C8	2.54	0.42
26:A:2393:U:O2'	37:L:59:ARG:O	2.33	0.42
51:Z:31:ILE:HD13	51:Z:31:ILE:HG21	1.91	0.42
9:i:80:HIS:HA	9:i:83:THR:HG22	2.01	0.42
12:l:23:LEU:HD22	12:l:94:TYR:HE1	1.84	0.42
15:o:21:THR:HA	15:o:26:VAL:HG11	2.01	0.42
20:t:79:THR:HA	20:t:82:ILE:HG12	2.00	0.42
25:z:288:HIS:HB2	25:z:321:LEU:HD22	2.01	0.42
26:A:568:U:H1'	26:A:2030:6MZ:H9C1	2.01	0.42
26:A:706:A:OP1	28:C:6:LYS:NZ	2.52	0.42
26:A:1681:G:OP2	26:A:1757:A:N6	2.52	0.42
41:P:88:ARG:NH1	41:P:114:ASN:OD1	2.52	0.42
52:0:27:LEU:HD12	52:0:36:LYS:HE3	2.01	0.42
1:a:1404:C:N4	1:a:1405:G:O6	2.52	0.42
24:y:12:U:C4	24:y:23:G:O6	2.72	0.42
26:A:6:A:H2'	26:A:7:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1798:U:OP2	28:C:269:ARG:NH2	2.53	0.42
29:D:177:VAL:HG22	29:D:189:VAL:HG12	2.01	0.42
37:L:85:VAL:HG11	37:L:90:VAL:HG12	2.01	0.42
39:N:103:ARG:HG2	39:N:105:GLY:H	1.85	0.42
41:P:29:VAL:HG12	41:P:80:VAL:HG22	2.00	0.42
45:T:29:THR:O	45:T:29:THR:OG1	2.35	0.42
1:a:18:C:H5''	5:e:131:ASN:HD21	1.84	0.42
1:a:987:G:H2'	1:a:988:G:H8	1.84	0.42
1:a:1452:C:O2'	1:a:1453:G:N2	2.52	0.42
2:b:66:ILE:HD13	2:b:220:VAL:HG21	2.02	0.42
3:c:113:LYS:HA	3:c:184:ASN:HD22	1.85	0.42
4:d:68:GLU:OE1	4:d:68:GLU:N	2.50	0.42
5:e:44:ARG:HG2	5:e:72:ASN:HA	2.00	0.42
11:k:13:LYS:HB3	11:k:15:VAL:HG23	2.01	0.42
13:m:80:MET:HE3	13:m:91:ARG:HG3	2.02	0.42
14:n:83:VAL:O	14:n:87:ALA:HB2	2.19	0.42
19:s:15:LEU:HA	19:s:18:VAL:HG12	2.00	0.42
25:z:265:PHE:HZ	25:z:315:LEU:HB2	1.85	0.42
26:A:1409:U:H2'	26:A:1410:G:H8	1.84	0.42
26:A:2141:G:H2'	26:A:2142:A:C8	2.55	0.42
26:A:2684:U:O2'	36:K:78:ARG:NH2	2.52	0.42
28:C:146:LYS:HB3	28:C:149:LYS:HE2	2.02	0.42
32:G:83:THR:HA	32:G:132:LEU:O	2.20	0.42
33:I:131:THR:HG22	33:I:135:MET:HE2	2.01	0.42
36:K:90:ASN:OD1	36:K:91:SER:N	2.50	0.42
41:P:47:ILE:HG22	41:P:99:LEU:HD21	2.01	0.42
1:a:1048:G:H2'	1:a:1050:G:H8	1.84	0.42
1:a:1052:U:O2'	1:a:1055:A:OP2	2.33	0.42
1:a:1520:C:H2'	1:a:1521:C:C6	2.54	0.42
4:d:170:LEU:HD12	4:d:181:PHE:HD1	1.84	0.42
5:e:140:ILE:HA	5:e:143:LEU:HG	2.02	0.42
26:A:223:A:O2'	26:A:420:C:O2	2.37	0.42
26:A:680:C:H2'	26:A:681:G:H8	1.84	0.42
26:A:1273:U:O2'	26:A:1275:A:OP1	2.37	0.42
26:A:2109:U:H3	26:A:2180:U:H3	1.68	0.42
27:B:93:C:H2'	27:B:94:A:H8	1.85	0.42
33:I:102:ARG:O	33:I:106:GLN:HB3	2.20	0.42
37:L:77:ILE:HG13	37:L:78:ARG:H	1.85	0.42
41:P:8:GLU:OE2	41:P:12:MET:HE2	2.19	0.42
1:a:79:G:H2'	1:a:80:A:H8	1.84	0.42
1:a:180:U:H2'	1:a:181:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:477:C:H2'	1:a:478:A:C8	2.55	0.42
1:a:564:C:OP1	12:l:11:ARG:NE	2.52	0.42
1:a:564:C:OP2	12:l:11:ARG:NH2	2.53	0.42
1:a:1412:C:H2'	1:a:1413:A:H8	1.85	0.42
2:b:92:ASN:OD1	2:b:93:HIS:N	2.52	0.42
2:b:185:ILE:HA	2:b:199:ILE:O	2.20	0.42
11:k:92:ARG:HG3	11:k:93:GLU:H	1.84	0.42
24:y:61:C:H2'	24:y:62:C:O4'	2.20	0.42
24:y:76:A:O2'	60:y:701:SEC:O	2.28	0.42
25:z:280:GLN:HG2	25:z:299:LEU:H	1.84	0.42
26:A:784:G:N2	26:A:792:A:O4'	2.53	0.42
26:A:1664:A:H61	26:A:1996:C:N4	2.17	0.42
26:A:2135:A:H61	26:A:2156:G:H2'	1.85	0.42
27:B:111:U:H2'	27:B:112:G:H8	1.85	0.42
32:G:37:ASN:OD1	32:G:38:ASP:N	2.53	0.42
45:T:56:GLU:HB2	45:T:86:THR:HG23	2.01	0.42
1:a:3:A:N1	1:a:628:G:O2'	2.49	0.42
1:a:625:U:H2'	1:a:626:G:H8	1.85	0.42
2:b:71:THR:HG22	2:b:94:ARG:HA	2.01	0.42
4:d:28:ASP:C	4:d:30:LYS:H	2.27	0.42
4:d:151:GLN:O	4:d:154:VAL:HG22	2.19	0.42
25:z:9:VAL:HA	61:z:701:GNP:O3G	2.19	0.42
26:A:1614:A:H61	44:S:88:ARG:H	1.67	0.42
26:A:2037:A:H2'	26:A:2038:G:C8	2.55	0.42
26:A:2698:U:H2'	26:A:2699:C:C6	2.54	0.42
29:D:9:VAL:O	29:D:26:VAL:HB	2.20	0.42
1:a:235:C:H2'	1:a:236:A:C8	2.55	0.42
1:a:475:C:H2'	1:a:476:U:C6	2.55	0.42
6:f:67:PRO:HG2	6:f:70:VAL:HG22	2.01	0.42
26:A:479:A:N3	26:A:481:G:H5''	2.35	0.42
26:A:657:U:H2'	26:A:658:U:C6	2.54	0.42
26:A:793:A:OP2	26:A:2071:A:O2'	2.29	0.42
26:A:1252:G:OP2	42:Q:13:HIS:NE2	2.50	0.42
26:A:2107:G:H2'	26:A:2108:A:C4	2.55	0.42
26:A:2567:G:H2'	26:A:2568:U:C6	2.55	0.42
26:A:2899:A:H2'	26:A:2900:A:H8	1.84	0.42
27:B:49:C:H2'	27:B:50:A:C8	2.54	0.42
31:F:125:GLY:O	31:F:157:THR:OG1	2.37	0.42
37:L:19:LEU:HD23	37:L:27:LEU:HD13	2.02	0.42
46:U:32:LYS:HE3	46:U:63:ALA:HB3	2.02	0.42
1:a:406:G:H5'	4:d:4:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:684:U:O2'	11:k:40:ALA:O	2.35	0.42
1:a:1485:U:H5'	26:A:1961:C:H5''	2.00	0.42
20:t:74:HIS:O	20:t:78:LEU:CB	2.68	0.42
24:y:8:G:N2	24:y:48:G:H21	2.17	0.42
24:y:20:G:O6	24:y:48:G:N1	2.53	0.42
24:y:64:G:N2	25:z:327:SER:OG	2.47	0.42
26:A:1754:A:O3'	41:P:102:ARG:NH2	2.51	0.42
30:E:128:ALA:HB3	30:E:133:LEU:HD21	2.02	0.42
32:G:36:LEU:HD21	32:G:70:LEU:HD11	2.02	0.42
34:H:70:GLU:HB2	34:H:134:VAL:HG11	2.01	0.42
43:R:4:VAL:HG23	43:R:39:LEU:HB2	2.01	0.42
57:6:11:GLU:OE1	57:6:25:ARG:NH1	2.46	0.42
1:a:619:U:H3	4:d:130:ASN:HB2	1.85	0.41
1:a:883:C:H2'	1:a:884:U:C6	2.54	0.41
7:g:38:ALA:O	7:g:42:VAL:HG23	2.20	0.41
11:k:64:VAL:HG12	11:k:68:ARG:HH11	1.85	0.41
15:o:45:HIS:O	15:o:47:LYS:N	2.53	0.41
24:y:52:G:N1	24:y:53:G:C6	2.88	0.41
26:A:596:U:H2'	26:A:597:G:H8	1.84	0.41
26:A:1353:A:H2'	26:A:1354:A:H8	1.84	0.41
26:A:1386:C:H2'	26:A:1387:A:C8	2.55	0.41
26:A:1737:G:O2'	26:A:1738:G:N3	2.53	0.41
26:A:2183:A:H2'	26:A:2184:A:C8	2.55	0.41
26:A:2514:U:H2'	26:A:2515:C:C6	2.55	0.41
28:C:36:ASN:HB2	28:C:61:TYR:HB2	2.02	0.41
32:G:4:ALA:HB2	32:G:65:GLY:HA2	2.02	0.41
39:N:79:LEU:O	39:N:84:GLY:N	2.49	0.41
1:a:234:C:H4'	17:q:65:PRO:HG3	2.02	0.41
5:e:70:MET:HE3	5:e:70:MET:HB2	1.95	0.41
6:f:18:VAL:HG21	6:f:58:HIS:CD2	2.55	0.41
25:z:495:TRP:HA	25:z:498:ALA:HB3	2.03	0.41
26:A:20:C:H2'	26:A:21:A:H8	1.85	0.41
26:A:576:U:H2'	26:A:577:G:C8	2.54	0.41
26:A:1503:A:H2'	26:A:1504:A:H8	1.85	0.41
34:H:5:LEU:HB2	34:H:16:GLY:H	1.85	0.41
37:L:80:SER:OG	37:L:115:GLU:OE2	2.38	0.41
39:N:56:LYS:NZ	39:N:90:ARG:O	2.51	0.41
46:U:52:ASN:OD1	46:U:53:GLN:N	2.52	0.41
10:j:25:ILE:HA	10:j:28:THR:HG22	2.02	0.41
16:p:76:LYS:O	16:p:80:LYS:HG2	2.20	0.41
26:A:445:C:O2'	26:A:449:A:N3	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:466:A:OP1	54:2:34:ARG:NH1	2.54	0.41
26:A:1039:A:H61	26:A:1116:G:H1	1.68	0.41
26:A:1190:G:OP1	37:L:30:THR:OG1	2.28	0.41
26:A:1693:U:O4	26:A:1976:U:O2'	2.33	0.41
32:G:51:PHE:HE2	32:G:68:ARG:HA	1.85	0.41
33:I:9:LYS:HB3	33:I:55:PRO:HB2	2.03	0.41
51:Z:16:LEU:HB3	51:Z:19:HIS:ND1	2.35	0.41
1:a:458:U:H2'	1:a:459:A:C8	2.56	0.41
1:a:579:A:O2'	15:o:53:ARG:NH2	2.49	0.41
1:a:618:C:O2	1:a:622:A:N6	2.52	0.41
3:c:19:SER:HB3	3:c:21:TRP:NE1	2.35	0.41
9:i:8:THR:OG1	9:i:9:GLY:N	2.50	0.41
10:j:28:THR:O	10:j:32:THR:OG1	2.32	0.41
11:k:30:ILE:HD12	11:k:45:THR:HG22	2.02	0.41
16:p:58:ALA:HA	16:p:61:VAL:HG22	2.01	0.41
25:z:373:LEU:HD22	25:z:411:LEU:HA	2.02	0.41
26:A:1028:A:OP2	26:A:1126:A:N6	2.36	0.41
26:A:1197:G:N2	26:A:1249:U:O2'	2.54	0.41
26:A:1250:G:P	37:L:21:ARG:HE	2.42	0.41
33:I:2:LYS:HE2	33:I:61:TYR:CD1	2.55	0.41
33:I:82:ALA:HB1	33:I:108:ILE:HD13	2.02	0.41
35:J:45:THR:HB	35:J:48:VAL:HG12	2.01	0.41
1:a:405:U:H1'	1:a:498:A:H2'	2.02	0.41
6:f:9:MET:HB2	6:f:85:ILE:O	2.21	0.41
20:t:19:HIS:CE1	20:t:23:ARG:HH22	2.37	0.41
20:t:55:PRO:HB2	20:t:59:ARG:HH12	1.85	0.41
25:z:265:PHE:CZ	25:z:315:LEU:HB2	2.55	0.41
26:A:1751:U:H2'	26:A:1752:C:C6	2.55	0.41
26:A:2047:C:H2'	26:A:2048:G:H8	1.85	0.41
26:A:2428:G:H21	37:L:60:ARG:HH22	1.69	0.41
39:N:59:SER:OG	39:N:62:ASN:OD1	2.27	0.41
57:6:16:CYS:SG	57:6:18:CYS:HB2	2.60	0.41
1:a:543:U:OP1	4:d:13:ARG:NE	2.50	0.41
1:a:1315:U:O2'	1:a:1360:A:N3	2.48	0.41
24:y:47:G:H2'	24:y:47(A):G:C8	2.56	0.41
25:z:91:GLN:HE21	25:z:95:HIS:CD2	2.39	0.41
25:z:212:VAL:HG22	25:z:249:GLN:HB3	2.02	0.41
26:A:796:C:H2'	26:A:797:G:C8	2.55	0.41
26:A:1078:U:H5'	26:A:1079:C:H5''	2.02	0.41
26:A:2295:C:OP1	40:O:10:ARG:NH1	2.51	0.41
47:V:35:GLU:HB2	47:V:93:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:6:41:HIS:HD2	57:6:43:PHE:HB2	1.85	0.41
1:a:77:A:H2'	1:a:78:A:C8	2.56	0.41
1:a:154:U:H2'	1:a:155:A:C8	2.55	0.41
1:a:203:G:O2'	1:a:465:A:N1	2.53	0.41
1:a:332:G:OP2	20:t:2:ASN:N	2.54	0.41
1:a:917:G:H2'	1:a:918:A:C8	2.55	0.41
2:b:14:HIS:HE1	2:b:211:LEU:HD21	1.85	0.41
8:h:53:ASP:OD1	8:h:53:ASP:N	2.54	0.41
24:y:33:U:H1'	24:y:37:6IA:H131	2.01	0.41
25:z:239:LEU:HG	25:z:241:ILE:HG23	2.03	0.41
26:A:569:U:O2'	26:A:971:G:N2	2.48	0.41
26:A:882:G:H2'	26:A:883:G:C8	2.55	0.41
26:A:1171:G:H2'	26:A:1172:C:O4'	2.20	0.41
31:F:37:MET:HB2	31:F:86:CYS:SG	2.60	0.41
34:H:96:THR:O	34:H:99:ILE:HG22	2.21	0.41
42:Q:78:PHE:CE1	42:Q:109:VAL:HG22	2.55	0.41
1:a:591:U:H2'	1:a:592:G:C8	2.56	0.41
1:a:1030:U:O2'	1:a:1033:G:N3	2.54	0.41
1:a:1248:A:H2	9:i:71:ILE:HD11	1.85	0.41
10:j:12:ALA:HB2	10:j:96:VAL:HG23	2.01	0.41
13:m:6:ILE:HG23	13:m:7:ASN:H	1.86	0.41
14:n:46:LYS:O	14:n:49:THR:OG1	2.28	0.41
21:u:49:ALA:O	21:u:53:LYS:HD3	2.21	0.41
26:A:58:G:O2'	26:A:73:A:N1	2.42	0.41
26:A:242:G:H1'	26:A:243:U:H5	1.85	0.41
26:A:922:C:H1'	48:W:22:PHE:CD2	2.55	0.41
26:A:935:C:H2'	26:A:936:A:H8	1.85	0.41
26:A:1927:A:H2'	26:A:1928:A:C8	2.56	0.41
32:G:42:VAL:HG23	32:G:51:PHE:CE1	2.55	0.41
47:V:40:ILE:HD12	47:V:40:ILE:HG23	1.87	0.41
1:a:208:U:H2'	1:a:210:C:H1'	2.03	0.41
1:a:448:A:H3'	1:a:449:G:H8	1.86	0.41
1:a:499:A:H1'	1:a:500:G:C8	2.56	0.41
1:a:1213:A:O2'	1:a:1215:G:N7	2.45	0.41
1:a:1520:C:H2'	1:a:1521:C:H6	1.86	0.41
7:g:129:ASN:HA	7:g:134:VAL:HG21	2.03	0.41
14:n:98:ALA:HB1	14:n:100:TRP:HZ3	1.85	0.41
25:z:65:LEU:HD22	25:z:324:ARG:HH11	1.85	0.41
25:z:96:LEU:HD22	25:z:138:PHE:CE2	2.56	0.41
25:z:293:VAL:HG13	25:z:311:THR:HB	2.02	0.41
26:A:213:A:H2'	26:A:214:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:223:A:N1	26:A:407:G:O2'	2.50	0.41
26:A:514:A:H2'	26:A:515:A:C8	2.55	0.41
26:A:679:C:H2'	26:A:680:C:C6	2.56	0.41
26:A:1244:A:O2'	30:E:29:HIS:NE2	2.42	0.41
26:A:2260:C:O2'	26:A:2388:A:O2'	2.38	0.41
28:C:171:VAL:O	28:C:182:LYS:HA	2.20	0.41
32:G:86:LEU:HG	32:G:163:TYR:HD1	1.85	0.41
46:U:7:ASP:HB2	46:U:23:LYS:HB2	2.02	0.41
1:a:185:U:O2	20:t:75:LYS:NZ	2.54	0.41
1:a:332:G:O3'	20:t:2:ASN:N	2.54	0.41
1:a:579:A:H2'	1:a:580:C:H6	1.86	0.41
1:a:769:G:H4'	1:a:1513:A:H4'	2.02	0.41
9:i:101:GLY:C	9:i:103:VAL:H	2.29	0.41
10:j:41:PRO:O	10:j:72:ARG:NH1	2.54	0.41
16:p:69:ASP:OD1	16:p:70:ARG:N	2.53	0.41
24:y:66:G:H4'	25:z:292:HIS:CE1	2.55	0.41
26:A:191:A:O2'	26:A:678:C:O2	2.36	0.41
26:A:285:G:C6	26:A:356:G:C6	3.08	0.41
26:A:589:U:H2'	26:A:590:A:H8	1.86	0.41
26:A:1475:G:O2'	26:A:1514:G:O6	2.39	0.41
26:A:1808:A:O2'	26:A:1809:A:O4'	2.35	0.41
26:A:1939:5MU:OP1	26:A:2604:PSU:O2'	2.39	0.41
26:A:2012:G:N7	44:S:16:LYS:NZ	2.69	0.41
26:A:2591:C:H2'	26:A:2592:G:C8	2.55	0.41
27:B:57:A:H1'	31:F:26:GLN:HG3	2.03	0.41
48:W:42:HIS:CD2	48:W:73:ARG:HD3	2.56	0.41
57:6:14:ALA:HB1	57:6:34:LEU:HD11	2.03	0.41
4:d:51:GLY:O	4:d:55:ARG:CB	2.69	0.40
4:d:191:SER:OG	4:d:192:ALA:N	2.51	0.40
5:e:51:LYS:HB2	5:e:51:LYS:HE2	1.87	0.40
25:z:445:LEU:HA	25:z:445:LEU:HD23	1.91	0.40
26:A:48:G:O2'	26:A:118:A:N1	2.40	0.40
26:A:1274:A:OP1	26:A:1646:C:N4	2.45	0.40
26:A:2086:U:H2'	26:A:2087:G:C8	2.56	0.40
30:E:133:LEU:HA	30:E:136:GLN:HG2	2.02	0.40
31:F:12:VAL:HG12	31:F:27:VAL:HG21	2.02	0.40
41:P:19:PHE:HE2	41:P:46:VAL:HG11	1.87	0.40
1:a:429:U:OP2	4:d:12:ARG:NH1	2.55	0.40
4:d:85:THR:O	4:d:89:LEU:HB3	2.21	0.40
16:p:71:VAL:O	16:p:75:ILE:HG12	2.21	0.40
23:x:91:A:H1'	23:x:92:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:y:25:G:H2'	24:y:26:G:H8	1.85	0.40
25:z:122:VAL:HG13	25:z:145:ILE:HG12	2.03	0.40
26:A:924:G:H2'	26:A:925:A:C8	2.56	0.40
26:A:1265:A:H61	26:A:2013:A:H5''	1.87	0.40
26:A:1687:G:N1	26:A:1700:A:OP1	2.44	0.40
26:A:1972:G:OP2	28:C:237:ARG:NH1	2.54	0.40
26:A:2229:U:H2'	26:A:2230:G:C8	2.57	0.40
29:D:110:THR:HB	29:D:202:ILE:HG13	2.04	0.40
35:J:91:GLU:HG3	35:J:95:ARG:HH22	1.86	0.40
38:M:57:VAL:HG12	38:M:112:LEU:HG	2.03	0.40
57:6:7:PRO:HB2	57:6:27:THR:HG23	2.03	0.40
1:a:21:G:H2'	1:a:22:G:C8	2.56	0.40
1:a:409:U:H3	1:a:433:G:H1	1.69	0.40
1:a:443:C:H2'	1:a:444:G:C8	2.56	0.40
1:a:600:A:H2'	1:a:601:G:C8	2.57	0.40
1:a:647:C:H2'	1:a:648:A:C8	2.56	0.40
1:a:1523:G:H5''	11:k:124:LYS:HE2	2.03	0.40
2:b:77:GLU:O	2:b:80:LYS:HB3	2.21	0.40
25:z:269:ILE:HG13	25:z:355:TRP:CZ3	2.57	0.40
26:A:83:A:N6	26:A:101:A:O2'	2.49	0.40
26:A:744:U:H2'	26:A:745:1MG:O4'	2.21	0.40
26:A:1857:G:H22	26:A:1884:G:H2'	1.86	0.40
26:A:1899:A:H4'	26:A:1901:A:H5''	2.03	0.40
26:A:1997:C:H2'	26:A:1998:A:H8	1.86	0.40
26:A:2185:U:H2'	26:A:2186:G:C8	2.56	0.40
26:A:2392:A:H2	37:L:55:MET:HE2	1.86	0.40
27:B:13:G:N2	27:B:16:G:N3	2.69	0.40
32:G:3:VAL:HG22	32:G:68:ARG:NH2	2.37	0.40
47:V:21:ARG:NH1	47:V:87:GLN:O	2.46	0.40
52:0:32:THR:OG1	52:0:33:SER:N	2.55	0.40
1:a:1376:U:H2'	1:a:1377:A:C8	2.57	0.40
1:a:1479:C:H2'	1:a:1480:A:C8	2.56	0.40
3:c:121:SER:HA	3:c:124:GLU:HG2	2.04	0.40
4:d:51:GLY:O	4:d:55:ARG:HB2	2.22	0.40
5:e:134:ASN:O	5:e:138:ALA:HB2	2.22	0.40
12:l:113:ARG:NE	12:l:120:ARG:HE	2.20	0.40
25:z:82:VAL:HG22	25:z:92:THR:HG21	2.02	0.40
25:z:436:ASP:HB3	25:z:488:SER:OG	2.21	0.40
26:A:500:G:N1	26:A:503:A:OP2	2.50	0.40
26:A:697:G:H2'	26:A:698:C:C6	2.57	0.40
26:A:1151:A:H4'	42:Q:80:ASN:ND2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2041:U:H2'	26:A:2042:A:C8	2.56	0.40
26:A:2699:C:H2'	26:A:2700:A:C8	2.57	0.40
27:B:49:C:H2'	27:B:50:A:H8	1.87	0.40
37:L:89:VAL:HG13	37:L:123:ARG:NH1	2.37	0.40
39:N:33:ILE:HB	39:N:114:GLU:HG3	2.03	0.40
46:U:70:ALA:HB3	46:U:79:ALA:HB1	2.03	0.40
48:W:19:VAL:HA	48:W:34:VAL:HG22	2.03	0.40
1:a:8:A:N7	4:d:204:SER:OG	2.55	0.40
1:a:41:G:H2'	1:a:42:G:H8	1.86	0.40
3:c:30:ASP:OD1	3:c:31:ASN:N	2.54	0.40
15:o:57:ARG:O	15:o:60:SER:OG	2.30	0.40
25:z:2:ILE:HD11	25:z:235:GLN:HA	2.04	0.40
26:A:1123:C:H2'	26:A:1124:G:C8	2.56	0.40
26:A:2022:U:H3	52:0:5:ASN:ND2	2.20	0.40
26:A:2087:G:H2'	26:A:2088:A:H8	1.86	0.40
28:C:175:LEU:HA	28:C:175:LEU:HD23	1.84	0.40
37:L:123:ARG:NH2	37:L:143:GLU:OE2	2.55	0.40
40:O:31:THR:HG23	40:O:33:ARG:O	2.22	0.40
43:R:98:ILE:HD12	43:R:98:ILE:HA	1.92	0.40
47:V:77:VAL:HG23	47:V:89:ILE:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	216/218 (99%)	188 (87%)	24 (11%)	4 (2%)	6	30
3	c	204/206 (99%)	191 (94%)	10 (5%)	3 (2%)	8	38
4	d	203/205 (99%)	190 (94%)	8 (4%)	5 (2%)	4	25
5	e	155/157 (99%)	142 (92%)	6 (4%)	7 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	98/100 (98%)	81 (83%)	13 (13%)	4 (4%)	2	17
7	g	149/151 (99%)	139 (93%)	7 (5%)	3 (2%)	6	30
8	h	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	16	52
9	i	125/127 (98%)	108 (86%)	13 (10%)	4 (3%)	3	20
10	j	96/98 (98%)	83 (86%)	7 (7%)	6 (6%)	1	12
11	k	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	6	32
12	l	121/123 (98%)	110 (91%)	7 (6%)	4 (3%)	3	20
13	m	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	4	24
14	n	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
15	o	86/88 (98%)	76 (88%)	7 (8%)	3 (4%)	3	19
16	p	80/82 (98%)	72 (90%)	5 (6%)	3 (4%)	2	18
17	q	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	2	18
18	r	63/65 (97%)	57 (90%)	3 (5%)	3 (5%)	2	15
19	s	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
20	t	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	42
21	u	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	2	15
25	z	613/614 (100%)	587 (96%)	20 (3%)	6 (1%)	12	47
28	C	269/271 (99%)	254 (94%)	13 (5%)	2 (1%)	18	55
29	D	207/209 (99%)	197 (95%)	8 (4%)	2 (1%)	12	47
30	E	199/201 (99%)	189 (95%)	8 (4%)	2 (1%)	12	47
31	F	175/177 (99%)	163 (93%)	9 (5%)	3 (2%)	7	34
32	G	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	3	22
33	I	139/141 (99%)	121 (87%)	14 (10%)	4 (3%)	3	22
34	H	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	3	20
35	J	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	18	55
36	K	120/122 (98%)	116 (97%)	2 (2%)	2 (2%)	7	34
37	L	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	9	38
38	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	8	38
39	N	118/120 (98%)	108 (92%)	9 (8%)	1 (1%)	16	52
40	O	114/116 (98%)	103 (90%)	10 (9%)	1 (1%)	14	49
41	P	112/114 (98%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	Q	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
43	R	101/103 (98%)	93 (92%)	6 (6%)	2 (2%)	6	30
44	S	108/110 (98%)	102 (94%)	4 (4%)	2 (2%)	6	30
45	T	91/93 (98%)	79 (87%)	11 (12%)	1 (1%)	11	45
46	U	100/102 (98%)	89 (89%)	5 (5%)	6 (6%)	1	12
47	V	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
48	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
49	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
50	Y	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	7	36
51	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
52	0	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	6	30
53	1	48/50 (96%)	46 (96%)	1 (2%)	1 (2%)	5	28
54	2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	26
55	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	7	36
56	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
57	6	64/66 (97%)	57 (89%)	5 (8%)	2 (3%)	3	21
All	All	6330/6431 (98%)	5844 (92%)	368 (6%)	118 (2%)	8	30

