



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 01:55 pm BST

PDB ID : 7OT5 / pdb_00007ot5
EMDB ID : EMD-13055
Title : CspA-70 cotranslational folding intermediate 1
Authors : Agirrezabala, X.; Samatova, E.; Macher, M.; Liutkute, M.; Gil-Carton, D.;
Novacek, J.; Valle, M.; Rodnina, M.V.
Deposited on : 2021-06-09
Resolution : 2.90 Å(reported)
Based on initial model : 6ORE

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:

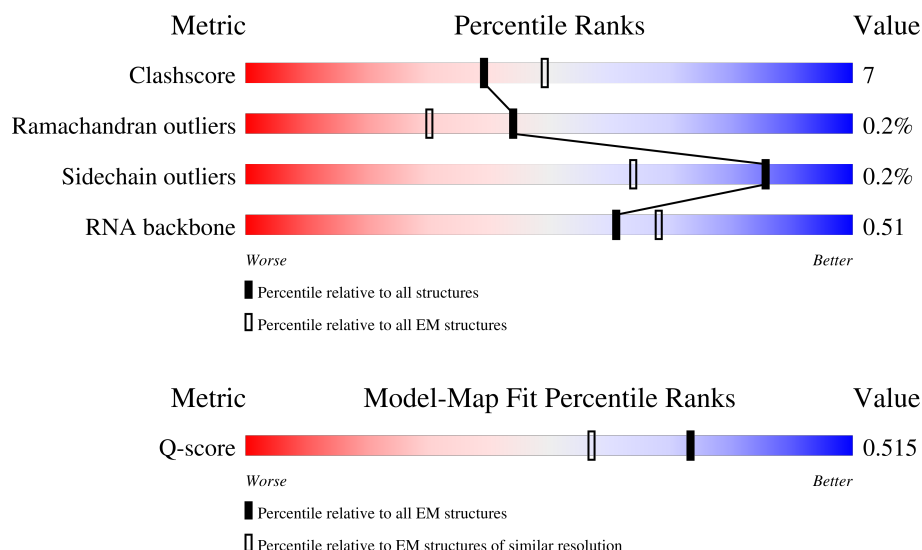
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	1	2903	 67% 27% 5%
2	2	1534	 67% 28% 5%
3	3	120	 75% 22% 3%

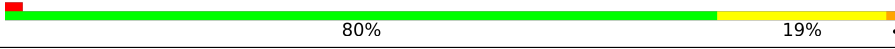
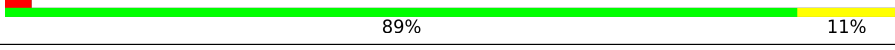
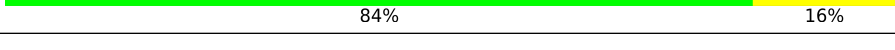
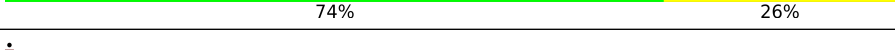
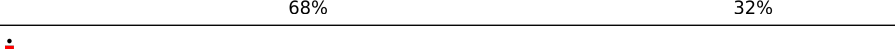
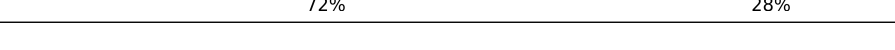
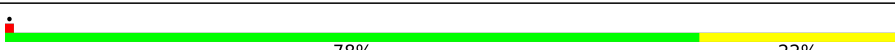
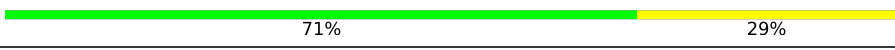
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Mol	Chain	Length	Quality of chain
4	C	271	
5	D	209	
6	E	201	
7	F	177	
8	G	175	
9	H	149	
10	I	142	
11	J	123	
12	K	144	
13	L	136	
14	M	119	
15	N	116	
16	O	114	
17	P	117	
18	Q	103	
19	R	110	
20	S	94	
21	T	103	
22	U	94	
23	V	81	
24	W	77	
25	X	62	
26	Y	58	
27	Z	66	
28	a	56	

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Mol	Chain	Length	Quality of chain
29	b	52	 90%10%
30	c	46	 74%26%
31	d	64	 80%19%.
32	e	38	 89%11%
33	f	225	 65%35%
34	g	208	 72%28%
35	h	205	 84%16%
36	i	156	 74%26%
37	j	104	 68%32%
38	k	151	 72%28%
39	l	129	 80%20%
40	m	127	 76%24%
41	n	99	 62%38%
42	o	117	 81%19%
43	p	123	 76%23%.
44	q	116	 78%22%
45	r	100	 75%25%
46	s	88	 83%16%.
47	t	82	 83%17%
48	u	80	 72%28%
49	v	66	 89%11%
50	w	83	 71%29%
51	x	86	 74%26%
52	y	70	 9%69%31%
53	4	6	 67%17%17%

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Mol	Chain	Length	Quality of chain
54	z	85	47% 22% 24% 7%
55	B	66	5% 30% 64% 5%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145365 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 9 is a protein called 50S ribosomal protein L9.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	117	Total	C	N	O	S	0	0
			947	604	192	151			

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 21 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	103	Total	C	N	O		
			788	498	148	142	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	V	81	Total	C	N	O	S	
			610	376	123	110	1	0

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	58	Total	C	N	O	S	
			448	281	87	78	2	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	66	Total	C	N	O	S	
			522	323	99	94	6	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	52	Total	C	N	O	S	0	0
			426	275	78	73			

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

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

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

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

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

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

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

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

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

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

- Molecule 43 is a protein called 30S ribosomal protein S12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S14.

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

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 50 is a protein called Ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 52 is a protein called 30S ribosomal protein S21.

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	6	Total	C	N	O	P	0	0
			122	55	17	44	6		

- Molecule 54 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	85	Total	C	N	O	P	0	0
			1830	822	328	595	85		

- Molecule 55 is a protein called Cold shock protein CspB.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B	66	Total	C	N	O	S	0	0
			496	316	81	98	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	45	LYS	LEU	conflict	UNP A0A7U8W1U7
B	61	ALA	GLY	conflict	UNP A0A7U8W1U7

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

Mol	Chain	Residues	Atoms		AltConf
56	1	261	Total 261	Mg 261	0
56	2	113	Total 113	Mg 113	0
56	3	8	Total 8	Mg 8	0
56	C	1	Total 1	Mg 1	0
56	D	2	Total 2	Mg 2	0
56	P	1	Total 1	Mg 1	0
56	T	1	Total 1	Mg 1	0
56	a	2	Total 2	Mg 2	0
56	h	1	Total 1	Mg 1	0
56	m	1	Total 1	Mg 1	0
56	q	1	Total 1	Mg 1	0
56	z	2	Total 2	Mg 2	0

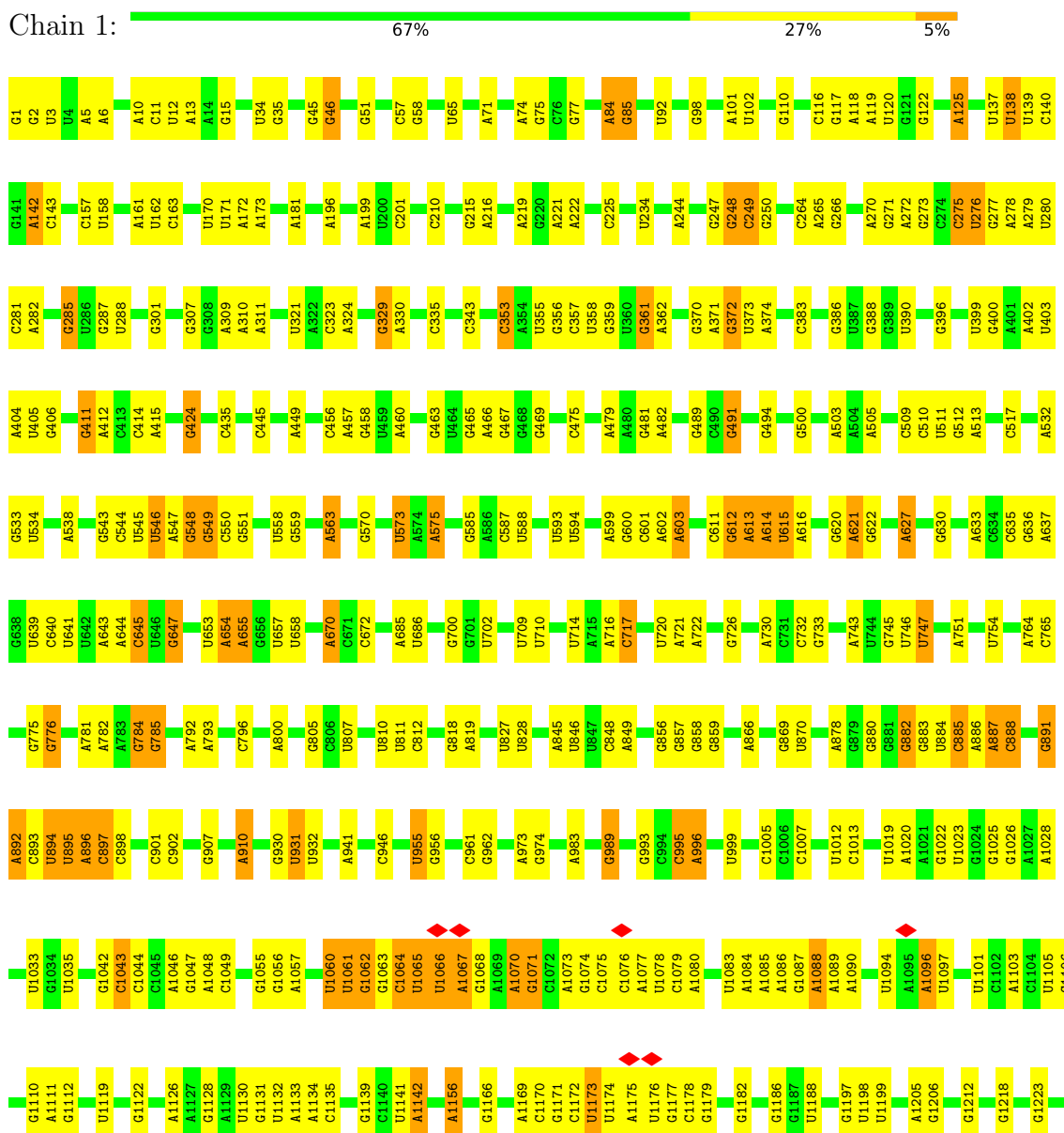
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	Z	1	Total 1	Zn 1	0
57	e	1	Total 1	Zn 1	0

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.

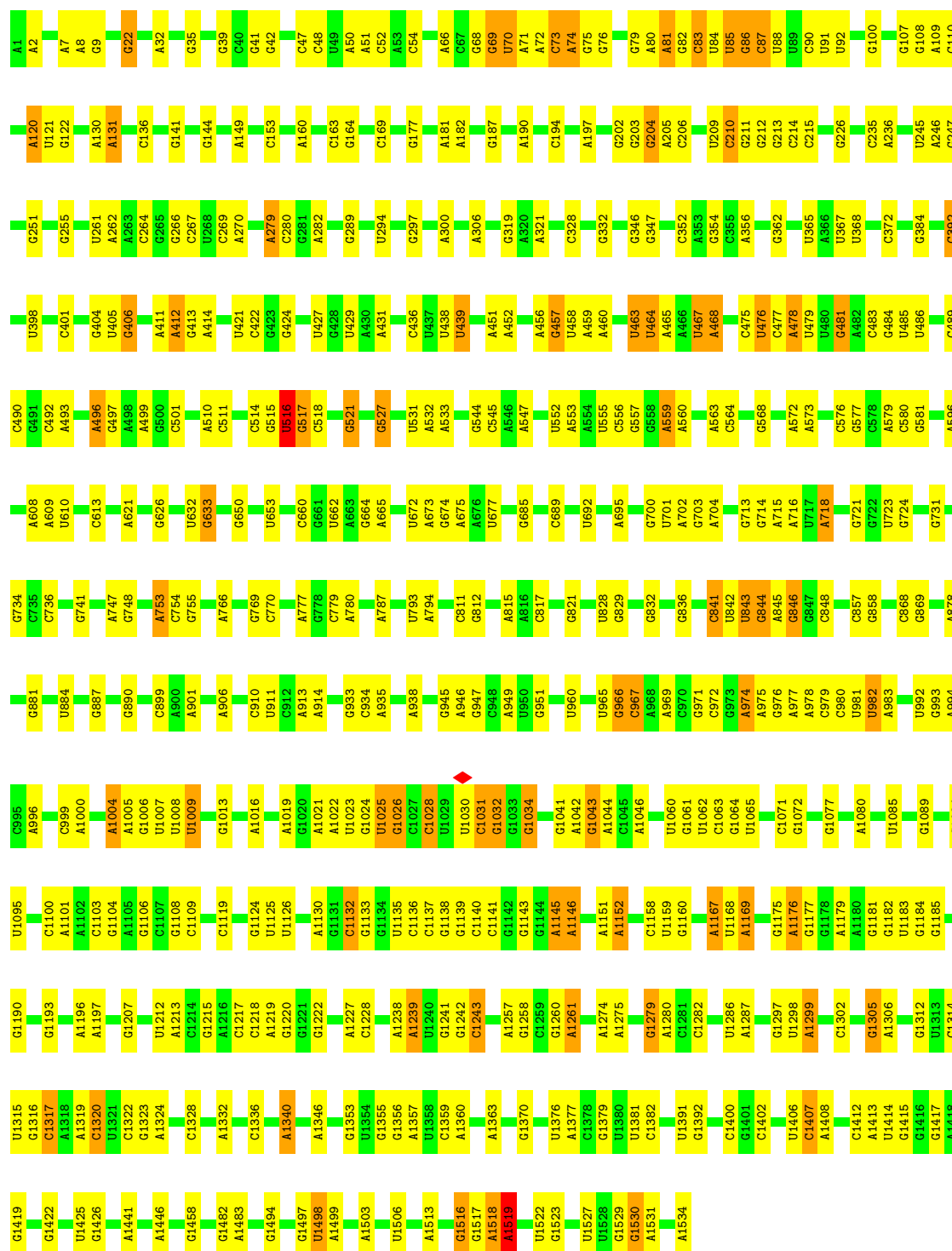
• Molecule 1: 23S rRNA



G2819	A2820	A2821	G2822	A2823	G2824	G2825																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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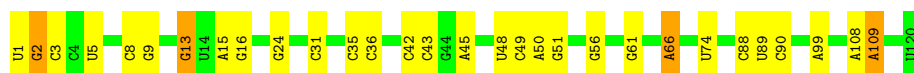
• Molecule 2: 16S rRNA