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
2	b	151	LYS
5	e	89	THR
6	f	94	HIS
9	i	57	VAL
9	i	125	GLN
10	j	34	ALA
10	j	57	VAL
10	j	92	LEU
11	k	92	ARG
12	l	101	LEU
13	m	4	ALA
13	m	6	ILE
15	o	46	LYS
15	o	87	ARG

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Mol	Chain	Res	Type
16	p	44	SER
17	q	16	MET
17	q	49	ASN
25	z	191	VAL
25	z	301	GLU
25	z	328	ALA
28	C	121	ALA
30	E	83	VAL
32	G	174	LYS
32	G	175	LYS
33	I	64	ARG
34	H	9	VAL
35	J	81	ILE
37	L	36	LYS
38	M	58	LYS
44	S	64	ALA
46	U	51	LEU
46	U	88	ASP
52	0	2	VAL
53	1	4	ILE
55	3	31	ILE
3	c	60	ALA
3	c	79	LYS
4	d	165	GLU
4	d	191	SER
5	e	77	ASN
5	e	93	VAL
8	h	44	PHE
9	i	107	ALA
10	j	42	LEU
11	k	91	GLY
12	l	25	ALA
18	r	11	ARG
18	r	18	GLN
21	u	25	ALA
25	z	487	PHE
32	G	108	PHE
33	I	24	GLY
34	H	3	VAL
34	H	41	LYS
36	K	35	VAL
39	N	117	ASP

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Mol	Chain	Res	Type
43	R	52	PRO
43	R	53	PHE
46	U	6	ARG
46	U	18	LYS
57	6	40	CYS
57	6	43	PHE
4	d	47	LEU
5	e	23	THR
6	f	99	ALA
7	g	129	ASN
9	i	12	LYS
15	o	2	LEU
16	p	43	ALA
21	u	24	LYS
21	u	34	ARG
28	C	204	LEU
29	D	140	HIS
29	D	149	ASN
32	G	118	ALA
33	I	69	VAL
34	H	15	LEU
37	L	29	LYS
2	b	17	HIS
3	c	156	LEU
5	e	122	VAL
7	g	57	GLU
10	j	58	ASN
12	l	2	THR
12	l	46	SER
17	q	72	TRP
20	t	26	MET
31	F	20	ASN
32	G	173	ALA
34	H	89	LYS
44	S	3	THR
45	T	88	LYS
54	2	40	ALA
2	b	120	SER
4	d	150	LYS
5	e	158	LYS
6	f	92	THR
7	g	56	SER

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Mol	Chain	Res	Type
10	j	75	ASP
25	z	345	ARG
30	E	122	GLU
31	F	149	ARG
36	K	92	GLU
40	O	101	GLY
46	U	97	SER
46	U	98	ASN
50	Y	24	GLU
4	d	4	LEU
13	m	11	HIS
38	M	69	PRO
5	e	24	VAL
16	p	49	GLY
18	r	17	VAL
25	z	600	GLY
31	F	135	ILE
6	f	19	PRO
33	I	12	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	180 (100%)	0	100	100
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	172 (100%)	0	100	100
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	102 (99%)	1 (1%)	68	76
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
25	z	502/501 (100%)	502 (100%)	0	100	100
28	C	216/216 (100%)	216 (100%)	0	100	100
29	D	164/164 (100%)	164 (100%)	0	100	100
30	E	165/165 (100%)	164 (99%)	1 (1%)	78	81
31	F	148/148 (100%)	147 (99%)	1 (1%)	76	80
32	G	137/137 (100%)	137 (100%)	0	100	100
33	I	109/109 (100%)	109 (100%)	0	100	100
34	H	114/114 (100%)	113 (99%)	1 (1%)	70	77
35	J	116/116 (100%)	116 (100%)	0	100	100
36	K	103/103 (100%)	103 (100%)	0	100	100
37	L	102/102 (100%)	102 (100%)	0	100	100
38	M	109/109 (100%)	109 (100%)	0	100	100
39	N	100/100 (100%)	100 (100%)	0	100	100
40	O	86/86 (100%)	86 (100%)	0	100	100
41	P	99/99 (100%)	99 (100%)	0	100	100
42	Q	89/89 (100%)	89 (100%)	0	100	100
43	R	84/84 (100%)	84 (100%)	0	100	100
44	S	93/93 (100%)	93 (100%)	0	100	100
45	T	80/80 (100%)	80 (100%)	0	100	100
46	U	83/83 (100%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	V	78/78 (100%)	78 (100%)	0	100	100
48	W	57/57 (100%)	57 (100%)	0	100	100
49	X	67/67 (100%)	67 (100%)	0	100	100
50	Y	55/55 (100%)	55 (100%)	0	100	100
51	Z	48/48 (100%)	47 (98%)	1 (2%)	47	64
52	0	47/47 (100%)	47 (100%)	0	100	100
53	1	45/45 (100%)	45 (100%)	0	100	100
54	2	38/38 (100%)	38 (100%)	0	100	100
55	3	51/51 (100%)	51 (100%)	0	100	100
56	4	34/34 (100%)	34 (100%)	0	100	100
57	6	59/59 (100%)	59 (100%)	0	100	100
All	All	5230/5252 (100%)	5225 (100%)	5 (0%)	87	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	23	LEU
30	E	83	VAL
31	F	39	VAL
34	H	3	VAL
51	Z	47	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	24	ASN
4	d	53	GLN
5	e	60	GLN
5	e	120	HIS
5	e	121	ASN
5	e	147	ASN
6	f	46	GLN
9	i	4	GLN
9	i	109	GLN
9	i	125	GLN
12	l	95	HIS
14	n	42	ASN

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Mol	Chain	Res	Type
14	n	65	GLN
15	o	36	ASN
15	o	45	HIS
15	o	79	GLN
16	p	9	HIS
16	p	63	GLN
17	q	44	HIS
17	q	46	HIS
19	s	68	HIS
20	t	47	GLN
20	t	60	GLN
25	z	47	GLN
25	z	91	GLN
25	z	100	GLN
25	z	232	ASN
25	z	292	HIS
25	z	483	HIS
25	z	491	GLN
25	z	529	GLN
28	C	20	ASN
28	C	85	ASN
28	C	133	ASN
28	C	199	HIS
28	C	250	GLN
29	D	36	GLN
29	D	134	HIS
29	D	150	GLN
29	D	164	GLN
30	E	46	GLN
30	E	62	GLN
30	E	90	GLN
31	F	26	GLN
31	F	80	GLN
32	G	114	HIS
32	G	138	GLN
34	H	2	GLN
34	H	11	ASN
34	H	18	GLN
34	H	20	ASN
36	K	29	HIS
36	K	93	GLN
37	L	35	HIS