Chain 2:  67% 28% 5%



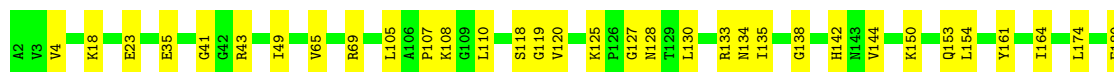
• Molecule 3: 5S rRNA

Chain 3:  75% 22%



- Molecule 4: 50S ribosomal protein L2

Chain C: 82% 18%



- Molecule 5: 50S ribosomal protein L3

Chain D: 86% 12%



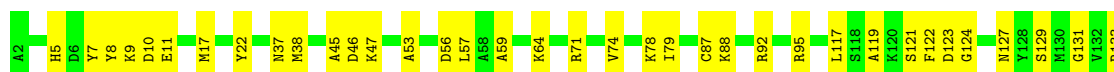
- Molecule 6: 50S ribosomal protein L4

Chain E: 84% 16%



- Molecule 7: 50S ribosomal protein L5

Chain F: 70% 30%

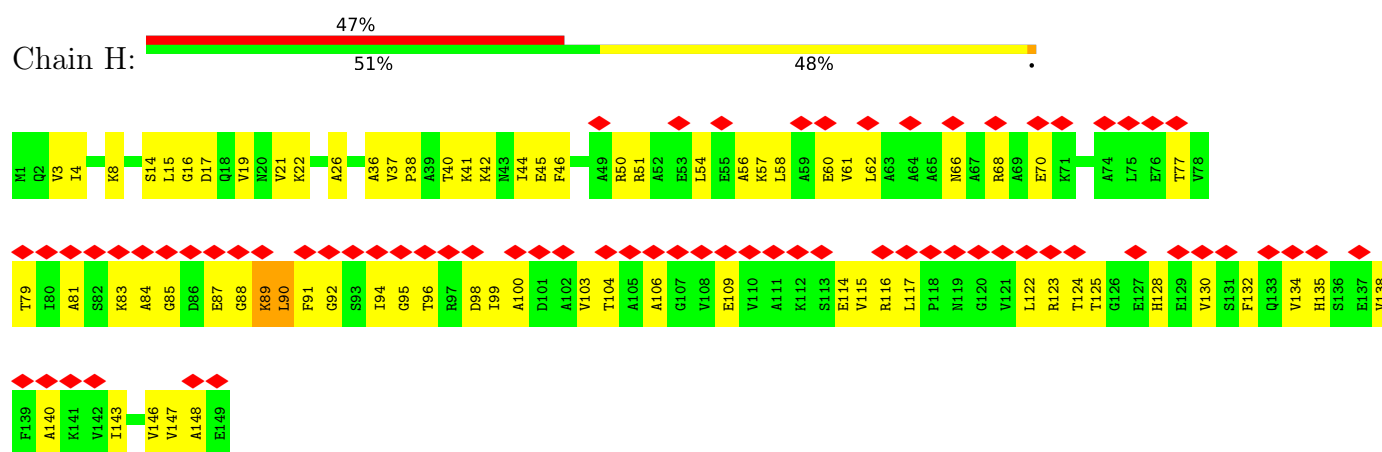


- Molecule 8: 50S ribosomal protein L6

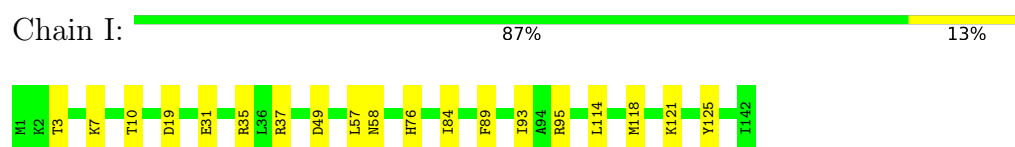
Chain G: 80% 19%



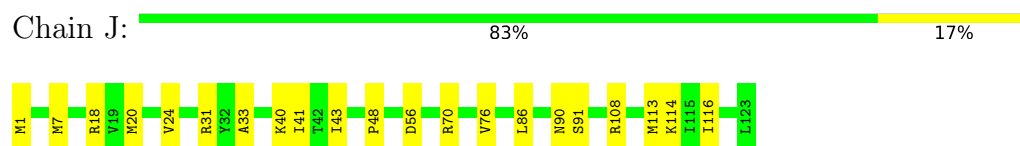
- Molecule 9: 50S ribosomal protein L9



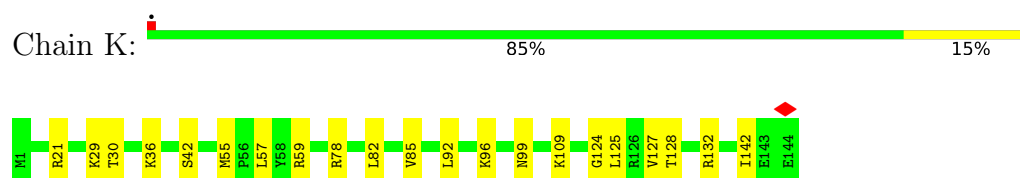
- Molecule 10: 50S ribosomal protein L13



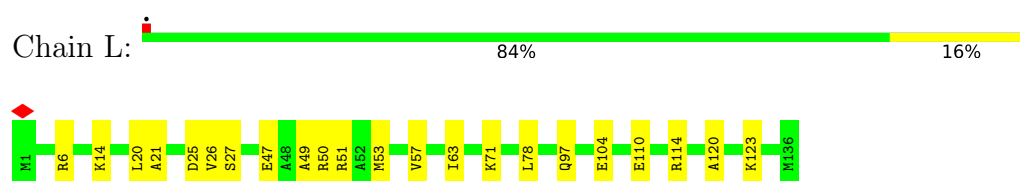
- Molecule 11: 50S ribosomal protein L14



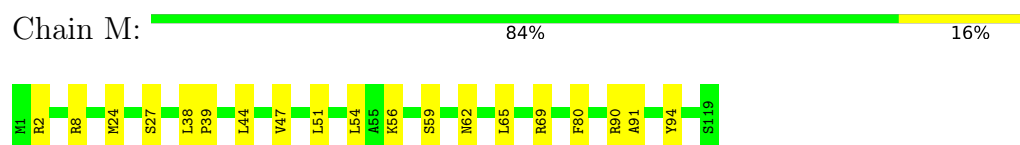
- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L17



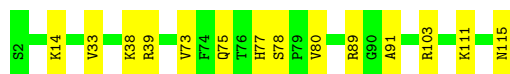
- Molecule 15: 50S ribosomal protein L18

Chain N:  77% 23%



- Molecule 16: 50S ribosomal protein L19

Chain O:  88% 12%



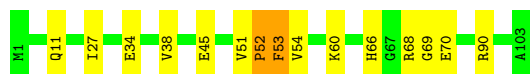
- Molecule 17: 50S ribosomal protein L20

Chain P:  90% 10%



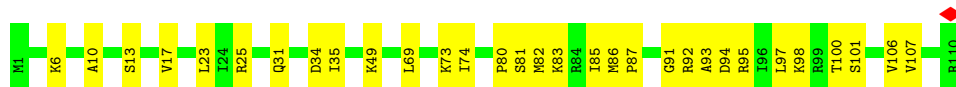
- Molecule 18: 50S ribosomal protein L21

Chain Q:  85% 13% .