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Mol	Chain	Res	Type
40	O	19	GLN
40	O	61	GLN
41	P	51	ASN
41	P	55	HIS
42	Q	51	GLN
42	Q	71	ASN
43	R	89	HIS
43	R	91	GLN
46	U	73	ASN
50	Y	39	GLN
52	0	5	ASN
55	3	25	HIS
56	4	33	HIS
57	6	65	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1538/1539 (99%)	197 (12%)	0
22	v	76/77 (98%)	10 (13%)	0
23	x	47/48 (97%)	30 (63%)	0
24	y	94/95 (98%)	23 (24%)	0
26	A	2902/2903 (99%)	417 (14%)	5 (0%)
27	B	119/120 (99%)	11 (9%)	0
58	w	2/3 (66%)	0	0
All	All	4778/4785 (99%)	688 (14%)	5 (0%)

All (688) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	8	A
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	49	U
1	a	50	A
1	a	51	A
1	a	86	G

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Mol	Chain	Res	Type
1	a	94	G
1	a	95	C
1	a	96	U
1	a	121	U
1	a	127	G
1	a	131	A
1	a	141	G
1	a	164	G
1	a	173	U
1	a	177	G
1	a	183	C
1	a	197	A
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	237	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	254	G
1	a	266	G
1	a	267	C
1	a	289	G
1	a	298	A
1	a	316	C
1	a	319	G
1	a	328	C
1	a	330	C
1	a	347	G
1	a	352	C
1	a	354	G
1	a	356	A
1	a	367	U
1	a	368	U
1	a	372	C
1	a	392	C
1	a	406	G
1	a	407	U
1	a	411	A
1	a	412	A

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Mol	Chain	Res	Type
1	a	414	A
1	a	420	U
1	a	426	U
1	a	429	U
1	a	430	A
1	a	436	C
1	a	438	U
1	a	439	U
1	a	467	U
1	a	481	G
1	a	482	A
1	a	491	G
1	a	497	G
1	a	499	A
1	a	509	A
1	a	511	C
1	a	512	U
1	a	517	G
1	a	518	C
1	a	524	G
1	a	527	G7M
1	a	528	C
1	a	531	U
1	a	532	A
1	a	546	A
1	a	547	A
1	a	551	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	633	G
1	a	642	A
1	a	653	U
1	a	661	G
1	a	665	A
1	a	686	U
1	a	723	U
1	a	724	G
1	a	733	G

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Mol	Chain	Res	Type
1	a	748	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	816	A
1	a	817	C
1	a	819	A
1	a	832	G
1	a	841	C
1	a	842	U
1	a	843	U
1	a	844	G
1	a	845	A
1	a	876	C
1	a	878	A
1	a	889	A
1	a	890	G
1	a	926	G
1	a	934	C
1	a	935	A
1	a	942	G
1	a	960	U
1	a	966	2MG
1	a	968	A
1	a	969	A
1	a	974	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	991	U
1	a	993	G
1	a	1004	A
1	a	1020	G
1	a	1032	G
1	a	1034	G
1	a	1043	G
1	a	1065	U
1	a	1085	U
1	a	1089	G
1	a	1094	G
1	a	1095	U

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Mol	Chain	Res	Type
1	a	1101	A
1	a	1105	A
1	a	1134	G
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1158	C
1	a	1159	U
1	a	1160	G
1	a	1168	U
1	a	1169	A
1	a	1182	G
1	a	1196	A
1	a	1197	A
1	a	1213	A
1	a	1227	A
1	a	1238	A
1	a	1240	U
1	a	1241	G
1	a	1260	G
1	a	1278	G
1	a	1280	A
1	a	1287	A
1	a	1297	G
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1317	C
1	a	1320	C
1	a	1338	G
1	a	1345	U
1	a	1346	A
1	a	1363	A
1	a	1364	U
1	a	1394	A
1	a	1396	A
1	a	1397	C
1	a	1398	A
1	a	1406	U

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Mol	Chain	Res	Type
1	a	1419	G
1	a	1429	A
1	a	1441	A
1	a	1491	G
1	a	1492	A
1	a	1493	A
1	a	1497	G
1	a	1503	A
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1520	C
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1536	C
1	a	1537	U
22	v	9	G
22	v	18	G
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	31	G
22	v	52	G
22	v	54	5MU
22	v	59	A
22	v	75	C
23	x	88	A
23	x	90	G
23	x	96	C
23	x	98	U
23	x	104	U
23	x	108	A
23	x	109	C
23	x	110	G
23	x	111	G
23	x	112	C
23	x	113	C
23	x	114	C
23	x	115	A
23	x	116	U

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Mol	Chain	Res	Type
23	x	117	C
23	x	118	G
23	x	119	G
23	x	120	U
23	x	121	U
23	x	122	G
23	x	123	C
23	x	125	G
23	x	126	G
23	x	127	U
23	x	128	C
23	x	129	U
23	x	130	G
23	x	131	C
23	x	133	C
23	x	134	C
24	y	8	G
24	y	15	C
24	y	18	G
24	y	20	G
24	y	29	G
24	y	31	A
24	y	40	C
24	y	45	U
24	y	46	G
24	y	47(F)	C
24	y	47(G)	C
24	y	47(H)	A
24	y	47(I)	G
24	y	47(J)	C
24	y	49	G
24	y	54	5MU
24	y	55	PSU
24	y	56	C
24	y	60	U
24	y	61	C
24	y	64	G
24	y	66	G
24	y	73	G
26	A	10	A
26	A	15	G
26	A	23	G

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Mol	Chain	Res	Type
26	A	27	G
26	A	34	U
26	A	60	G
26	A	63	A
26	A	71	A
26	A	74	A
26	A	75	G
26	A	91	A
26	A	101	A
26	A	102	U
26	A	118	A
26	A	120	U
26	A	125	A
26	A	131	A
26	A	138	U
26	A	139	U
26	A	142	A
26	A	181	A
26	A	196	A
26	A	199	A
26	A	204	A
26	A	205	G
26	A	216	A
26	A	222	A
26	A	228	C
26	A	230	G
26	A	232	G
26	A	248	G
26	A	255	A
26	A	277	G
26	A	278	A
26	A	279	A
26	A	285	G
26	A	311	A
26	A	322	A
26	A	329	G
26	A	330	A
26	A	362	A
26	A	367	G
26	A	372	G
26	A	386	G
26	A	396	G

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Mol	Chain	Res	Type
26	A	404	A
26	A	405	U
26	A	411	G
26	A	448	U
26	A	451	U
26	A	456	C
26	A	473	G
26	A	479	A
26	A	480	A
26	A	481	G
26	A	490	C
26	A	491	G
26	A	504	A
26	A	505	A
26	A	508	A
26	A	509	C
26	A	529	A
26	A	530	G
26	A	531	C
26	A	532	A
26	A	533	G
26	A	549	G
26	A	562	U
26	A	563	A
26	A	573	U
26	A	603	A
26	A	614	A
26	A	615	U
26	A	616	A
26	A	622	G
26	A	637	A
26	A	646	U
26	A	647	G
26	A	655	A
26	A	664	G
26	A	668	A
26	A	675	A
26	A	686	U
26	A	695	G
26	A	711	G
26	A	717	C
26	A	726	G

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Mol	Chain	Res	Type
26	A	730	A
26	A	747	5MU
26	A	748	G
26	A	765	C
26	A	775	G
26	A	782	A
26	A	784	G
26	A	789	A
26	A	805	G
26	A	812	C
26	A	819	A
26	A	827	U
26	A	830	G
26	A	846	U
26	A	859	G
26	A	869	G
26	A	885	C
26	A	887	U
26	A	888	C
26	A	889	C
26	A	890	C
26	A	910	A
26	A	932	U
26	A	941	A
26	A	946	C
26	A	959	A
26	A	961	C
26	A	965	C
26	A	973	A
26	A	974	G
26	A	983	A
26	A	990	A
26	A	1009	A
26	A	1012	U
26	A	1013	C
26	A	1022	G
26	A	1023	U
26	A	1026	G
26	A	1033	U
26	A	1040	A
26	A	1042	G
26	A	1043	C

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Mol	Chain	Res	Type
26	A	1045	C
26	A	1046	A
26	A	1047	G
26	A	1057	A
26	A	1058	U
26	A	1059	G
26	A	1061	U
26	A	1062	G
26	A	1064	C
26	A	1065	U
26	A	1066	U
26	A	1067	A
26	A	1068	G
26	A	1069	A
26	A	1070	A
26	A	1071	G
26	A	1073	A
26	A	1076	C
26	A	1077	A
26	A	1078	U
26	A	1079	C
26	A	1084	A
26	A	1088	A
26	A	1092	C
26	A	1094	U
26	A	1100	C
26	A	1101	U
26	A	1110	G
26	A	1112	G
26	A	1119	U
26	A	1132	U
26	A	1133	A
26	A	1134	A
26	A	1135	C
26	A	1142	A
26	A	1143	A
26	A	1157	G
26	A	1171	G
26	A	1175	A
26	A	1178	C
26	A	1180	U
26	A	1206	G

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Mol	Chain	Res	Type
26	A	1210	G
26	A	1211	C
26	A	1236	G
26	A	1248	G
26	A	1253	A
26	A	1255	U
26	A	1256	G
26	A	1271	G
26	A	1272	A
26	A	1273	U
26	A	1300	G
26	A	1301	A
26	A	1311	G
26	A	1314	C
26	A	1325	U
26	A	1329	U
26	A	1345	C
26	A	1359	A
26	A	1365	A
26	A	1378	A
26	A	1379	U
26	A	1383	A
26	A	1392	A
26	A	1394	U
26	A	1395	A
26	A	1401	G
26	A	1403	A
26	A	1407	G
26	A	1416	G
26	A	1417	C
26	A	1420	A
26	A	1428	C
26	A	1437	C
26	A	1452	G
26	A	1455	G
26	A	1458	U
26	A	1460	U
26	A	1468	U
26	A	1482	G
26	A	1490	A
26	A	1493	C
26	A	1497	U

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Mol	Chain	Res	Type
26	A	1509	A
26	A	1515	A
26	A	1532	A
26	A	1534	U
26	A	1535	A
26	A	1536	C
26	A	1537	G
26	A	1566	A
26	A	1569	A
26	A	1578	U
26	A	1583	A
26	A	1608	A
26	A	1609	A
26	A	1618	6MZ
26	A	1639	C
26	A	1646	C
26	A	1648	U
26	A	1649	G
26	A	1654	A
26	A	1660	G
26	A	1674	G
26	A	1675	C
26	A	1715	G
26	A	1738	G
26	A	1758	U
26	A	1764	C
26	A	1773	A
26	A	1784	A
26	A	1791	A
26	A	1799	G
26	A	1800	C
26	A	1801	A
26	A	1808	A
26	A	1816	C
26	A	1829	A
26	A	1833	C
26	A	1847	A
26	A	1870	C
26	A	1871	A
26	A	1876	A
26	A	1906	G
26	A	1913	A

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Mol	Chain	Res	Type
26	A	1915	3TD
26	A	1927	A
26	A	1929	G
26	A	1930	G
26	A	1937	A
26	A	1941	C
26	A	1955	U
26	A	1960	A
26	A	1962	5MC
26	A	1963	U
26	A	1964	G
26	A	1967	C
26	A	1971	U
26	A	1972	G
26	A	1991	U
26	A	1992	G
26	A	1993	U
26	A	1997	C
26	A	2002	G
26	A	2021	C
26	A	2022	U
26	A	2023	C
26	A	2030	6MZ
26	A	2031	A
26	A	2032	G
26	A	2043	C
26	A	2051	A
26	A	2052	A
26	A	2055	C
26	A	2056	G
26	A	2060	A
26	A	2061	G
26	A	2062	A
26	A	2069	G7M
26	A	2070	A
26	A	2080	A
26	A	2100	G
26	A	2105	U
26	A	2107	G
26	A	2110	G
26	A	2111	U
26	A	2112	G

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Mol	Chain	Res	Type
26	A	2113	U
26	A	2116	G
26	A	2118	U
26	A	2119	A
26	A	2120	G
26	A	2125	G
26	A	2127	G
26	A	2129	C
26	A	2131	U
26	A	2132	U
26	A	2133	G
26	A	2134	A
26	A	2146	C
26	A	2147	A
26	A	2157	G
26	A	2159	G
26	A	2160	C
26	A	2162	G
26	A	2168	G
26	A	2171	A
26	A	2172	U
26	A	2173	A
26	A	2177	C
26	A	2178	C
26	A	2179	C
26	A	2182	U
26	A	2198	A
26	A	2204	G
26	A	2210	U
26	A	2211	A
26	A	2212	A
26	A	2225	A
26	A	2238	G
26	A	2239	G
26	A	2250	G
26	A	2251	OMG
26	A	2268	A
26	A	2278	A
26	A	2283	C
26	A	2287	A
26	A	2305	U
26	A	2308	G

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Mol	Chain	Res	Type
26	A	2310	C
26	A	2312	U
26	A	2319	G
26	A	2322	A
26	A	2333	A
26	A	2334	U
26	A	2335	A
26	A	2336	A
26	A	2342	C
26	A	2347	C
26	A	2350	C
26	A	2354	C
26	A	2357	G
26	A	2383	G
26	A	2385	C
26	A	2402	U
26	A	2403	C
26	A	2428	G
26	A	2429	G
26	A	2430	A
26	A	2434	A
26	A	2436	G
26	A	2441	U
26	A	2445	2MG
26	A	2447	G
26	A	2448	A
26	A	2470	G
26	A	2476	A
26	A	2478	A
26	A	2480	C
26	A	2484	G
26	A	2494	G
26	A	2502	G
26	A	2503	2MA
26	A	2504	PSU
26	A	2505	G
26	A	2506	U
26	A	2513	A
26	A	2518	A
26	A	2520	C
26	A	2525	G
26	A	2529	G

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Mol	Chain	Res	Type
26	A	2547	A
26	A	2554	U
26	A	2567	G
26	A	2581	G
26	A	2582	G
26	A	2585	U
26	A	2602	A
26	A	2609	U
26	A	2613	U
26	A	2629	U
26	A	2630	G
26	A	2639	A
26	A	2663	G
26	A	2689	U
26	A	2690	U
26	A	2714	G
26	A	2718	G
26	A	2726	A
26	A	2733	A
26	A	2744	G
26	A	2755	C
26	A	2758	A
26	A	2764	A
26	A	2765	A
26	A	2778	A
26	A	2791	G
26	A	2793	C
26	A	2797	U
26	A	2809	A
26	A	2818	U
26	A	2821	A
26	A	2833	U
26	A	2849	U
26	A	2872	A
26	A	2879	A
26	A	2884	U
27	B	24	G
27	B	26	C
27	B	35	C
27	B	38	C
27	B	42	C
27	B	45	A

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Mol	Chain	Res	Type
27	B	57	A
27	B	87	U
27	B	90	C
27	B	108	A
27	B	109	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	818	G
26	A	960	A
26	A	1042	G
26	A	1358	G
26	A	1875	G