- Molecule 19: 50S ribosomal protein L22

Chain R:  72% 28%



- Molecule 20: 50S ribosomal protein L23

Chain S:  82% 18%



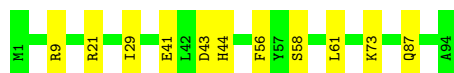
- Molecule 21: Ribosomal protein L24

Chain T:  71% 29%



- Molecule 22: 50S ribosomal protein L25

Chain U:  88% 12%



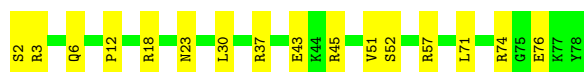
- Molecule 23: 50S ribosomal protein L27

Chain V:  5% 75% 25%



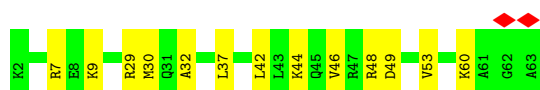
- Molecule 24: 50S ribosomal protein L28

Chain W:  79% 21%



- Molecule 25: 50S ribosomal protein L29

Chain X:  79% 21%



- Molecule 26: 50S ribosomal protein L30

Chain Y:  76% 24%



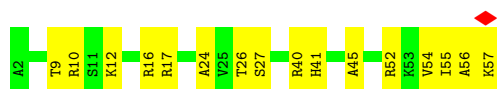
- Molecule 27: 50S ribosomal protein L31

Chain Z:  6% 67% 33%

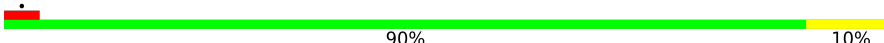


- Molecule 28: 50S ribosomal protein L32

Chain a:  71% 29%



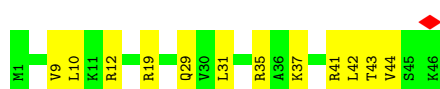
- Molecule 29: 50S ribosomal protein L33

Chain b:  90% 10%



- Molecule 30: 50S ribosomal protein L34

Chain c:  74% 26%



- Molecule 31: 50S ribosomal protein L35

Chain d:  80% 19%



- Molecule 32: 50S ribosomal protein L36

Chain e:  89% 11%



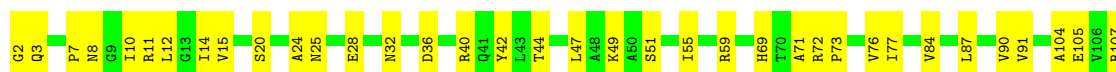
- Molecule 33: 30S ribosomal protein S2

Chain f:  65% 35%



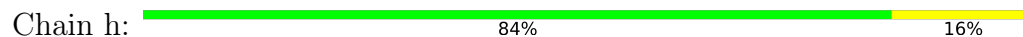
- Molecule 34: 30S ribosomal protein S3

Chain g:  72% 28%





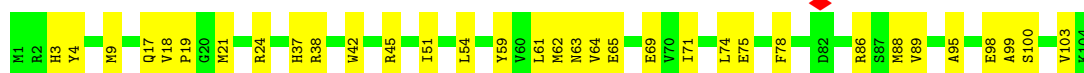
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



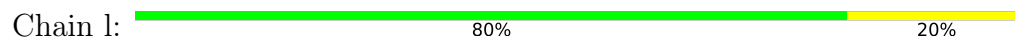
- Molecule 37: 30S ribosomal protein S6



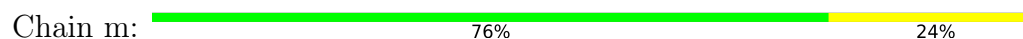
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

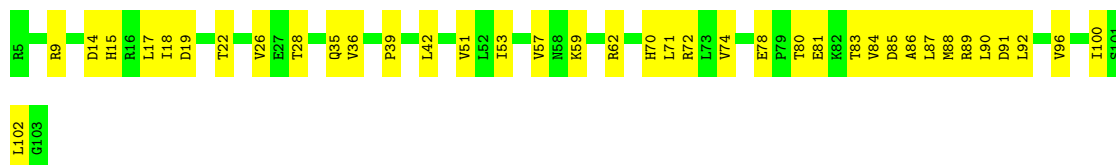


- Molecule 40: 30S ribosomal protein S9

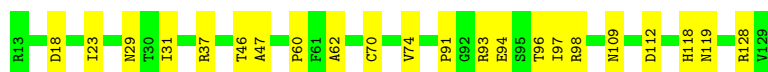
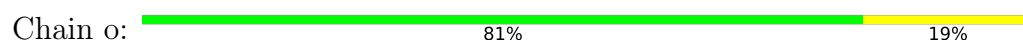




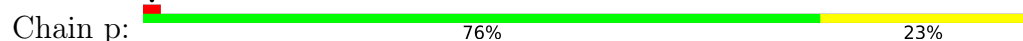
- Molecule 41: 30S ribosomal protein S10



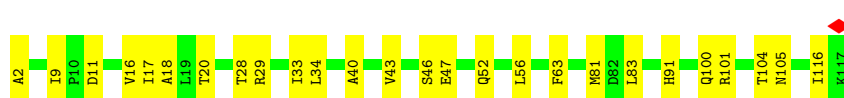
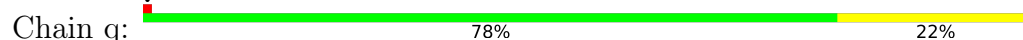
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



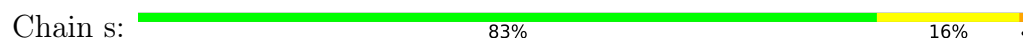
- Molecule 44: 30S ribosomal protein S13



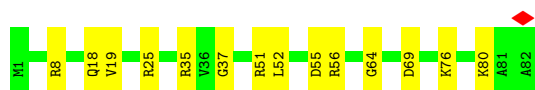
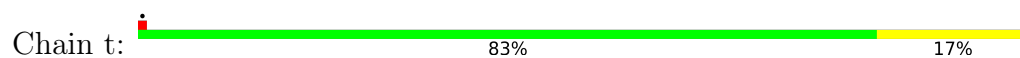
- Molecule 45: 30S ribosomal protein S14



- Molecule 46: 30S ribosomal protein S15



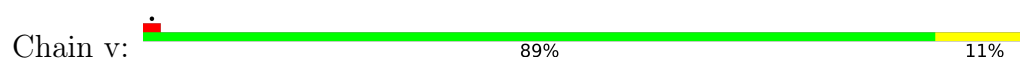
● Molecule 47: 30S ribosomal protein S16



● Molecule 48: 30S ribosomal protein S17



● Molecule 49: 30S ribosomal protein S18



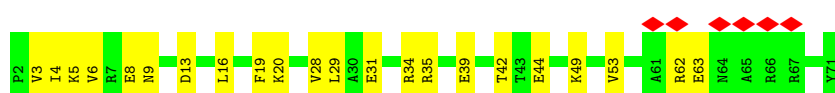
● Molecule 50: Ribosomal protein S19



● Molecule 51: 30S ribosomal protein S20



● Molecule 52: 30S ribosomal protein S21

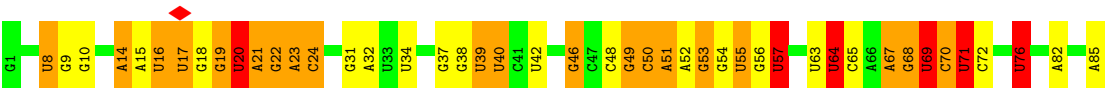


● Molecule 53: mRNA





● Molecule 54: tRNA-Leu



● Molecule 55: Cold shock protein CspB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26765	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.2	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.055	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, 2MG, OMG, 2MA, UR3, MA6, G7M, PSU, MG, 5MU, 0TD, OMC, OMU, ZN, 1MG, 3TD, 6MZ, 5MC

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	1	0.43	0/69286	0.46	2/108087 (0.0%)
2	2	0.39	0/36590	0.44	0/57074
3	3	0.37	0/2872	0.41	0/4478
4	C	0.57	0/2121	0.54	0/2852
5	D	0.56	0/1586	0.55	0/2134
6	E	0.51	0/1571	0.59	0/2113
7	F	0.44	0/1434	0.60	0/1926
8	G	0.37	0/1333	0.55	0/1805
9	H	0.32	0/1122	0.83	0/1515
10	I	0.55	0/1152	0.54	0/1551
11	J	0.53	0/955	0.53	0/1279
12	K	0.53	0/1062	0.59	0/1413
13	L	0.53	0/1093	0.56	0/1460
14	M	0.57	0/964	0.64	0/1289
15	N	0.48	0/902	0.62	0/1209
16	O	0.52	0/929	0.49	0/1242
17	P	0.62	0/960	0.65	0/1278
18	Q	0.53	0/829	0.62	0/1107
19	R	0.59	0/864	0.62	0/1156
20	S	0.50	0/752	0.52	0/1005
21	T	0.45	0/796	0.53	0/1062
22	U	0.49	0/766	0.57	0/1025
23	V	0.56	0/617	0.52	0/815
24	W	0.53	0/635	0.58	0/848
25	X	0.46	0/502	0.70	0/667
26	Y	0.52	0/452	0.56	0/605
27	Z	0.32	0/531	0.59	0/709
28	a	0.53	0/450	0.58	0/599
29	b	0.43	0/433	0.55	0/576
30	c	0.61	0/380	0.59	0/498
31	d	0.62	0/513	0.66	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.53	0/303	0.48	0/397
33	f	0.41	0/1791	0.71	1/2413 (0.0%)
34	g	0.45	0/1663	0.59	0/2241
35	h	0.46	0/1665	0.60	0/2227
36	i	0.51	0/1165	0.62	0/1568
37	j	0.42	0/867	0.64	0/1171
38	k	0.43	0/1195	0.64	0/1602
39	l	0.49	0/989	0.55	0/1326
40	m	0.45	0/1034	0.66	1/1375 (0.1%)
41	n	0.42	0/800	0.71	0/1082
42	o	0.43	0/893	0.61	0/1205
43	p	0.48	0/960	0.57	0/1286
44	q	0.44	0/909	0.63	0/1215
45	r	0.46	0/817	0.61	0/1088
46	s	0.46	0/722	0.60	0/964
47	t	0.48	0/659	0.58	0/884
48	u	0.42	0/657	0.51	0/881
49	v	0.47	0/553	0.58	0/743
50	w	0.40	0/680	0.52	0/915
51	x	0.50	0/675	0.70	0/895
52	y	0.40	0/597	0.66	0/792
53	4	0.47	0/134	0.88	0/205
54	z	0.38	0/1768	0.49	1/2759 (0.0%)
55	B	0.46	0/507	0.80	1/682 (0.1%)
All	All	0.44	0/156455	0.50	6/233969 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	67	A	C1'-C2'-O2'	-6.85	101.53	111.80
1	1	2171	A	C1'-C2'-O2'	-6.10	102.66	111.80
1	1	2133	G	N9-C1'-C2'	5.54	122.31	114.00
40	m	54	LEU	N-CA-C	-5.30	105.15	111.03
55	B	53	PHE	CB-CA-C	5.14	118.15	110.08
33	f	127	ASP	N-CA-C	-5.11	103.74	110.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62336	0	31363	512	0
2	2	32929	0	16582	254	0
3	3	2569	0	1299	14	0
4	C	2082	0	2154	34	0
5	D	1565	0	1616	26	0
6	E	1552	0	1619	23	0
7	F	1410	0	1444	51	0
8	G	1313	0	1358	21	0
9	H	1111	0	1148	66	0
10	I	1129	0	1162	13	0
11	J	946	0	1023	16	0
12	K	1053	0	1129	17	0
13	L	1074	0	1157	16	0
14	M	951	0	994	14	0
15	N	892	0	923	22	0
16	O	917	0	962	10	0
17	P	947	0	1019	13	0
18	Q	816	0	839	13	0
19	R	857	0	922	34	0
20	S	746	0	811	13	0
21	T	788	0	844	23	0
22	U	753	0	780	6	0
23	V	610	0	628	15	0
24	W	625	0	652	12	0
25	X	501	0	531	8	0
26	Y	448	0	488	12	0
27	Z	522	0	520	18	0
28	a	444	0	458	13	0
29	b	426	0	464	3	0
30	c	377	0	418	10	0
31	d	504	0	572	13	0
32	e	302	0	340	4	0
33	f	1760	0	1787	76	0
34	g	1636	0	1710	42	0
35	h	1643	0	1706	24	0
36	i	1152	0	1196	34	0
37	j	848	0	846	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	k	1181	0	1238	33	0
39	l	979	0	1031	22	0
40	m	1022	0	1070	22	0
41	n	790	0	831	27	0
42	o	877	0	887	17	0
43	p	957	0	1017	20	0
44	q	900	0	965	27	0
45	r	805	0	844	26	0
46	s	714	0	734	16	0
47	t	649	0	666	10	0
48	u	648	0	691	16	0
49	v	544	0	560	6	0
50	w	663	0	688	23	0
51	x	669	0	719	15	0
52	y	589	0	629	17	0
53	4	122	0	64	2	0
54	z	1830	0	942	47	0
55	B	496	0	475	77	0
56	1	261	0	0	0	0
56	2	113	0	0	0	0
56	3	8	0	0	0	0
56	C	1	0	0	0	0
56	D	2	0	0	0	0
56	P	1	0	0	0	0
56	T	1	0	0	0	0
56	a	2	0	0	0	0
56	h	1	0	0	0	0
56	m	1	0	0	0	0
56	q	1	0	0	0	0
56	z	2	0	0	0	0
57	Z	1	0	0	0	0
57	e	1	0	0	0	0
All	All	145365	0	97515	1674	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 7.