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

43 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	$\# Z > 2$
26	PSU	A	2457	26	18,21,22	1.35	2 (11%)	22,30,33	1.95	5 (22%)
1	5MC	a	967	1	18,22,23	0.89	2 (11%)	26,32,35	1.00	3 (11%)
26	PSU	A	1917	26	18,21,22	1.46	4 (22%)	22,30,33	1.88	4 (18%)
22	4SU	v	8	22	18,21,22	1.77	5 (27%)	26,30,33	2.25	5 (19%)
26	PSU	A	955	26	18,21,22	1.45	3 (16%)	22,30,33	2.07	3 (13%)
26	2MG	A	2445	26	23,26,27	1.29	4 (17%)	32,38,41	2.34	7 (21%)
1	2MG	a	1207	1	23,26,27	1.27	4 (17%)	32,38,41	2.27	7 (21%)
26	2MA	A	2503	26	22,25,26	1.62	5 (22%)	33,37,40	2.40	8 (24%)
22	5MU	v	54	22	19,22,23	1.45	6 (31%)	28,32,35	2.08	9 (32%)
26	OMG	A	2251	26,22	23,26,27	1.24	3 (13%)	33,38,41	1.92	5 (15%)
26	3TD	A	1915	26	18,22,23	4.08	7 (38%)	22,32,35	1.90	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	G7M	A	2069	26	23,26,27	1.70	4 (17%)	35,39,42	2.14	8 (22%)
26	OMC	A	2498	26	19,22,23	0.91	0	26,31,34	1.29	4 (15%)
1	PSU	a	516	1	18,21,22	1.34	2 (11%)	22,30,33	1.83	4 (18%)
26	5MC	A	1962	26	18,22,23	0.89	1 (5%)	26,32,35	1.49	4 (15%)
1	2MG	a	966	1	23,26,27	1.32	4 (17%)	32,38,41	2.26	5 (15%)
24	H2U	y	19	24	18,21,22	1.25	3 (16%)	21,30,33	2.79	5 (23%)
26	6MZ	A	2030	26	22,25,26	1.58	3 (13%)	30,36,39	3.05	12 (40%)
24	5MU	y	54	24	19,22,23	1.51	4 (21%)	28,32,35	2.61	8 (28%)
1	MA6	a	1519	1	23,26,27	1.56	3 (13%)	34,38,41	2.50	12 (35%)
26	5MU	A	747	26	19,22,23	1.52	5 (26%)	28,32,35	1.95	6 (21%)
26	H2U	A	2449	26	18,21,22	1.16	3 (16%)	21,30,33	1.54	3 (14%)
1	4OC	a	1402	1	20,23,24	0.77	1 (5%)	26,32,35	1.15	2 (7%)
22	H2U	v	20	22	18,21,22	1.01	2 (11%)	21,30,33	1.44	2 (9%)
24	6IA	y	37	24	26,29,30	1.36	4 (15%)	37,41,44	1.98	9 (24%)
22	PSU	v	55	22	18,21,22	1.48	3 (16%)	22,30,33	1.93	4 (18%)
26	PSU	A	2580	26	18,21,22	1.38	2 (11%)	22,30,33	1.89	4 (18%)
26	PSU	A	746	26	18,21,22	1.33	2 (11%)	22,30,33	1.88	4 (18%)
1	UR3	a	1498	1	19,22,23	1.05	1 (5%)	26,32,35	1.90	5 (19%)
1	MA6	a	1518	1	23,26,27	1.54	3 (13%)	34,38,41	2.58	15 (44%)
24	PSU	y	55	24	18,21,22	1.38	3 (16%)	22,30,33	2.88	9 (40%)
1	2MG	a	1516	1	23,26,27	1.27	4 (17%)	32,38,41	2.17	6 (18%)
26	PSU	A	2504	26	18,21,22	1.42	4 (22%)	22,30,33	1.93	3 (13%)
26	6MZ	A	1618	26	22,25,26	1.55	3 (13%)	30,36,39	2.38	10 (33%)
26	PSU	A	1911	26	18,21,22	1.42	3 (16%)	22,30,33	1.92	4 (18%)
26	5MU	A	1939	26	19,22,23	1.40	6 (31%)	28,32,35	2.11	6 (21%)
1	5MC	a	1407	1	18,22,23	0.96	2 (11%)	26,32,35	1.31	3 (11%)
26	PSU	A	2604	26	18,21,22	1.43	2 (11%)	22,30,33	2.01	3 (13%)
26	2MG	A	1835	26	23,26,27	1.23	3 (13%)	32,38,41	2.53	9 (28%)
26	PSU	A	2605	26	18,21,22	1.36	3 (16%)	22,30,33	1.94	4 (18%)
26	OMU	A	2552	26	19,22,23	1.22	3 (15%)	26,31,34	1.88	7 (26%)
26	1MG	A	745	26	22,26,27	1.20	1 (4%)	33,39,42	1.86	9 (27%)
1	G7M	a	527	1	23,26,27	1.77	5 (21%)	35,39,42	2.34	10 (28%)

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
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
26	PSU	A	1917	26	-	2/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
26	2MG	A	2445	26	-	2/9/27/28	0/3/3/3
1	2MG	a	1207	1	-	1/9/27/28	0/3/3/3
26	2MA	A	2503	26	-	4/7/25/26	0/3/3/3
22	5MU	v	54	22	-	2/7/25/26	0/2/2/2
26	OMG	A	2251	26,22	-	1/9/27/28	0/3/3/3
26	3TD	A	1915	26	-	5/7/25/26	0/2/2/2
26	G7M	A	2069	26	2/2/5/5	2/7/25/26	0/3/3/3
26	OMC	A	2498	26	-	0/9/27/28	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
26	5MC	A	1962	26	-	5/7/25/26	0/2/2/2
1	2MG	a	966	1	-	0/9/27/28	0/3/3/3
24	H2U	y	19	24	-	4/7/38/39	0/2/2/2
26	6MZ	A	2030	26	-	4/9/27/28	0/3/3/3
24	5MU	y	54	24	-	3/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	3/11/29/30	0/3/3/3
26	5MU	A	747	26	-	0/7/25/26	0/2/2/2
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
1	4OC	a	1402	1	-	0/9/29/30	0/2/2/2
22	H2U	v	20	22	-	1/7/38/39	0/2/2/2
24	6IA	y	37	24	-	1/13/31/32	0/3/3/3
22	PSU	v	55	22	-	2/7/25/26	0/2/2/2
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2
26	PSU	A	746	26	-	1/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	4/11/29/30	0/3/3/3
24	PSU	y	55	24	-	5/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	2/9/27/28	0/3/3/3
26	PSU	A	2504	26	-	2/7/25/26	0/2/2/2
26	6MZ	A	1618	26	-	2/9/27/28	0/3/3/3
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
26	2MG	A	1835	26	-	0/9/27/28	0/3/3/3
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
26	OMU	A	2552	26	-	2/9/27/28	0/2/2/2
26	1MG	A	745	26	-	0/7/25/26	0/3/3/3
1	G7M	a	527	1	2/2/5/5	0/7/25/26	0/3/3/3

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1915	3TD	C6-C5	11.65	1.48	1.35
26	A	1915	3TD	C2-N1	9.25	1.49	1.37
26	A	1915	3TD	C6-N1	5.96	1.46	1.36
26	A	1618	6MZ	C5-C4	5.23	1.48	1.39
26	A	2030	6MZ	C5-C4	5.19	1.48	1.39
26	A	2503	2MA	C5-C4	5.11	1.48	1.39
1	a	527	G7M	C5-N7	-4.93	1.33	1.39
1	a	1518	MA6	C5-C4	4.76	1.47	1.39
1	a	1519	MA6	C5-C4	4.70	1.47	1.39
24	y	37	6IA	C5-C4	4.66	1.47	1.39
22	v	8	4SU	C4-S4	-4.65	1.59	1.68
26	A	2069	G7M	C5-N7	-4.50	1.34	1.39
1	a	527	G7M	C5-C4	4.07	1.48	1.38
24	y	54	5MU	C2-N1	3.86	1.44	1.38
24	y	55	PSU	C2-N1	-3.85	1.31	1.36
26	A	2069	G7M	C5-C4	3.81	1.47	1.38
26	A	745	1MG	C5-C4	3.56	1.48	1.38
26	A	1915	3TD	O4-C4	-3.49	1.15	1.23
26	A	955	PSU	C6-C5	3.49	1.39	1.35
26	A	1911	PSU	C6-C5	3.47	1.39	1.35
26	A	1917	PSU	C6-C5	3.44	1.39	1.35
1	a	1519	MA6	C5-C6	3.40	1.50	1.41
26	A	2504	PSU	C6-C5	3.37	1.39	1.35
1	a	516	PSU	C6-C5	3.36	1.39	1.35
22	v	55	PSU	C6-C5	3.36	1.39	1.35
26	A	1915	3TD	C2-N3	3.35	1.46	1.38
24	y	19	H2U	C2-N3	-3.34	1.32	1.38
1	a	1518	MA6	C5-C6	3.30	1.50	1.41
26	A	2604	PSU	C6-C5	3.30	1.39	1.35
1	a	966	2MG	C5-C4	3.28	1.47	1.38
1	a	1516	2MG	C5-C4	3.21	1.47	1.38
26	A	2580	PSU	C6-C5	3.20	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	55	PSU	C4-N3	-3.20	1.32	1.38
26	A	2503	2MA	C5-C6	3.19	1.49	1.41
22	v	8	4SU	C5-C4	-3.16	1.38	1.42
1	a	1207	2MG	C5-C4	3.13	1.47	1.38
26	A	2445	2MG	C5-C4	3.12	1.47	1.38
26	A	2457	PSU	C6-C5	3.08	1.38	1.35
26	A	746	PSU	C6-C5	3.07	1.38	1.35
26	A	2251	OMG	C5-C4	3.06	1.47	1.38
26	A	1835	2MG	C5-C4	3.06	1.47	1.38
26	A	2604	PSU	C4-N3	-3.00	1.33	1.38
26	A	2030	6MZ	C5-C6	2.99	1.49	1.41
26	A	747	5MU	C6-C5	2.98	1.39	1.34
22	v	8	4SU	C4-N3	-2.96	1.34	1.37
26	A	747	5MU	C2-N1	2.95	1.43	1.38
26	A	2449	H2U	C2-N3	-2.92	1.32	1.38
26	A	2605	PSU	C4-N3	-2.91	1.33	1.38
24	y	54	5MU	C4-N3	-2.90	1.33	1.38
26	A	2605	PSU	C6-C5	2.89	1.38	1.35
26	A	1618	6MZ	C5-C6	2.82	1.49	1.41
22	v	54	5MU	C2-N1	2.81	1.42	1.38
26	A	747	5MU	C4-N3	-2.81	1.33	1.38
22	v	54	5MU	C4-N3	-2.79	1.33	1.38
26	A	2504	PSU	C4-N3	-2.78	1.33	1.38
26	A	1911	PSU	C4-N3	-2.78	1.33	1.38
26	A	955	PSU	C4-N3	-2.77	1.33	1.38
1	a	1498	UR3	C2-N1	2.76	1.42	1.38
1	a	527	G7M	C6-N1	-2.76	1.33	1.38
26	A	1939	5MU	C6-C5	2.75	1.39	1.34
1	a	966	2MG	C6-N1	-2.71	1.33	1.38
26	A	746	PSU	C4-N3	-2.71	1.33	1.38
26	A	1939	5MU	C4-N3	-2.69	1.33	1.38
24	y	37	6IA	C5-C6	2.68	1.48	1.41
26	A	2457	PSU	C4-N3	-2.67	1.33	1.38
26	A	2445	2MG	C6-N1	-2.65	1.33	1.38
22	v	20	H2U	C2-N3	-2.63	1.33	1.38
24	y	55	PSU	C6-N1	-2.63	1.31	1.36
26	A	2580	PSU	C4-N3	-2.62	1.34	1.38
26	A	2069	G7M	C6-N1	-2.62	1.34	1.38
26	A	2449	H2U	C4-N3	-2.60	1.33	1.37
26	A	1917	PSU	C4-N3	-2.60	1.34	1.38
1	a	1407	5MC	C6-C5	2.58	1.38	1.34
1	a	527	G7M	O2'-C2'	-2.57	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2069	G7M	O2'-C2'	-2.57	1.36	1.43
24	y	19	H2U	O4-C4	-2.54	1.18	1.23
1	a	1207	2MG	C6-N1	-2.54	1.34	1.38
26	A	1915	3TD	O2-C2	-2.54	1.18	1.23
26	A	2552	OMU	C4-N3	-2.53	1.34	1.38
22	v	55	PSU	C2-N3	-2.51	1.33	1.37
24	y	37	6IA	C8-N7	2.50	1.36	1.31
26	A	2251	OMG	C6-N1	-2.50	1.34	1.38
26	A	1962	5MC	C6-N1	-2.46	1.33	1.38
1	a	966	2MG	C2-N3	2.45	1.36	1.31
22	v	54	5MU	C6-C5	2.43	1.38	1.34
1	a	1516	2MG	C6-N1	-2.43	1.34	1.38
1	a	967	5MC	C6-C5	2.42	1.38	1.34
22	v	20	H2U	C4-N3	-2.39	1.33	1.37
26	A	2449	H2U	C2-N1	-2.39	1.32	1.35
24	y	55	PSU	C4-N3	-2.38	1.34	1.38
26	A	2030	6MZ	C5-N7	-2.37	1.34	1.39
26	A	747	5MU	C4-C5	2.36	1.48	1.44
24	y	54	5MU	C6-C5	2.36	1.38	1.34
26	A	1835	2MG	C6-N1	-2.35	1.34	1.38
1	a	516	PSU	C4-N3	-2.35	1.34	1.38
1	a	966	2MG	C5-N7	-2.32	1.34	1.39
24	y	19	H2U	C4-N3	-2.31	1.33	1.37
1	a	1516	2MG	C2-N3	2.26	1.36	1.31
26	A	2445	2MG	C2-N3	2.25	1.36	1.31
26	A	1939	5MU	C4-C5	2.24	1.48	1.44
24	y	54	5MU	C6-N1	-2.24	1.34	1.38
22	v	54	5MU	C6-N1	-2.22	1.34	1.38
26	A	1939	5MU	C6-N1	-2.22	1.34	1.38
26	A	1915	3TD	C4-N3	2.21	1.45	1.40
26	A	2445	2MG	C5-N7	-2.19	1.34	1.39
26	A	2251	OMG	C5-N7	-2.18	1.34	1.39
1	a	1207	2MG	C5-N7	-2.18	1.34	1.39
1	a	1518	MA6	C4-N9	-2.18	1.32	1.37
1	a	1207	2MG	C2-N3	2.17	1.36	1.31
1	a	1519	MA6	C8-N7	2.17	1.35	1.31
26	A	2503	2MA	C8-N7	2.15	1.35	1.31
26	A	2552	OMU	C2-N3	-2.15	1.34	1.38
26	A	1917	PSU	C4-C5	2.14	1.50	1.44
26	A	1835	2MG	C5-N7	-2.13	1.35	1.39
26	A	1618	6MZ	C8-N7	2.13	1.35	1.31
26	A	2605	PSU	C2-N3	-2.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1939	5MU	C2-N1	2.12	1.41	1.38
22	v	54	5MU	C2-N3	-2.11	1.34	1.38
1	a	1407	5MC	C6-N1	-2.10	1.34	1.38
1	a	527	G7M	C5-C6	2.10	1.49	1.43
26	A	1939	5MU	C2-N3	-2.09	1.34	1.38
26	A	2504	PSU	C2-N3	-2.09	1.33	1.37
1	a	967	5MC	C6-N1	-2.09	1.34	1.38
22	v	54	5MU	C4-C5	2.09	1.48	1.44
26	A	2503	2MA	C4-N9	-2.07	1.33	1.37
26	A	2504	PSU	C4-C5	2.07	1.50	1.44
26	A	2503	2MA	C5-N7	-2.06	1.35	1.39
26	A	747	5MU	C2-N3	-2.04	1.34	1.38
26	A	1917	PSU	C2-N1	-2.04	1.34	1.36
26	A	1911	PSU	C2-N3	-2.04	1.34	1.37
26	A	2552	OMU	C2-N1	2.03	1.41	1.38
24	y	37	6IA	C5-N7	-2.03	1.35	1.39
26	A	955	PSU	C2-N1	-2.02	1.34	1.36
22	v	8	4SU	C2-N3	-2.02	1.34	1.38
1	a	1516	2MG	C5-N7	-2.02	1.35	1.39
22	v	8	4SU	C2-N1	2.01	1.41	1.38
1	a	1402	4OC	C6-C5	2.00	1.39	1.35

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2030	6MZ	C5-C4-N3	-8.83	115.23	126.75
26	A	1835	2MG	C2-N3-C4	8.77	122.91	112.04
24	y	19	H2U	C4-N3-C2	-8.63	118.63	125.79
26	A	2503	2MA	C5-C4-N3	-7.79	118.43	127.19
1	a	1207	2MG	C2-N3-C4	7.62	121.49	112.04
26	A	2445	2MG	C2-N3-C4	7.60	121.46	112.04
26	A	2030	6MZ	N3-C4-N9	7.21	138.96	127.08
1	a	966	2MG	C2-N3-C4	7.20	120.97	112.04
1	a	1516	2MG	C2-N3-C4	7.18	120.95	112.04
26	A	1835	2MG	C5-C4-N3	-7.02	117.08	128.46
26	A	2503	2MA	N3-C4-N9	6.84	136.47	126.99
26	A	2445	2MG	C5-C4-N3	-6.75	117.51	128.46
24	y	55	PSU	C6-C5-C4	-6.71	113.51	118.20
1	a	966	2MG	C5-C4-N3	-6.70	117.59	128.46
26	A	955	PSU	N1-C2-N3	6.62	122.63	115.13
26	A	2604	PSU	N1-C2-N3	6.61	122.62	115.13
24	y	19	H2U	C5-C4-N3	6.49	123.94	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1207	2MG	C5-C4-N3	-6.46	117.98	128.46
1	a	527	G7M	C5-C4-N3	-6.39	115.90	128.15
26	A	2504	PSU	N1-C2-N3	6.24	122.20	115.13
1	a	527	G7M	N9-C4-N3	6.17	138.33	125.94
26	A	1618	6MZ	C5-C4-N3	-6.12	118.77	126.75
1	a	1516	2MG	C5-C4-N3	-6.11	118.55	128.46
26	A	2457	PSU	N1-C2-N3	6.08	122.02	115.13
1	a	1498	UR3	C4-N3-C2	-6.06	118.86	124.56
26	A	2580	PSU	N1-C2-N3	6.05	121.98	115.13
26	A	2605	PSU	N1-C2-N3	6.05	121.98	115.13
22	v	55	PSU	N1-C2-N3	6.03	121.97	115.13
22	v	8	4SU	C4-N3-C2	-5.97	121.55	127.34
26	A	2251	OMG	C5-C4-N3	-5.93	118.85	128.46
26	A	746	PSU	N1-C2-N3	5.91	121.83	115.13
26	A	1917	PSU	N1-C2-N3	5.86	121.76	115.13
22	v	8	4SU	C5-C4-N3	5.83	120.10	114.69
24	y	54	5MU	O4-C4-C5	-5.81	118.17	124.90
26	A	1911	PSU	N1-C2-N3	5.75	121.65	115.13
24	y	37	6IA	C5-C4-N3	-5.67	119.35	126.75
1	a	966	2MG	N9-C4-N3	5.64	137.27	125.94
24	y	55	PSU	O2-C2-N1	-5.61	116.61	122.79
24	y	55	PSU	N1-C2-N3	5.50	121.36	115.13
26	A	1618	6MZ	N3-C4-N9	5.45	136.05	127.08
1	a	516	PSU	N1-C2-N3	5.42	121.27	115.13
26	A	2069	G7M	N9-C4-N3	5.38	136.75	125.94
26	A	2449	H2U	C4-N3-C2	-5.38	121.33	125.79
1	a	1518	MA6	C5-C4-N3	-5.37	119.74	126.75
26	A	2069	G7M	C5-C4-N3	-5.36	117.87	128.15
22	v	8	4SU	C5-C4-S4	-5.35	117.57	124.47
1	a	1519	MA6	C5-C4-N3	-5.33	119.79	126.75
26	A	1939	5MU	C4-N3-C2	-5.28	120.52	127.35
24	y	54	5MU	C5-C4-N3	5.23	119.78	115.31
24	y	54	5MU	C1'-N1-C2	5.19	126.96	117.57
1	a	1518	MA6	C9-N6-C6	-5.07	107.25	120.40
26	A	747	5MU	N3-C2-N1	5.07	121.62	114.89
1	a	1519	MA6	C2-N1-C6	5.02	123.62	111.75
26	A	1835	2MG	N9-C4-N3	5.00	135.97	125.94
26	A	1915	3TD	N1-C2-N3	4.98	120.07	116.14
1	a	1519	MA6	C4-C5-N7	-4.90	104.65	110.62
1	a	527	G7M	C2-N3-C4	4.89	121.01	112.30
26	A	2251	OMG	C2-N3-C4	4.88	120.99	112.30
1	a	1518	MA6	C2-N1-C6	4.87	123.25	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1939	5MU	N3-C2-N1	4.86	121.34	114.89
26	A	2030	6MZ	C4-C5-N7	-4.84	104.73	110.62
26	A	2445	2MG	N9-C4-N3	4.82	135.61	125.94
1	a	1207	2MG	N9-C4-N3	4.80	135.58	125.94
26	A	1939	5MU	C5-C4-N3	4.77	119.38	115.31
26	A	2030	6MZ	C5-N7-C8	4.75	110.27	103.51
1	a	1519	MA6	C10-N6-C6	-4.74	108.10	120.40
26	A	2030	6MZ	C2-N3-C4	4.73	122.93	111.75
24	y	54	5MU	C4-N3-C2	-4.70	121.26	127.35
24	y	55	PSU	C4-N3-C2	-4.67	119.61	126.34
26	A	1915	3TD	C4-N3-C2	-4.66	119.56	124.61
26	A	747	5MU	C4-N3-C2	-4.66	121.32	127.35
24	y	54	5MU	N3-C2-N1	4.61	121.01	114.89
1	a	1516	2MG	N9-C4-N3	4.61	135.19	125.94
24	y	19	H2U	O4-C4-C5	-4.59	112.36	122.17
22	v	54	5MU	C4-N3-C2	-4.58	121.42	127.35
1	a	1518	MA6	C4-C5-N7	-4.49	105.15	110.62
22	v	54	5MU	N3-C2-N1	4.43	120.78	114.89
22	v	54	5MU	C5-C4-N3	4.43	119.09	115.31
26	A	2552	OMU	N3-C2-N1	4.38	120.70	114.89
26	A	955	PSU	O2-C2-N1	-4.35	118.00	122.79
26	A	1618	6MZ	C9-N6-C6	-4.31	119.16	122.87
24	y	37	6IA	N3-C4-N9	4.30	134.17	127.08
26	A	2605	PSU	C4-N3-C2	-4.27	120.18	126.34
26	A	2069	G7M	C2-N3-C4	4.24	119.85	112.30
1	a	1498	UR3	C1'-N1-C2	4.23	124.14	116.99
26	A	1618	6MZ	C6-C5-N7	4.21	136.95	132.39
26	A	1911	PSU	C4-N3-C2	-4.17	120.33	126.34
26	A	745	1MG	C5-C4-N3	-4.17	121.70	128.46
26	A	2069	G7M	CN7-N7-C5	4.16	131.94	126.77
24	y	37	6IA	C6-C5-N7	4.14	136.87	132.39
26	A	1962	5MC	C5-C6-N1	-4.11	119.11	123.34
26	A	2030	6MZ	C6-C5-N7	4.11	136.83	132.39
26	A	2552	OMU	C1'-N1-C2	4.09	124.97	117.57
26	A	1939	5MU	O4-C4-C5	-4.06	120.19	124.90
24	y	54	5MU	O2-C2-N3	-4.04	113.97	121.50
26	A	2457	PSU	C4-N3-C2	-4.04	120.52	126.34
26	A	1915	3TD	O4-C4-N3	-4.04	112.90	120.30
26	A	745	1MG	C2-N3-C4	4.04	121.05	111.98
26	A	746	PSU	C4-N3-C2	-4.03	120.53	126.34
26	A	747	5MU	C5-C4-N3	4.02	118.74	115.31
26	A	1939	5MU	C5-C6-N1	-3.98	119.25	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1518	MA6	C2-N3-C4	3.98	121.14	111.75
24	y	37	6IA	C2-N3-C4	3.96	121.10	111.75
26	A	1618	6MZ	C2-N3-C4	3.96	121.10	111.75
26	A	2604	PSU	C4-N3-C2	-3.96	120.64	126.34
26	A	2503	2MA	C2-N1-C6	3.94	124.22	118.08
1	a	1519	MA6	C5-N7-C8	3.93	109.09	103.51
26	A	2251	OMG	N9-C4-N3	3.92	133.81	125.94
1	a	1519	MA6	C2-N3-C4	3.92	121.01	111.75
26	A	2552	OMU	C4-N3-C2	-3.92	121.41	126.58
22	v	20	H2U	C4-N3-C2	-3.92	122.54	125.79
26	A	2069	G7M	O3'-C3'-C4'	3.91	122.36	111.05
26	A	2504	PSU	C4-N3-C2	-3.89	120.73	126.34
22	v	55	PSU	C4-N3-C2	-3.88	120.74	126.34
1	a	1518	MA6	N3-C4-N9	3.88	133.48	127.08
24	y	55	PSU	O4-C4-C5	-3.88	113.90	124.05
26	A	2498	OMC	O2-C2-N3	-3.86	116.05	122.33
24	y	37	6IA	N3-C2-N1	-3.86	122.56	128.60
26	A	955	PSU	C4-N3-C2	-3.86	120.78	126.34
1	a	1519	MA6	N3-C4-N9	3.80	133.35	127.08
26	A	745	1MG	N9-C4-N3	3.79	133.56	125.94
1	a	516	PSU	C4-N3-C2	-3.77	120.91	126.34
26	A	2030	6MZ	C4-N9-C8	3.76	109.80	105.73
24	y	54	5MU	C1'-N1-C6	-3.74	114.89	121.12
26	A	2580	PSU	C4-N3-C2	-3.74	120.95	126.34
26	A	1917	PSU	O2-C2-N1	-3.73	118.69	122.79
1	a	1519	MA6	N1-C2-N3	-3.72	122.78	128.60
22	v	8	4SU	N3-C2-N1	3.71	119.81	114.89
26	A	2503	2MA	C4-N9-C8	3.71	109.75	105.73
22	v	54	5MU	O4-C4-C5	-3.69	120.62	124.90
26	A	2604	PSU	O2-C2-N1	-3.66	118.76	122.79
1	a	1518	MA6	N1-C6-N6	-3.64	113.11	117.08
1	a	1518	MA6	N1-C2-N3	-3.59	122.99	128.60
1	a	1518	MA6	C6-C5-N7	3.59	139.31	133.28
26	A	2457	PSU	O2-C2-N1	-3.57	118.86	122.79
1	a	527	G7M	CN7-N7-C5	3.56	131.19	126.77
26	A	2251	OMG	C6-C5-N7	3.55	136.86	130.25
1	a	1498	UR3	O2-C2-N3	-3.53	116.36	121.34
1	a	1407	5MC	O2-C2-N3	-3.51	116.61	122.33
1	a	1519	MA6	C6-C5-N7	3.45	139.07	133.28
1	a	1519	MA6	C10-N6-C9	-3.45	105.01	116.12
26	A	2030	6MZ	C1'-N9-C8	-3.44	119.36	127.14
26	A	745	1MG	C6-C5-N7	3.39	137.02	129.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2580	PSU	O2-C2-N1	-3.39	119.06	122.79
1	a	1518	MA6	C5-N7-C8	3.37	108.30	103.51
26	A	746	PSU	O2-C2-N1	-3.36	119.09	122.79
26	A	1618	6MZ	C4-N9-C8	3.36	109.37	105.73
26	A	2030	6MZ	N9-C8-N7	-3.32	109.37	113.91
1	a	1519	MA6	C4-N9-C8	3.31	109.31	105.73
26	A	1835	2MG	C6-C5-N7	3.28	136.35	130.25
1	a	527	G7M	O3'-C3'-C4'	3.27	120.50	111.05
22	v	54	5MU	C1'-N1-C2	3.26	123.48	117.57
1	a	527	G7M	O3'-C3'-C2'	3.26	122.37	111.82
24	y	37	6IA	C4-C5-N7	-3.25	106.65	110.62
26	A	747	5MU	O4-C4-C5	-3.25	121.14	124.90
26	A	2552	OMU	C5-C4-N3	3.23	119.68	114.84
24	y	54	5MU	C6-N1-C2	-3.23	118.03	121.30
1	a	1402	4OC	O2-C2-N3	-3.21	117.11	122.33
26	A	1618	6MZ	C4-C5-N7	-3.19	106.73	110.62
26	A	745	1MG	C6-C5-C4	-3.19	116.44	119.97
24	y	55	PSU	C6-N1-C2	-3.14	119.47	122.68
26	A	1917	PSU	C4-N3-C2	-3.11	121.86	126.34
26	A	1618	6MZ	N1-C2-N3	-3.09	123.78	128.60
1	a	1516	2MG	C6-C5-N7	3.08	135.97	130.25
1	a	1498	UR3	C6-N1-C2	-3.07	119.03	121.79
1	a	1207	2MG	C6-C5-N7	3.05	135.93	130.25
26	A	2445	2MG	C6-C5-N7	3.05	135.93	130.25
26	A	2605	PSU	O2-C2-N1	-3.04	119.44	122.79
26	A	747	5MU	C5-C6-N1	-3.04	120.21	123.34
26	A	2504	PSU	O2-C2-N1	-3.01	119.48	122.79
26	A	1962	5MC	N4-C4-N3	3.00	123.95	118.48
26	A	2251	OMG	C4-C5-N7	-2.97	106.03	110.72
1	a	516	PSU	O2-C2-N1	-2.96	119.54	122.79
26	A	1962	5MC	C5-C4-N4	-2.94	117.08	121.48
26	A	1911	PSU	O2-C2-N1	-2.92	119.57	122.79
26	A	2030	6MZ	C9-N6-C6	-2.92	120.36	122.87
26	A	2503	2MA	C4-C5-N7	-2.89	107.10	110.62
26	A	2552	OMU	O2-C2-N3	-2.88	116.14	121.50
24	y	55	PSU	O4-C4-N3	2.86	125.60	120.12
26	A	2445	2MG	C4-C5-N7	-2.85	106.21	110.72
1	a	1518	MA6	C4-N9-C8	2.85	108.81	105.73
22	v	54	5MU	C1'-N1-C6	-2.81	116.44	121.12
1	a	1519	MA6	N9-C8-N7	-2.80	110.08	113.91
1	a	1407	5MC	C5-C6-N1	-2.80	120.46	123.34
22	v	54	5MU	C5-C6-N1	-2.78	120.48	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1835	2MG	CM2-N2-C2	-2.78	117.73	123.86
26	A	2069	G7M	O3'-C3'-C2'	2.75	120.71	111.82
26	A	1835	2MG	C4-C5-N7	-2.74	106.38	110.72
26	A	2503	2MA	N6-C6-N1	2.73	120.89	117.03
26	A	1618	6MZ	C5-N7-C8	2.71	107.36	103.51
26	A	1835	2MG	C2-N1-C6	-2.70	121.37	124.48
26	A	747	5MU	O2-C2-N3	-2.69	116.49	121.50
26	A	745	1MG	C4-C5-N7	-2.64	106.54	110.72
22	v	54	5MU	O2-C2-N3	-2.64	116.59	121.50
1	a	527	G7M	C5'-C4'-C3'	2.63	125.03	115.18
22	v	55	PSU	C6-C5-C4	-2.61	116.37	118.20
1	a	1407	5MC	C5-C4-N3	-2.60	118.87	121.67
26	A	1917	PSU	C6-C5-C4	-2.58	116.39	118.20
24	y	37	6IA	C5-N7-C8	2.58	107.17	103.51
1	a	1207	2MG	C4-C5-N7	-2.58	106.64	110.72
26	A	2445	2MG	C2-N1-C6	-2.57	121.52	124.48
26	A	2552	OMU	O4-C4-C5	-2.57	120.64	125.16
26	A	1939	5MU	O2-C2-N1	-2.57	119.37	122.79
26	A	2445	2MG	CM2-N2-C2	-2.56	118.21	123.86
26	A	1962	5MC	C5-C4-N3	-2.56	118.91	121.67
26	A	2498	OMC	O2-C2-N1	2.56	124.17	118.89
26	A	2503	2MA	C5-N7-C8	2.54	107.12	103.51
22	v	55	PSU	O2-C2-N3	-2.53	117.05	121.82
1	a	1516	2MG	C4-C5-N7	-2.47	106.81	110.72
1	a	527	G7M	C1'-N9-C4	2.45	133.79	126.50
1	a	1518	MA6	C5-C6-N6	2.44	129.55	125.30
24	y	19	H2U	C5-C6-N1	-2.43	103.61	111.61
24	y	37	6IA	C2-N1-C6	2.42	123.38	115.25
26	A	2498	OMC	CM2-O2'-C2'	-2.42	108.18	114.52
26	A	2069	G7M	C5'-C4'-C3'	2.37	124.07	115.18
26	A	745	1MG	C8-N9-C4	2.37	110.55	106.05
1	a	967	5MC	C5-C6-N1	-2.36	120.91	123.34
1	a	1402	4OC	C6-C5-C4	2.35	119.83	116.96
26	A	746	PSU	C5-C6-N1	-2.35	118.59	122.11
26	A	2498	OMC	C1'-N1-C2	2.35	123.66	118.42
1	a	1498	UR3	C3U-N3-C4	2.34	121.24	117.89
24	y	37	6IA	C4-N9-C8	2.34	108.26	105.73
1	a	1518	MA6	C10-N6-C9	-2.33	108.61	116.12
1	a	527	G7M	O4'-C4'-C5'	2.32	117.01	109.37
24	y	55	PSU	C5-C6-N1	2.29	125.53	122.11
1	a	516	PSU	C6-C5-C4	-2.27	116.61	118.20
22	v	54	5MU	C5M-C5-C4	2.26	121.26	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2449	H2U	C5-C6-N1	-2.25	104.21	111.61
26	A	2457	PSU	C5-C6-N1	-2.24	118.75	122.11
26	A	1835	2MG	C5-C6-N1	2.24	118.87	113.19
26	A	2605	PSU	C5-C6-N1	-2.22	118.77	122.11
26	A	2552	OMU	C6-N1-C2	-2.22	118.15	120.99
1	a	1518	MA6	N9-C8-N7	-2.21	110.89	113.91
1	a	966	2MG	C6-C5-N7	2.21	134.36	130.25
26	A	2069	G7M	C8-N7-C5	-2.21	105.02	107.78
26	A	1911	PSU	C6-C5-C4	-2.19	116.66	118.20
26	A	745	1MG	C1'-N9-C4	-2.18	120.02	126.50
1	a	1207	2MG	O6-C6-C5	-2.18	120.82	126.60
1	a	966	2MG	O6-C6-C5	-2.17	120.84	126.60
26	A	2503	2MA	N9-C8-N7	-2.17	110.95	113.91
26	A	1835	2MG	O6-C6-C5	-2.17	120.86	126.60
1	a	527	G7M	O2'-C2'-C1'	2.16	117.25	110.02
22	v	8	4SU	S4-C4-N3	2.16	122.33	120.21
24	y	19	H2U	O4-C4-N3	2.16	123.70	120.28
26	A	2580	PSU	O4'-C1'-C2'	2.14	108.16	105.14
26	A	2449	H2U	O2-C2-N1	-2.13	120.43	123.11
1	a	1516	2MG	O6-C6-C5	-2.12	120.98	126.60
24	y	55	PSU	O4'-C1'-C2'	2.12	108.13	105.14
26	A	745	1MG	C8-N7-C5	2.10	108.05	104.24
26	A	2030	6MZ	C4-C5-C6	2.10	118.44	116.81
22	v	20	H2U	C5-C4-N3	2.09	119.00	116.65
1	a	967	5MC	C5-C4-N3	-2.08	119.43	121.67
26	A	2030	6MZ	N1-C2-N3	-2.07	125.37	128.60
1	a	1207	2MG	C2-N1-C6	-2.06	122.11	124.48
1	a	967	5MC	CM5-C5-C6	-2.06	120.10	122.85
1	a	1518	MA6	C2'-C1'-N9	-2.02	108.20	113.30
26	A	1618	6MZ	C2-N1-C6	2.01	121.99	115.25
26	A	2457	PSU	O4'-C1'-C2'	2.00	107.97	105.14

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3'
1	a	527	G7M	C4'
26	A	2069	G7M	C3'
26	A	2069	G7M	C4'