All (1674) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1335:C:HO2'	55:B:5:MET:N	1.31	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:151:THR:HG23	5:D:152:PRO:HD3	1.31	1.08
19:R:69:LEU:HD22	19:R:107:VAL:HG22	1.40	1.01
1:1:621:A:H5'	1:1:621:A:H8	1.27	0.99
2:2:1028:C:C2	2:2:1034:G:N2	2.30	0.99
1:1:751:A:N3	55:B:56:GLU:OE1	2.00	0.94
1:1:1607:C:H4'	1:1:1608:A:H5'	1.49	0.94
1:1:2571:U:O2'	5:D:151:THR:HG21	1.69	0.93
33:f:129:LEU:HD21	33:f:134:ALA:HB2	1.51	0.91
1:1:891:G:O2'	1:1:892:A:OP1	1.89	0.91
2:2:1028:C:C2	2:2:1034:G:C2	2.59	0.91
19:R:85:ILE:HG21	55:B:45:LYS:HZ3	1.35	0.91
1:1:2102:G:O6	1:1:2187:U:C4	2.24	0.89
1:1:1779:U:OP2	1:1:1784:A:N6	2.06	0.89
2:2:951:G:OP2	44:q:101:ARG:NH2	2.06	0.88
1:1:1816:C:N4	4:C:35:GLU:OE2	2.06	0.88
1:1:1614:A:N3	55:B:49:GLN:NE2	2.22	0.87
1:1:2467:C:O2	13:L:123:LYS:NZ	2.07	0.87
1:1:796:C:OP1	6:E:57:LYS:NZ	2.06	0.87
2:2:501:C:OP1	43:p:114:ARG:NH2	2.07	0.87
1:1:1335:C:O2'	55:B:5:MET:N	2.07	0.87
1:1:2640:G:OP1	10:I:95:ARG:NH2	2.09	0.85
2:2:1382:C:O2'	38:k:79:ARG:NH1	2.09	0.85
1:1:1450:G:N2	1:1:1452:G:O6	2.09	0.85
50:w:33:THR:HG22	50:w:35:SER:H	1.42	0.84
2:2:1028:C:N3	2:2:1034:G:N1	2.25	0.84
3:3:43:C:O2	7:F:92:ARG:NH2	2.10	0.84
1:1:2133:G:O2'	1:1:2157:G:N2	2.10	0.84
1:1:1223:G:OP1	18:Q:68:ARG:NH2	2.11	0.83
2:2:356:A:N3	2:2:368:U:O2'	2.10	0.83
2:2:81:A:H62	2:2:87:C:N4	1.76	0.83
1:1:2133:G:N3	1:1:2158:A:N1	2.27	0.83
37:j:51:ILE:O	37:j:54:LEU:HD23	1.79	0.83
1:1:463:G:N2	1:1:466:A:OP2	2.11	0.82
55:B:64:ALA:O	55:B:68:THR:HG23	1.78	0.82
2:2:1028:C:O2	2:2:1034:G:C2	2.31	0.82
34:g:40:ARG:NH1	34:g:55:ILE:O	2.11	0.82
1:1:2683:C:O2	11:J:70:ARG:NH2	2.12	0.82
33:f:129:LEU:HD11	33:f:134:ALA:HA	1.62	0.82
1:1:621:A:H5'	1:1:621:A:C8	2.15	0.81
2:2:1005:A:N6	2:2:1024:G:O2'	2.13	0.81
44:q:11:ASP:OD1	44:q:46:SER:N	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:n:81:GLU:N	41:n:81:GLU:OE1	2.15	0.80
19:R:85:ILE:HD11	19:R:93:ALA:HB1	1.61	0.80
1:1:956:G:O6	13:L:14:LYS:NZ	2.16	0.79
1:1:475:C:O2	1:1:479:A:N6	2.16	0.79
1:1:1754:A:N1	1:1:2716:C:O2'	2.15	0.79
1:1:1869:G:N2	1:1:1871:A:O2'	2.15	0.79
49:v:35:GLU:OE1	49:v:35:GLU:N	2.15	0.79
45:r:41:ARG:NH2	50:w:6:LYS:O	2.15	0.79
40:m:84:THR:HG21	40:m:103:PHE:HB3	1.64	0.79
42:o:93:ARG:NH1	42:o:112:ASP:OD2	2.15	0.79
2:2:626:G:O3'	47:t:51:ARG:NH1	2.16	0.78
39:l:96:MET:SD	39:l:130:ALA:HB1	2.23	0.78
1:1:716:A:H3'	1:1:717:C:H5''	1.65	0.78
1:1:585:G:N7	17:P:6:ARG:NH1	2.30	0.78
44:q:9:ILE:HG23	44:q:18:ALA:HB1	1.64	0.78
1:1:2104:C:N4	1:1:2185:U:O2	2.15	0.78
2:2:411:A:OP2	35:h:26:ARG:NH1	2.17	0.78
2:2:1031:C:O3'	2:2:1032:G:N2	2.16	0.78
2:2:35:G:N3	43:p:115:SER:OG	2.17	0.77
2:2:1298:U:OP2	38:k:114:LYS:NZ	2.16	0.77
54:z:64:5MU:H5'	54:z:64:5MU:O2	1.83	0.77
40:m:36:GLU:OE1	40:m:45:ARG:NH1	2.18	0.77
44:q:16:VAL:O	44:q:20:THR:HG23	1.84	0.76
1:1:2478:A:OP2	32:e:2:LYS:NZ	2.19	0.75
2:2:881:G:OP2	43:p:9:ARG:NH1	2.20	0.75
40:m:25:ASN:OD1	40:m:27:LYS:NZ	2.16	0.75
2:2:1145:A:O2'	2:2:1146:A:OP2	2.03	0.75
9:H:125:THR:HA	9:H:146:VAL:HG13	1.69	0.75
34:g:25:ASN:N	34:g:28:GLU:OE2	2.20	0.75
34:g:156:ARG:NE	34:g:160:ALA:O	2.19	0.75
1:1:1172:C:O2'	1:1:1173:U:O4'	2.04	0.75
35:h:184:ARG:NH1	35:h:187:GLU:OE1	2.19	0.75
8:G:170:ARG:NH2	32:e:29:ALA:O	2.20	0.75
9:H:14:SER:N	9:H:17:ASP:OD2	2.19	0.75
35:h:188:ARG:NH1	35:h:192:SER:O	2.20	0.75
33:f:27:MET:HE2	33:f:193:PRO:HD3	1.68	0.74
21:T:28:VAL:HG22	21:T:34:VAL:HG12	1.67	0.74
1:1:2021:C:OP1	28:a:9:THR:HG21	1.87	0.74
1:1:2142:A:N6	1:1:2150:C:N3	2.34	0.74
2:2:1168:U:O2'	2:2:1169:A:OP1	2.05	0.74
19:R:91:GLY:HA3	55:B:53:PHE:CD2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:219:A:N3	1:1:234:U:O2'	2.20	0.74
34:g:49:LYS:O	34:g:72:ARG:NH1	2.20	0.74
38:k:116:MET:HA	38:k:119:ARG:HE	1.52	0.74
55:B:60:LYS:CG	55:B:64:ALA:HB3	2.17	0.74
1:1:2102:G:O6	1:1:2187:U:O4	2.05	0.74
2:2:107:G:N7	51:x:10:ARG:NH2	2.36	0.74
1:1:2298:A:OP1	7:F:71:ARG:NH2	2.20	0.74
15:N:111:ARG:NH2	15:N:117:PHE:OXT	2.21	0.74
1:1:1364:G:OP2	24:W:2:SER:N	2.20	0.73
2:2:1006:G:N2	2:2:1023:U:O2	2.21	0.73
1:1:930:G:H1'	26:Y:25:LEU:HD21	1.70	0.73
2:2:910:C:OP2	43:p:18:LYS:NZ	2.18	0.73
7:F:56:ASP:OD1	7:F:57:LEU:N	2.22	0.73
7:F:121:SER:OG	7:F:129:SER:O	2.06	0.73
2:2:1516:2MG:N2	2:2:1519:MA6:OP2	2.21	0.73
42:o:23:ILE:HD13	42:o:96:THR:HG21	1.70	0.73
2:2:1152:A:OP1	41:n:70:HIS:ND1	2.21	0.72
34:g:14:ILE:HG22	34:g:15:VAL:HG13	1.71	0.72
1:1:1094:U:O2'	1:1:1096:A:N7	2.19	0.72
44:q:83:LEU:HD21	50:w:65:GLU:HB2	1.71	0.72
2:2:1060:U:OP1	45:r:85:ARG:NH1	2.22	0.72
7:F:134:GLU:HG2	7:F:136:ILE:HD12	1.71	0.72
21:T:94:ARG:HB3	21:T:103:ILE:HD12	1.70	0.72
19:R:85:ILE:HG21	55:B:45:LYS:NZ	2.05	0.72
1:1:335:C:O2	21:T:68:SER:OG	2.08	0.72
9:H:62:LEU:O	9:H:66:ASN:ND2	2.23	0.72
1:1:301:G:OP2	21:T:82:ARG:NH1	2.23	0.71
1:1:309:A:N3	1:1:329:G:O2'	2.23	0.71
4:C:23:GLU:OE1	4:C:23:GLU:N	2.22	0.71
1:1:1652:A:OP1	14:M:8:ARG:NH2	2.22	0.71
23:V:33:ALA:N	23:V:64:ASP:OD1	2.24	0.71
33:f:10:LEU:HD23	33:f:10:LEU:O	1.89	0.71
2:2:401:C:O2'	2:2:621:A:N3	2.24	0.71
15:N:27:VAL:HG21	15:N:40:ILE:HD12	1.71	0.71
28:a:45:ALA:O	28:a:57:LYS:NZ	2.17	0.71
1:1:895:U:O2'	1:1:896:A:O4'	2.06	0.71
7:F:140:GLU:OE2	27:Z:26:SER:OG	2.08	0.71
33:f:57:LEU:HD13	33:f:217:VAL:HG13	1.72	0.71
1:1:563:A:N3	17:P:37:GLN:NE2	2.38	0.71
20:S:6:ARG:O	20:S:10:VAL:HG23	1.91	0.70
11:J:108:ARG:HG2	11:J:116:ILE:HG21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1317:C:OP2	45:r:28:LYS:NZ	2.19	0.70
2:2:464:U:N3	2:2:467:U:OP2	2.23	0.70
1:1:751:A:C2	55:B:56:GLU:OE1	2.44	0.70
2:2:110:C:O2'	47:t:25:ARG:O	2.09	0.70
18:Q:70:GLU:OE1	18:Q:70:GLU:N	2.24	0.70
2:2:2:A:N3	2:2:613:C:O2'	2.25	0.69
19:R:85:ILE:HD13	55:B:46:ASP:CG	2.16	0.69
34:g:40:ARG:O	34:g:44:THR:HG23	1.91	0.69
2:2:405:U:O4	35:h:2:ALA:N	2.25	0.69
33:f:129:LEU:CD2	33:f:134:ALA:HB2	2.22	0.69
1:1:2133:G:N2	1:1:2158:A:C2	2.60	0.69
1:1:1668:A:O2'	1:1:1674:G:N7	2.19	0.69
2:2:1028:C:O2	2:2:1034:G:N2	2.24	0.69
9:H:114:GLU:OE2	9:H:134:VAL:N	2.25	0.69
11:J:90:ASN:OD1	11:J:91:SER:N	2.24	0.69
1:1:621:A:OP2	12:K:99:ASN:ND2	2.26	0.69
3:3:5:U:OP1	3:3:61:G:O2'	2.11	0.69
33:f:119:THR:O	33:f:124:GLY:N	2.26	0.69
55:B:60:LYS:HG2	55:B:64:ALA:HB3	1.75	0.69
1:1:620:G:H4'	1:1:621:A:C5'	2.22	0.69
1:1:621:A:H8	1:1:621:A:C5'	2.04	0.68
4:C:180:GLU:OE2	4:C:267:ILE:HD12	1.92	0.68
8:G:2:SER:OG	8:G:3:ARG:N	2.26	0.68
34:g:77:ILE:HA	34:g:84:VAL:HG23	1.75	0.68
1:1:611:C:C2'	1:1:612:G:H5'	2.24	0.68
1:1:2118:U:H5''	1:1:2148:G:O2'	1.94	0.68
55:B:56:GLU:CD	55:B:56:GLU:H	2.01	0.68
48:u:76:VAL:HG23	48:u:77:ARG:HG2	1.75	0.68
1:1:1266:G:OP1	28:a:16:ARG:NE	2.23	0.68
4:C:43:ARG:NH2	4:C:49:ILE:HD11	2.09	0.68
13:L:25:ASP:OD1	13:L:26:VAL:N	2.26	0.68
1:1:482:A:OP1	21:T:47:LYS:NZ	2.23	0.67
1:1:2532:G:O2'	1:1:2657:A:N1	2.27	0.67
1:1:743:A:O2'	1:1:1659:G:OP1	2.10	0.67
39:l:5:ASP:OD2	39:l:77:ARG:NH1	2.28	0.67
54:z:69:5MU:O2	54:z:69:5MU:H2'	1.93	0.67
2:2:1167:A:O2'	2:2:1169:A:N7	2.28	0.67
38:k:67:GLU:OE1	38:k:70:ARG:NH1	2.27	0.67
1:1:2304:G:H22	1:1:2312:U:H3	1.41	0.67
1:1:1083:U:O2'	1:1:1085:A:OP2	2.05	0.67
2:2:736:C:OP1	49:v:61:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:982:U:H5''	45:r:6:MET:HE3	1.77	0.67
1:1:2445:2MG:OP1	6:E:69:ARG:NH1	2.23	0.67
1:1:1007:C:OP1	10:I:37:ARG:NH2	2.27	0.66
2:2:981:U:OP1	45:r:9:ARG:NH1	2.29	0.66
7:F:144:ASP:OD2	7:F:145:LYS:NZ	2.28	0.66
19:R:85:ILE:HG12	55:B:45:LYS:NZ	2.10	0.66
22:U:58:SER:O	22:U:73:LYS:NZ	2.29	0.66
40:m:130:ARG:NH1	54:z:34:U:O2	2.28	0.66
2:2:1340:A:O2'	54:z:32:A:O2'	2.13	0.66
2:2:1376:U:OP2	38:k:25:LYS:NZ	2.24	0.66
1:1:1028:A:OP2	1:1:1126:A:N6	2.27	0.66
38:k:78:ARG:HG2	38:k:80:VAL:HG13	1.78	0.66
54:z:69:5MU:O2	54:z:69:5MU:C2'	2.44	0.66
1:1:2258:C:O2'	1:1:2427:C:OP2	2.12	0.66
1:1:2848:G:O2'	1:1:2867:G:N2	2.26	0.66
9:H:84:ALA:HB1	9:H:90:LEU:HD12	1.77	0.66
2:2:933:G:O6	38:k:3:ARG:NH2	2.29	0.66
2:2:81:A:N6	2:2:87:C:N4	2.44	0.66
2:2:131:A:O2'	2:2:262:A:N3	2.29	0.66
1:1:2305:U:O2'	7:F:133:ARG:NH1	2.25	0.65
54:z:21:A:O2'	54:z:22:G:O5'	2.10	0.65
1:1:1266:G:OP2	28:a:17:ARG:NE	2.29	0.65
1:1:2125:G:H2'	1:1:2173:A:H61	1.59	0.65
36:i:157:ARG:NH1	39:l:43:GLU:OE1	2.30	0.65
1:1:2130:U:O2'	1:1:2158:A:N6	2.26	0.65
2:2:294:U:OP1	2:2:610:U:O2'	2.13	0.65
9:H:135:HIS:HB3	9:H:138:VAL:H	1.62	0.65
23:V:37:ILE:HG22	23:V:38:VAL:HG23	1.77	0.65
37:j:38:ARG:NH1	37:j:98:GLU:O	2.28	0.65
1:1:77:G:O3'	25:X:7:ARG:NH2	2.29	0.65
2:2:1006:G:C2	2:2:1023:U:O2	2.50	0.65
13:L:49:ALA:HB1	13:L:120:ALA:HB1	1.79	0.65
15:N:4:LYS:NZ	15:N:8:ILE:HD11	2.12	0.65
36:i:55:GLU:HG3	36:i:57:PRO:HD2	1.79	0.65
19:R:95:ARG:NH1	55:B:42:TYR:HE1	1.95	0.65
2:2:1315:U:O2'	2:2:1360:A:N3	2.24	0.64
33:f:129:LEU:HD21	33:f:134:ALA:CB	2.26	0.64
2:2:974:A:OP1	45:r:69:ARG:NH1	2.30	0.64
1:1:672:C:OP2	12:K:42:SER:OG	2.13	0.64
1:1:2753:A:O2'	32:e:15:LYS:NZ	2.30	0.64
34:g:47:LEU:HD12	34:g:47:LEU:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:500:G:N1	1:1:503:A:OP2	2.30	0.64
33:f:27:MET:HE1	33:f:187:VAL:CG1	2.26	0.64
33:f:68:LEU:HD11	33:f:92:VAL:HG23	1.80	0.64
1:1:125:A:OP2	30:c:19:ARG:NH2	2.31	0.64
1:1:402:A:H2'	1:1:403:U:H5'	1.80	0.64