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1498	UR3	O4'-C1'-N1-C6
1	a	1498	UR3	O4'-C1'-N1-C2
1	a	1518	MA6	O4'-C1'-N9-C8
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	N1-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C10
22	v	54	5MU	C3'-C4'-C5'-O5'
22	v	54	5MU	O4'-C4'-C5'-O5'
22	v	55	PSU	O4'-C1'-C5-C4
22	v	55	PSU	O4'-C1'-C5-C6
24	y	19	H2U	O4'-C1'-N1-C6
24	y	19	H2U	C2'-C1'-N1-C6
24	y	55	PSU	O4'-C4'-C5'-O5'
26	A	1618	6MZ	O4'-C4'-C5'-O5'
26	A	1618	6MZ	C3'-C4'-C5'-O5'
26	A	1915	3TD	O4'-C1'-C5-C4
26	A	1915	3TD	C2'-C1'-C5-C6
26	A	1915	3TD	O4'-C1'-C5-C6
26	A	1917	PSU	O4'-C4'-C5'-O5'
26	A	1962	5MC	C2'-C1'-N1-C2
26	A	1962	5MC	C2'-C1'-N1-C6
26	A	2030	6MZ	N1-C6-N6-C9
26	A	2445	2MG	O4'-C4'-C5'-O5'
26	A	2445	2MG	C3'-C4'-C5'-O5'
26	A	2504	PSU	O4'-C4'-C5'-O5'
26	A	2552	OMU	O4'-C1'-N1-C2
26	A	2552	OMU	O4'-C1'-N1-C6
24	y	19	H2U	C2'-C1'-N1-C2
26	A	1915	3TD	O4'-C4'-C5'-O5'
26	A	2030	6MZ	C3'-C4'-C5'-O5'
26	A	2069	G7M	O4'-C4'-C5'-O5'
26	A	2504	PSU	C3'-C4'-C5'-O5'
1	a	1518	MA6	O4'-C1'-N9-C4
24	y	55	PSU	C3'-C4'-C5'-O5'
26	A	1915	3TD	C3'-C4'-C5'-O5'
26	A	1917	PSU	C3'-C4'-C5'-O5'
1	a	1519	MA6	N1-C6-N6-C10
1	a	1516	2MG	O4'-C4'-C5'-O5'
24	y	54	5MU	C4'-C5'-O5'-P
1	a	1519	MA6	C5-C6-N6-C9
26	A	2503	2MA	O4'-C1'-N9-C8
26	A	2030	6MZ	O4'-C4'-C5'-O5'
26	A	2069	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
24	y	37	6IA	N6-C12-C13-C14
26	A	2503	2MA	O4'-C1'-N9-C4
26	A	2503	2MA	C4'-C5'-O5'-P
24	y	19	H2U	O4'-C1'-N1-C2
22	v	20	H2U	C4'-C5'-O5'-P
24	y	55	PSU	C4'-C5'-O5'-P
24	y	54	5MU	C2'-C1'-N1-C6
26	A	1962	5MC	O4'-C1'-N1-C6
26	A	2030	6MZ	C4'-C5'-O5'-P
1	a	1207	2MG	C3'-C4'-C5'-O5'
26	A	2251	OMG	O4'-C4'-C5'-O5'
24	y	55	PSU	O4'-C1'-C5-C4
1	a	1516	2MG	C3'-C4'-C5'-O5'
24	y	54	5MU	C2'-C1'-N1-C2
24	y	55	PSU	O4'-C1'-C5-C6
26	A	746	PSU	O4'-C1'-C5-C6
26	A	1962	5MC	O4'-C1'-N1-C2
26	A	2503	2MA	O4'-C4'-C5'-O5'
26	A	1962	5MC	C4'-C5'-O5'-P

There are no ring outliers.

15 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	2457	PSU	1	0
1	a	967	5MC	3	0
26	A	1915	3TD	1	0
26	A	1962	5MC	1	0
1	a	966	2MG	1	0
24	y	19	H2U	1	0
26	A	2030	6MZ	1	0
1	a	1519	MA6	1	0
24	y	37	6IA	2	0
22	v	55	PSU	1	0
26	A	2504	PSU	1	0
26	A	1939	5MU	1	0
26	A	2604	PSU	1	0
26	A	745	1MG	1	0
1	a	527	G7M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	FME	v	101	22	8,9,10	1.01	0	7,9,11	1.31	1 (14%)
60	SEC	y	701	24	2,5,6	0.63	0	0,5,7	-	-
61	GNP	z	701	62	33,34,34	1.54	5 (15%)	46,54,54	1.91	10 (21%)

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
59	FME	v	101	22	-	3/7/9/11	-
60	SEC	y	701	24	-	0/0/4/6	-
61	GNP	z	701	62	-	6/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	z	701	GNP	PB-N3B	4.30	1.74	1.63
61	z	701	GNP	PG-N3B	4.05	1.74	1.63
61	z	701	GNP	C6-N1	-2.92	1.33	1.38
61	z	701	GNP	C5-C4	2.72	1.46	1.38
61	z	701	GNP	C5-N7	-2.37	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	z	701	GNP	C5-C4-N3	-6.41	118.07	128.46
61	z	701	GNP	N9-C4-N3	5.34	136.66	125.94
61	z	701	GNP	C2-N3-C4	4.98	121.17	112.30
61	z	701	GNP	O6-C6-C5	-3.42	117.52	126.60
61	z	701	GNP	O3G-PG-O1G	-2.83	106.34	113.45
61	z	701	GNP	C5-C6-N1	2.72	120.11	113.19
61	z	701	GNP	C6-C5-N7	2.57	135.03	130.25
61	z	701	GNP	C2-N1-C6	-2.52	120.50	125.10
59	v	101	FME	CA-N-CN	2.51	126.68	122.82
61	z	701	GNP	C3'-C2'-C1'	2.18	105.56	101.43
61	z	701	GNP	PB-O3A-PA	-2.14	125.07	132.62

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	v	101	FME	O1-CN-N-CA
59	v	101	FME	CA-CB-CG-SD
61	z	701	GNP	PB-N3B-PG-O1G
61	z	701	GNP	PG-N3B-PB-O1B
61	z	701	GNP	PA-O3A-PB-O1B
61	z	701	GNP	PA-O3A-PB-O2B
61	z	701	GNP	C5'-O5'-PA-O1A
59	v	101	FME	CB-CG-SD-CE
61	z	701	GNP	C5'-O5'-PA-O3A

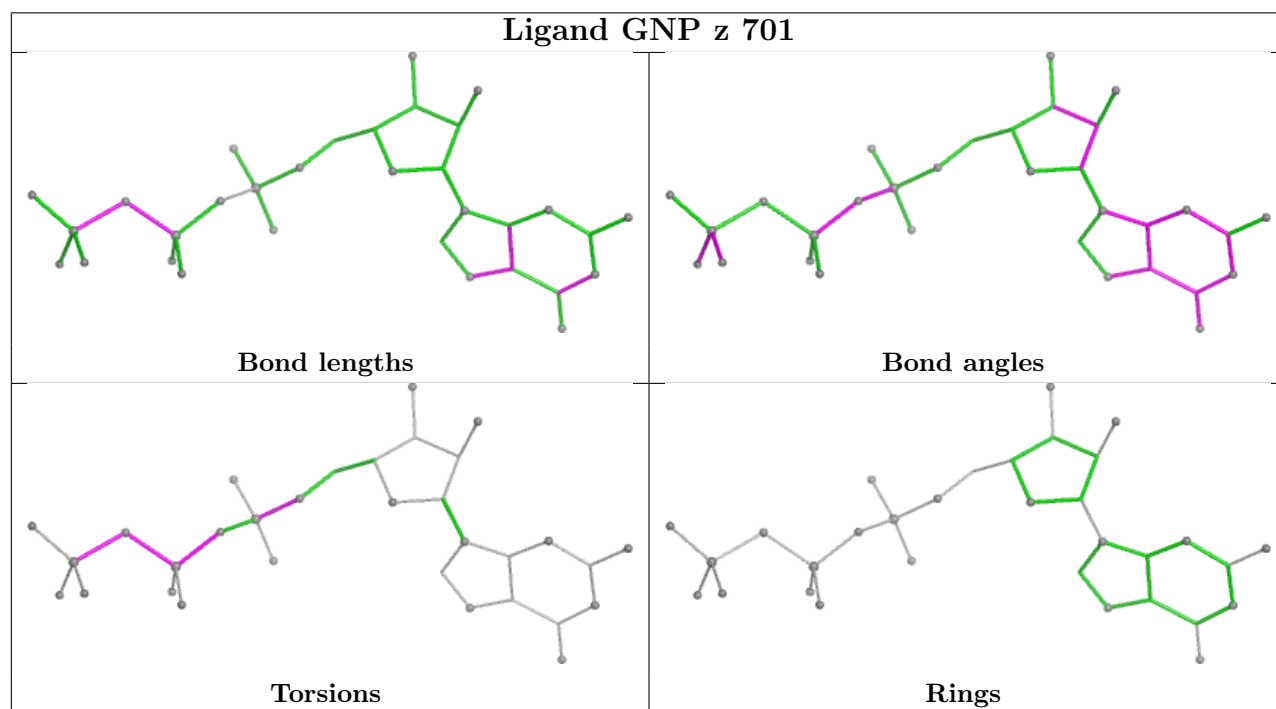
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	y	701	SEC	2	0
61	z	701	GNP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

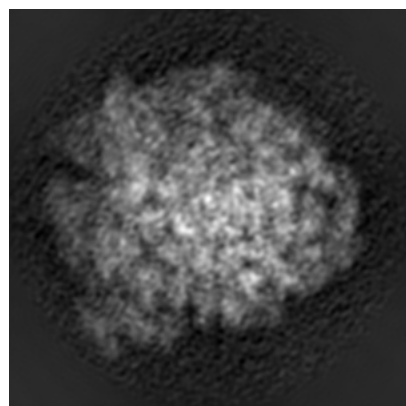
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4122. These allow visual inspection of the internal detail of the map and identification of artifacts.

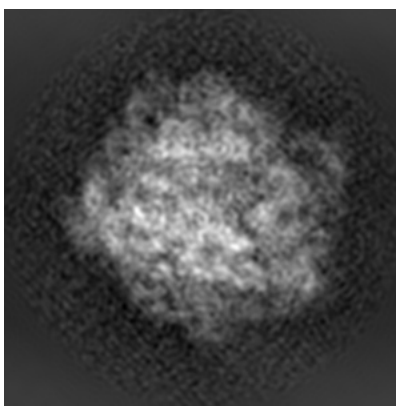
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

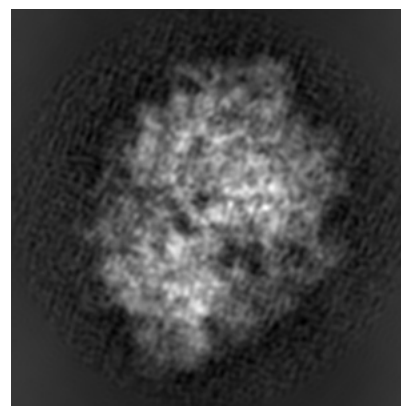
6.1.1 Primary map



X

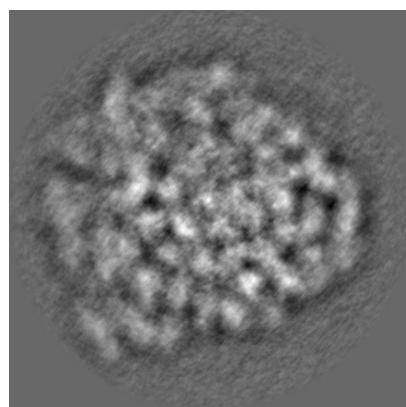


Y

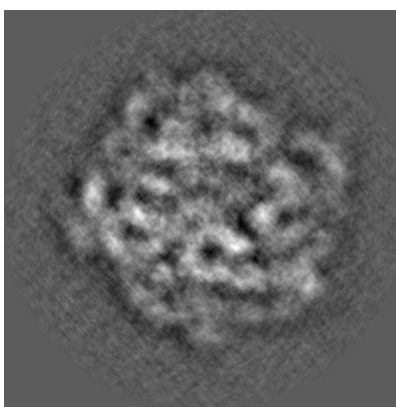


Z

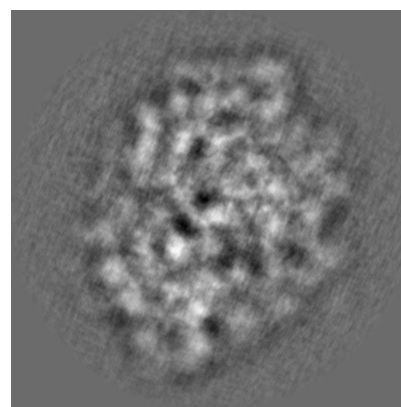
6.1.2 Raw map



X



Y

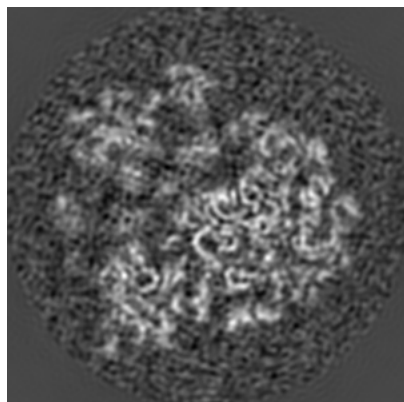


Z

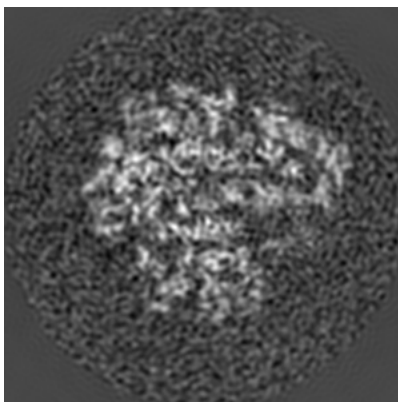
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

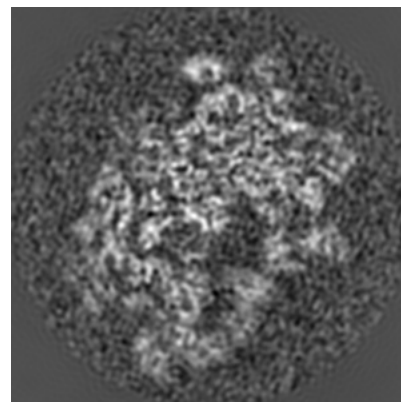
6.2.1 Primary map



X Index: 136

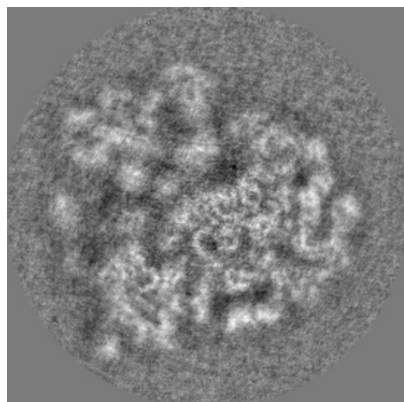


Y Index: 136

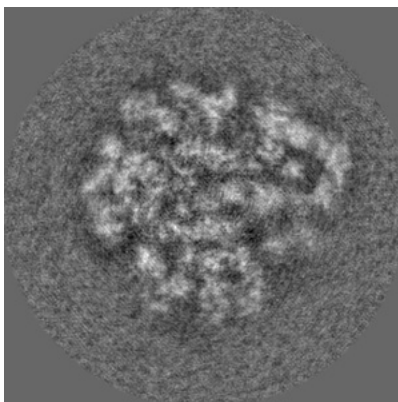


Z Index: 136

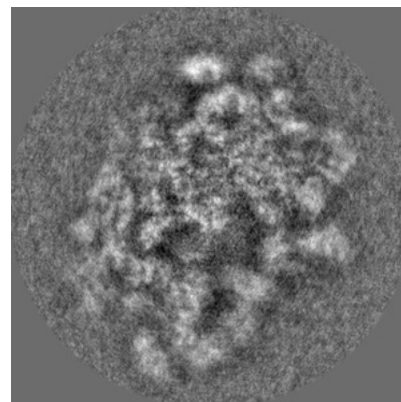
6.2.2 Raw map



X Index: 136



Y Index: 136

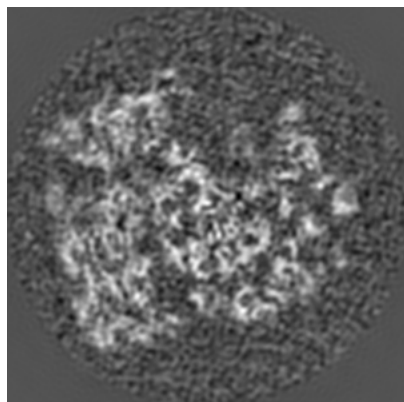


Z Index: 136

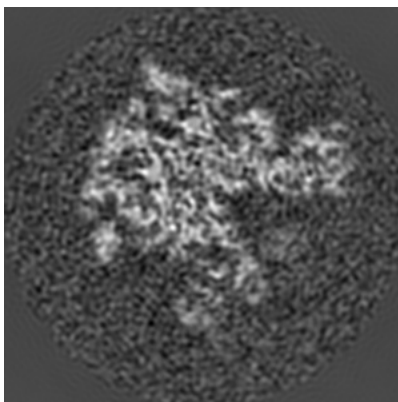
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

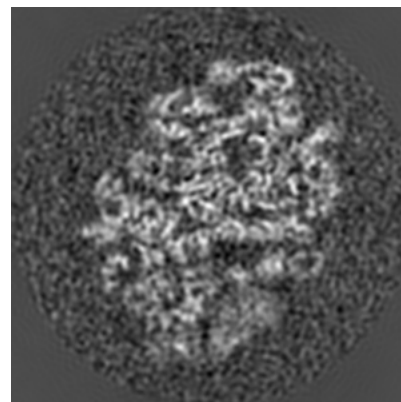
6.3.1 Primary map



X Index: 125

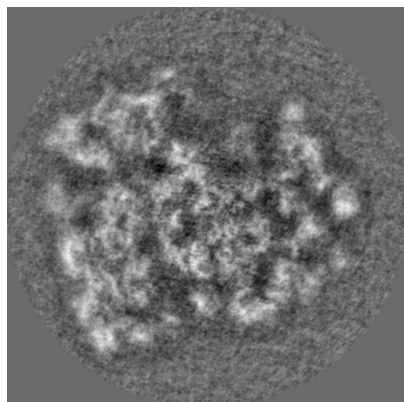


Y Index: 148

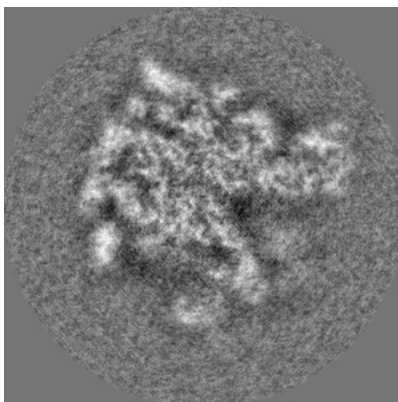


Z Index: 121

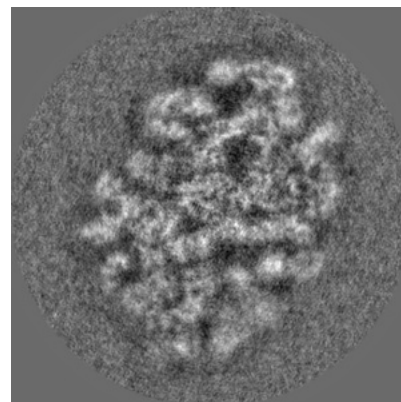
6.3.2 Raw map



X Index: 126



Y Index: 149

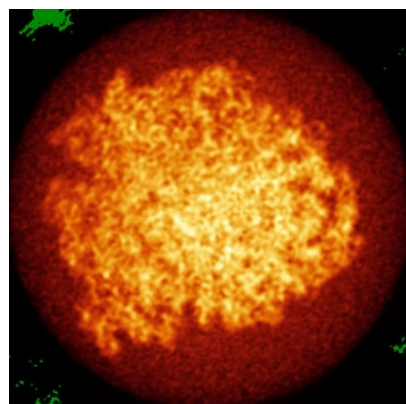


Z Index: 121

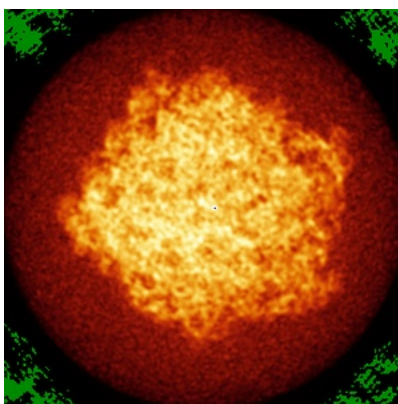
The images above show the largest variance slices of the map in three orthogonal directions.

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

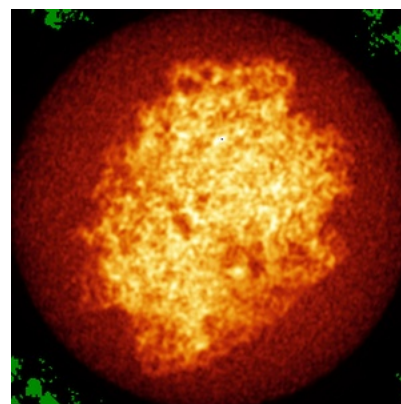
6.4.1 Primary map



X

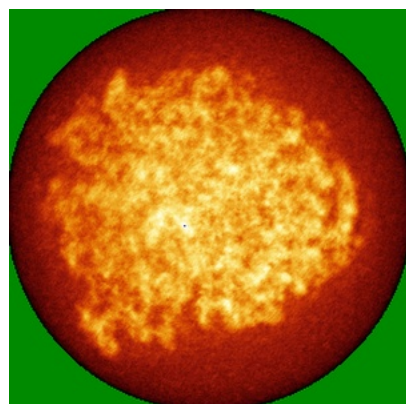


Y

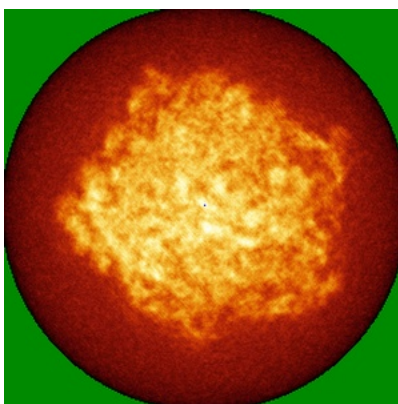


Z

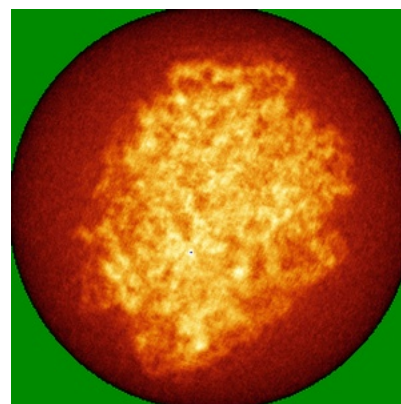
6.4.2 Raw map



X



Y

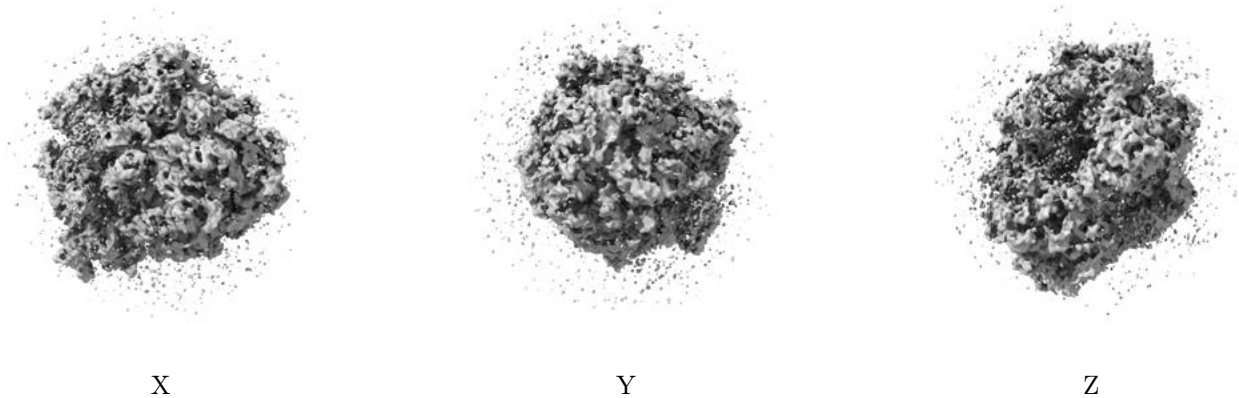


Z

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.

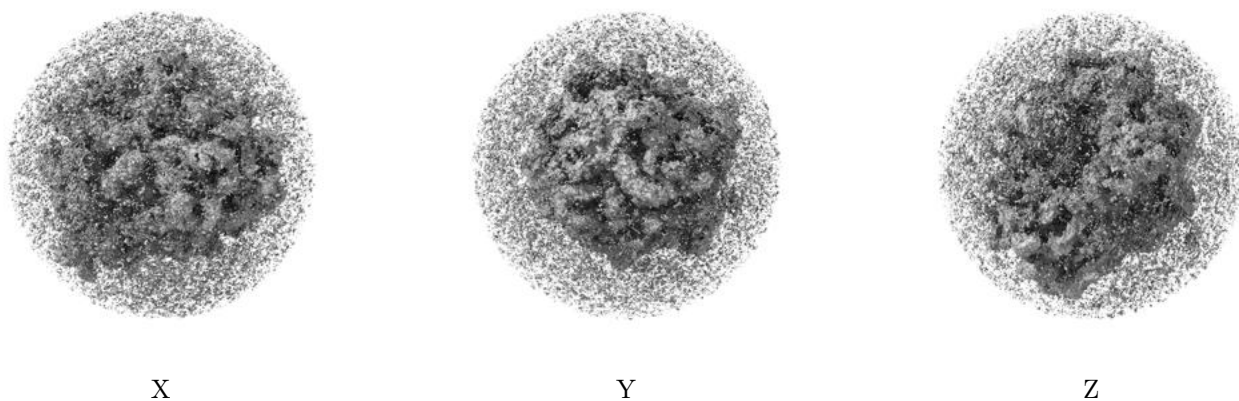
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.36. 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.

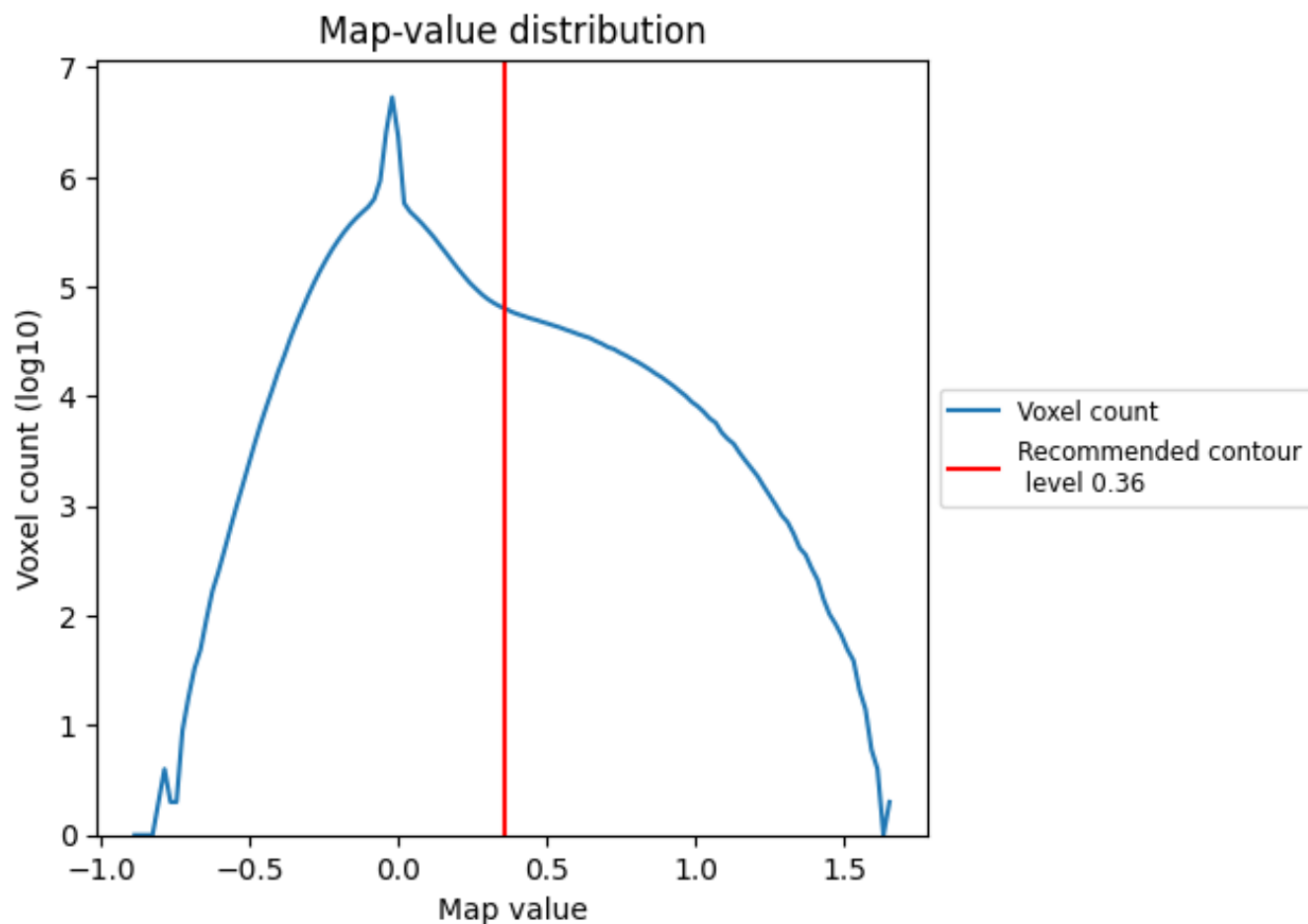
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

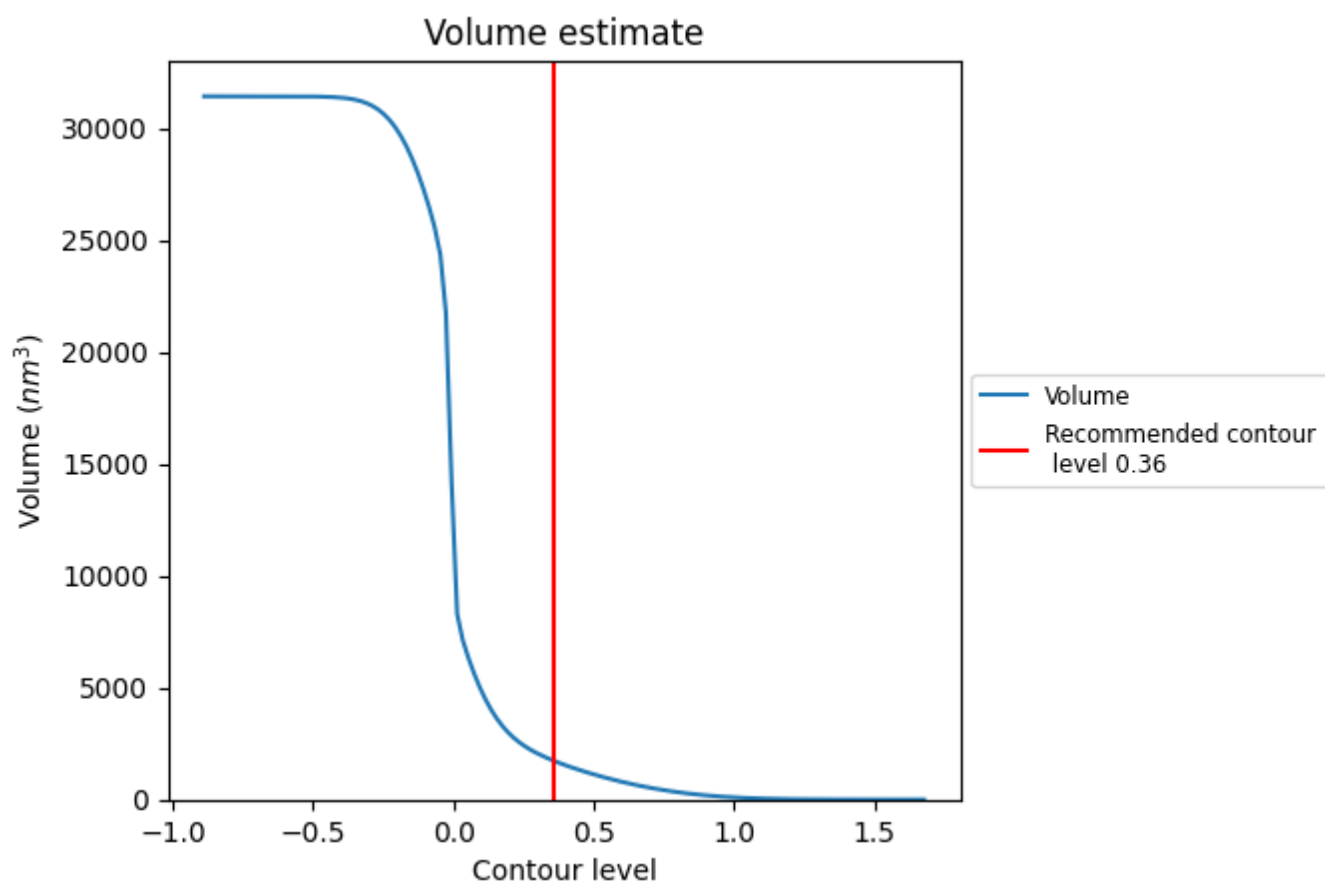
This section contains the results of statistical analysis of the map.

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.

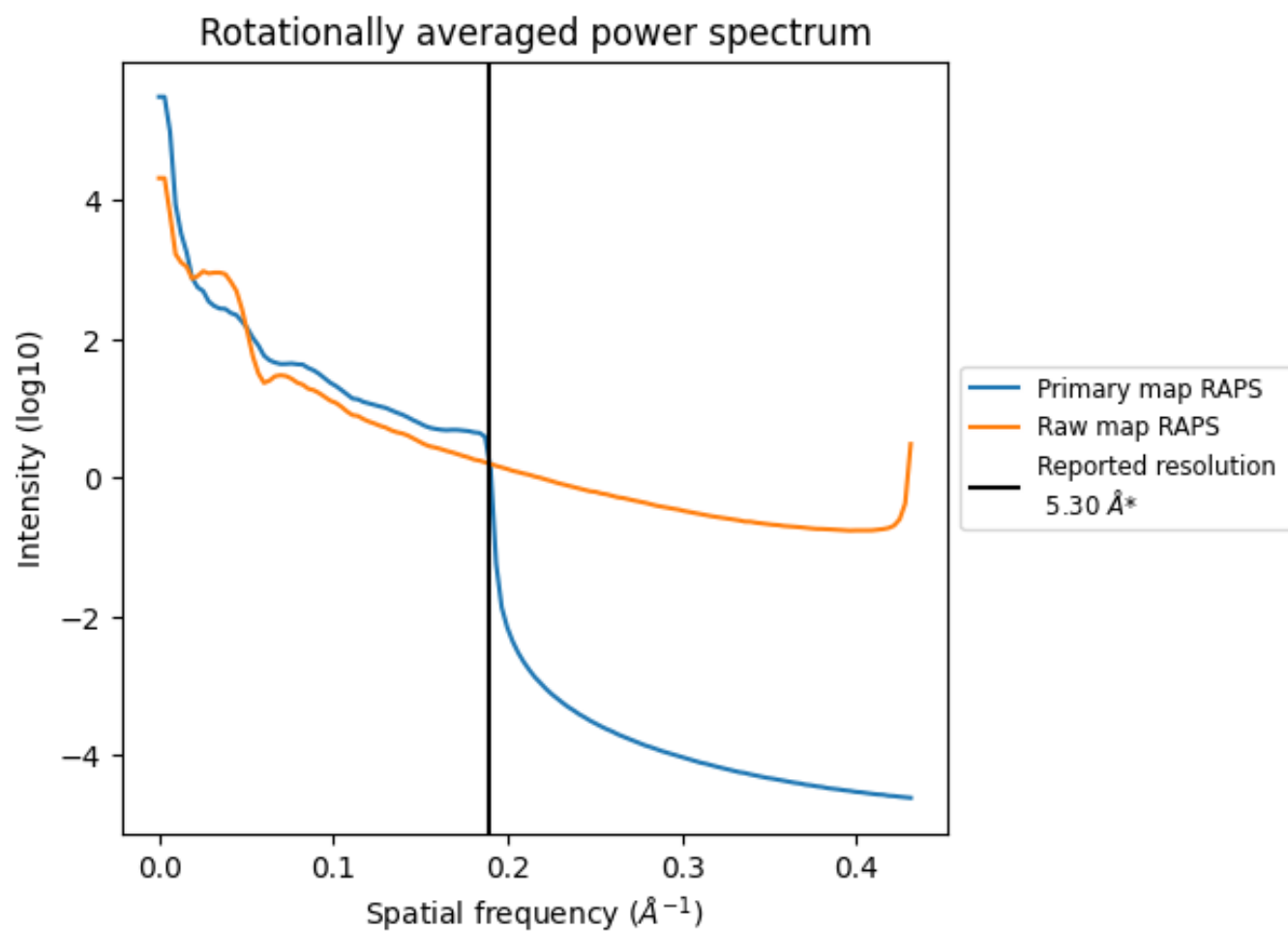
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1719 nm³; this corresponds to an approximate mass of 1553 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 ⓘ

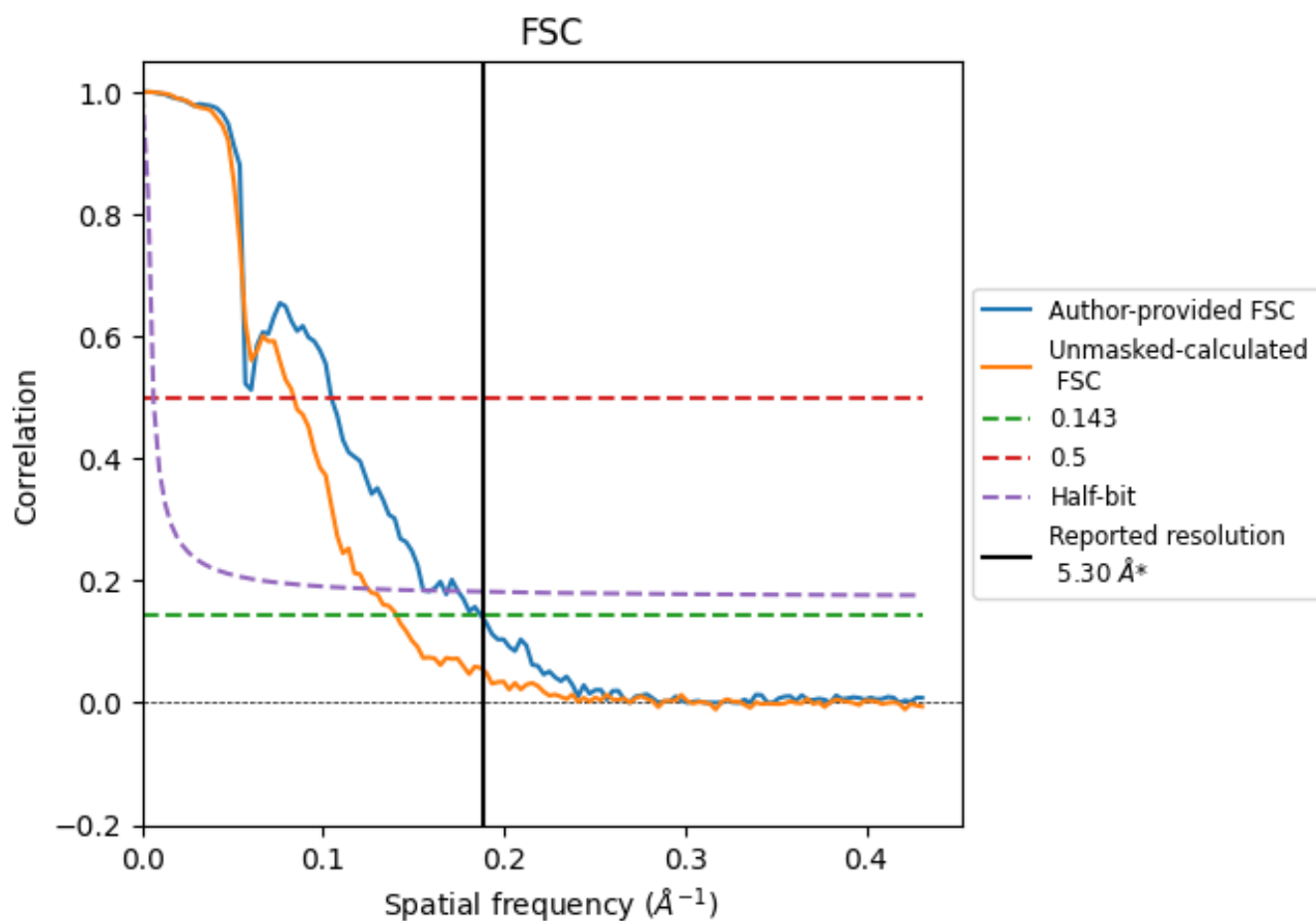


*Reported resolution corresponds to spatial frequency of 0.189 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.189 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

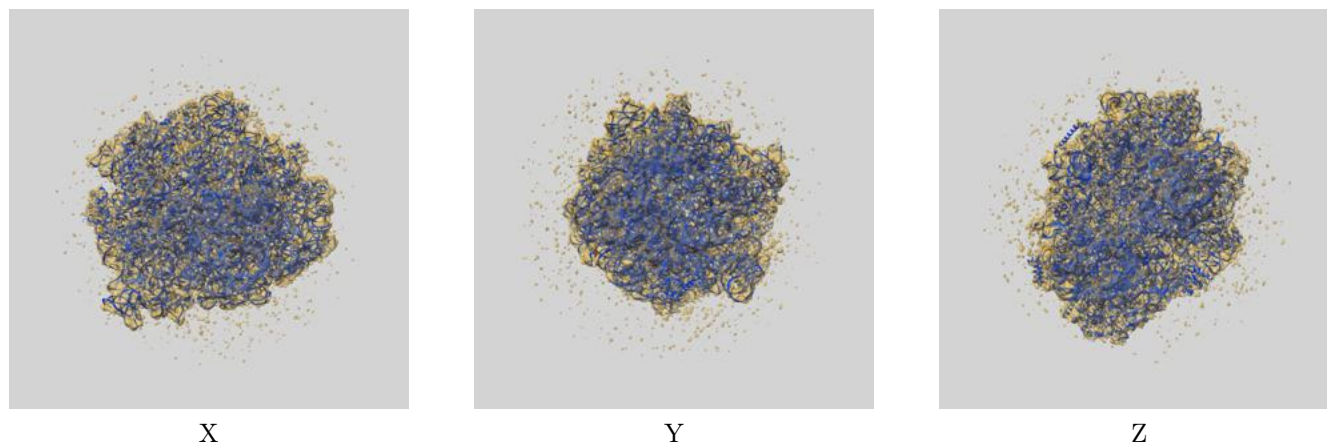
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.34	9.57	6.36
Unmasked-calculated*	7.12	11.95	8.01

*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 7.12 differs from the reported value 5.3 by more than 10 %

9 Map-model fit [i](#)

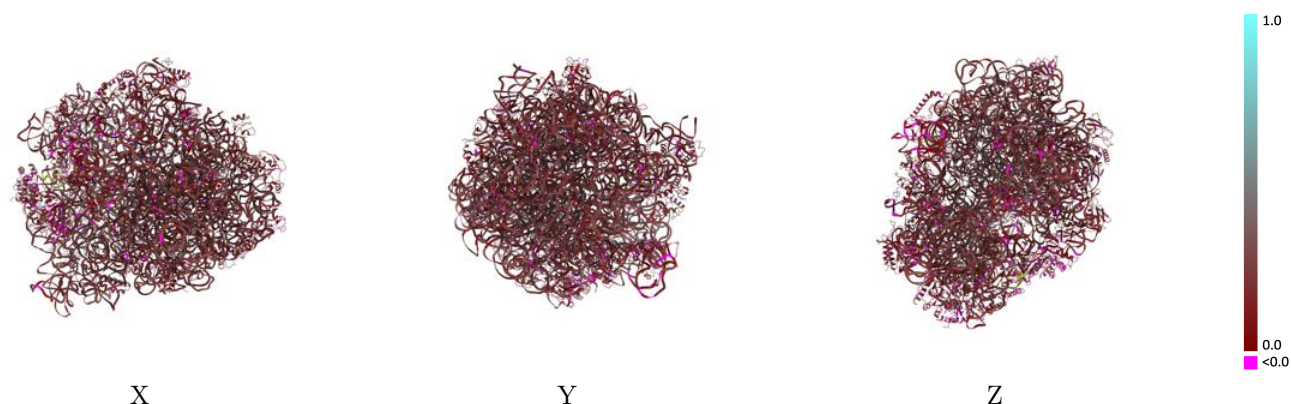
This section contains information regarding the fit between EMDB map EMD-4122 and PDB model 5LZB. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



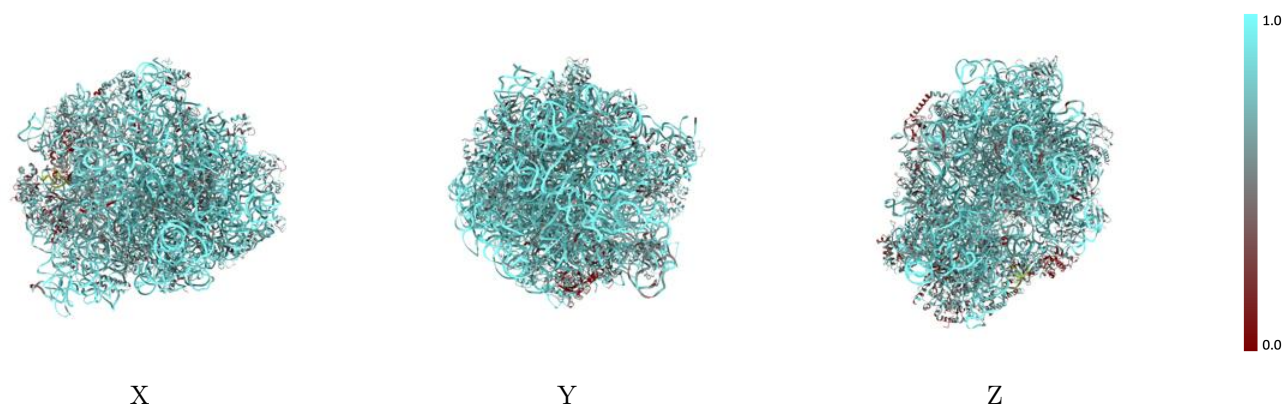
The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



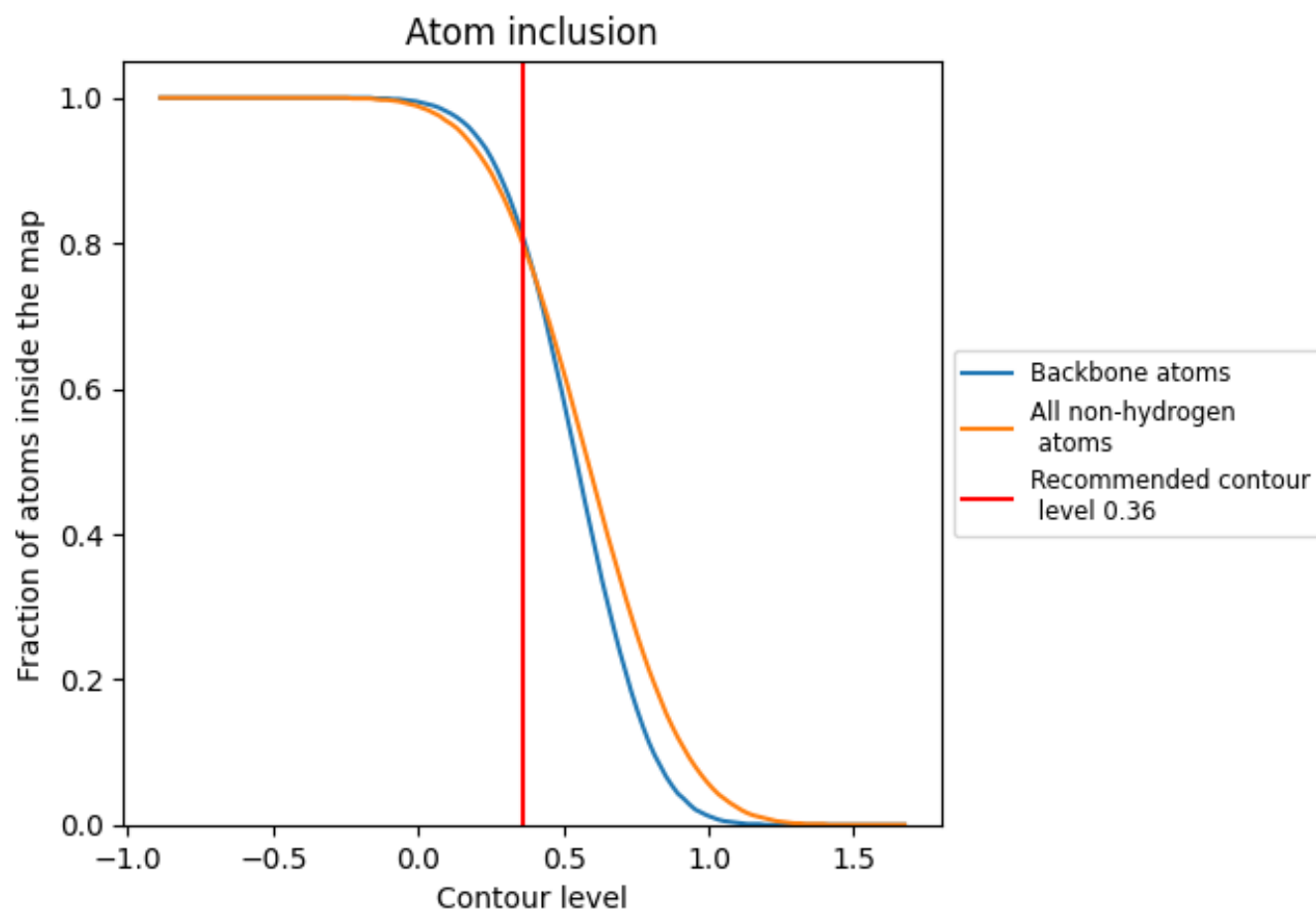
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.36).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8000	 0.2200
0	 0.5890	 0.1780
1	 0.4500	 0.1530
2	 0.6370	 0.1500
3	 0.6070	 0.1680
4	 0.6080	 0.1660
6	 0.6610	 0.1960
A	 0.9110	 0.2470
B	 0.9160	 0.2390
C	 0.6350	 0.1900
D	 0.6070	 0.1810
E	 0.6130	 0.1840
F	 0.6400	 0.1610
G	 0.6710	 0.1990
H	 0.2440	 0.1300
I	 0.2240	 0.0830
J	 0.6570	 0.1850
K	 0.5550	 0.1880
L	 0.6190	 0.2010
M	 0.6450	 0.1970
N	 0.6280	 0.1700
O	 0.6280	 0.1680
P	 0.6120	 0.1760
Q	 0.6340	 0.1690
R	 0.6250	 0.1760
S	 0.6240	 0.1700
T	 0.6060	 0.1810
U	 0.6380	 0.1720
V	 0.6250	 0.1730
W	 0.6240	 0.1840
X	 0.6490	 0.1950
Y	 0.6420	 0.1650
Z	 0.6450	 0.1800
a	 0.9080	 0.2430
b	 0.4710	 0.1670



Continued on next page...

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Chain	Atom inclusion	Q-score
c	 0.5780	 0.1860
d	 0.5310	 0.1750
e	 0.6060	 0.1940
f	 0.6340	 0.1880
g	 0.6410	 0.1780
h	 0.6060	 0.1730
i	 0.5860	 0.1640
j	 0.5410	 0.1670
k	 0.6420	 0.1680
l	 0.5680	 0.1910
m	 0.6540	 0.1750
n	 0.6020	 0.1610
o	 0.6710	 0.1630
p	 0.6190	 0.1840
q	 0.6940	 0.1740
r	 0.6580	 0.1920
s	 0.6320	 0.1750
t	 0.6520	 0.1690
u	 0.5390	 0.1590
v	 0.8960	 0.2380
w	 0.6770	 0.2190
x	 0.6290	 0.1880
y	 0.8100	 0.1590
z	 0.5460	 0.1390