1:1:2140:G:O6	1:1:2151:U:C2	2.50	0.64
6:E:117:ARG:NH2	6:E:183:PHE:O	2.28	0.63
1:1:1606:C:H5''	1:1:1607:C:H5'	1.80	0.63
5:D:13:ARG:NH1	16:O:75:GLN:OE1	2.29	0.63
8:G:84:THR:OG1	8:G:134:LYS:NZ	2.32	0.63
42:o:23:ILE:HD13	42:o:96:THR:CG2	2.28	0.63
45:r:46:LEU:O	45:r:50:THR:HG23	1.99	0.63
1:1:2146:C:O2'	1:1:2147:A:O5'	2.13	0.63
2:2:1314:C:N4	50:w:2:PRO:O	2.32	0.63
47:t:51:ARG:C	47:t:52:LEU:HD12	2.23	0.63
55:B:8:ILE:O	55:B:23:PRO:HD2	1.99	0.63
1:1:894:U:O2'	1:1:895:U:P	2.57	0.63
2:2:980:C:O2'	45:r:13:ARG:NH1	2.32	0.63
15:N:4:LYS:HZ3	15:N:8:ILE:HD11	1.64	0.63
1:1:627:A:OP1	12:K:78:ARG:NH1	2.31	0.63
7:F:38:MET:HE1	7:F:53:ALA:O	1.97	0.63
9:H:132:PHE:HD2	9:H:140:ALA:HB3	1.64	0.63
55:B:25:ASP:HA	55:B:30:VAL:HG21	1.81	0.63
2:2:120:A:O2'	2:2:122:G:N7	2.27	0.63
8:G:10:VAL:HA	8:G:49:THR:HG22	1.80	0.63
19:R:92:ARG:NH2	19:R:94:ASP:OD1	2.31	0.63
46:s:89:ARG:HH21	46:s:89:ARG:HB2	1.63	0.63
1:1:249:C:O2	31:d:12:LYS:NZ	2.32	0.62
18:Q:51:VAL:HB	18:Q:52:PRO:HD3	1.80	0.62
38:k:12:ILE:HG23	38:k:21:GLU:OE1	1.99	0.62
40:m:128:SER:OG	40:m:130:ARG:OXT	2.16	0.62
54:z:48:C:N4	54:z:49:G:O6	2.32	0.62
1:1:2497:A:N3	1:1:2498:OMC:N4	2.47	0.62
2:2:481:G:O2'	2:2:483:C:N4	2.32	0.62
2:2:911:U:OP2	43:p:94:ARG:NH2	2.32	0.62
5:D:152:PRO:O	5:D:154:LYS:N	2.32	0.62
9:H:98:ASP:OD1	9:H:99:ILE:N	2.32	0.62
2:2:662:U:O2'	2:2:836:G:OP1	2.17	0.62
2:2:1145:A:O2'	2:2:1146:A:P	2.57	0.62
14:M:59:SER:OG	14:M:62:ASN:OD1	2.16	0.62
26:Y:23:THR:HG23	26:Y:47:MET:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:115:LYS:O	33:f:119:THR:HG23	1.98	0.62
1:1:2134:A:H61	1:1:2157:G:H1'	1.64	0.62
16:O:89:ARG:NH2	16:O:115:ASN:OD1	2.33	0.62
42:o:94:GLU:OE1	42:o:98:ARG:NE	2.32	0.62
51:x:56:PRO:HA	51:x:59:ASP:OD1	1.99	0.62
55:B:24:ASP:O	55:B:27:SER:N	2.33	0.62
46:s:89:ARG:HH21	46:s:89:ARG:CB	2.13	0.62
1:1:125:A:H2	30:c:9:VAL:HG12	1.64	0.62
40:m:60:LYS:HB3	40:m:61:LEU:HD12	1.82	0.62
2:2:673:A:H2'	2:2:674:G:C8	2.34	0.62
8:G:23:VAL:HG22	8:G:36:THR:OG1	1.99	0.62
1:1:1452:G:O2'	1:1:2702:G:O6	2.18	0.61
2:2:1222:G:H5''	50:w:78:ARG:HD2	1.82	0.61
9:H:46:PHE:O	9:H:50:ARG:NH1	2.33	0.61
19:R:91:GLY:HA3	55:B:53:PHE:HD2	1.65	0.61
30:c:35:ARG:HG3	30:c:42:LEU:HD11	1.82	0.61
50:w:35:SER:OG	50:w:38:SER:OG	2.10	0.61
1:1:611:C:H2'	1:1:612:G:H5'	1.80	0.61
1:1:2079:U:O2'	24:W:23:ASN:OD1	2.16	0.61
9:H:15:LEU:HD23	9:H:16:GLY:N	2.16	0.61
2:2:545:C:OP1	35:h:58:LYS:NZ	2.33	0.61
2:2:1130:A:O2'	40:m:5:GLN:NE2	2.32	0.61
7:F:134:GLU:CG	7:F:136:ILE:HD12	2.29	0.61
43:p:46:ASN:ND2	43:p:89:0TD:SB	2.72	0.61
1:1:2469:A:N6	1:1:2481:G:O2'	2.34	0.61
54:z:71:5MU:H3'	54:z:71:5MU:OP2	2.00	0.61
1:1:2128:G:N3	1:1:2173:A:O2'	2.33	0.61
1:1:2133:G:C2	1:1:2158:A:C6	2.89	0.61
34:g:24:ALA:HB1	34:g:28:GLU:HG2	1.82	0.61
1:1:1056:G:O2'	1:1:1086:A:O2'	2.15	0.61
1:1:1664:A:H2	11:J:1:MET:HE1	1.64	0.61
46:s:4:SER:O	46:s:8:THR:HG23	2.01	0.61
1:1:2312:U:O2	7:F:37:ASN:ND2	2.34	0.61
2:2:1360:A:OP2	45:r:75:ARG:NH2	2.34	0.61
20:S:11:LEU:O	25:X:29:ARG:NH1	2.34	0.61
1:1:2635:A:O2'	5:D:81:GLU:OE1	2.15	0.60
41:n:19:ASP:HA	41:n:22:THR:HG22	1.83	0.60
1:1:2127:G:H8	1:1:2127:G:H5''	1.64	0.60
4:C:258:ARG:NH1	4:C:264:ASP:OD1	2.32	0.60
11:J:43:ILE:HD12	11:J:56:ASP:HB2	1.84	0.60
23:V:59:LEU:CD1	23:V:80:ILE:HD12	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:l:77:ARG:NE	39:l:79:SER:O	2.34	0.60
19:R:69:LEU:HD22	19:R:107:VAL:CG2	2.24	0.60
1:1:894:U:O2'	1:1:895:U:OP1	2.18	0.60
2:2:1305:G:H21	2:2:1332:A:H2	1.49	0.60
4:C:142:HIS:ND1	4:C:193:GLY:O	2.34	0.60
20:S:1:MET:HE3	20:S:2:ILE:O	2.01	0.60
40:m:12:ARG:HG3	40:m:13:LYS:H	1.67	0.60
1:1:1789:A:OP2	4:C:221:ARG:NH1	2.35	0.60
36:i:154:ALA:HA	36:i:164:ILE:HD11	1.84	0.60
1:1:324:A:OP2	1:1:1205:A:N6	2.35	0.60
1:1:1363:C:O2'	1:1:1809:A:N3	2.32	0.60
1:1:2831:G:N2	1:1:2884:U:OP2	2.35	0.60
2:2:673:A:O3'	37:j:86:ARG:NH2	2.34	0.60
7:F:74:VAL:HG22	7:F:79:ILE:HD11	1.84	0.60
1:1:1042:G:O2'	1:1:1043:C:H5''	2.02	0.59
38:k:66:LEU:HD21	38:k:97:ASN:OD1	2.02	0.59
51:x:4:ILE:HG22	51:x:6:SER:H	1.67	0.59
36:i:149:SER:H	36:i:152:MET:HE2	1.67	0.59
4:C:133:ARG:NE	4:C:187:ASP:OD1	2.33	0.59
15:N:94:ARG:NH2	15:N:97:PHE:O	2.35	0.59
35:h:27:ALA:O	35:h:30:THR:OG1	2.17	0.59
1:1:511:U:H2'	1:1:512:G:H5'	1.83	0.59
1:1:811:U:H2'	12:K:21:ARG:HA	1.84	0.59
37:j:86:ARG:NH1	49:v:64:TYR:O	2.36	0.59
52:y:8:GLU:O	52:y:9:ASN:OD1	2.20	0.59
1:1:517:C:P	28:a:10:ARG:HH22	2.26	0.59
1:1:1801:A:OP2	4:C:150:LYS:NZ	2.33	0.59
2:2:1016:A:HO2'	2:2:1217:C:HO2'	1.50	0.59
2:2:1193:G:O6	34:g:3:GLN:NE2	2.36	0.59
33:f:72:THR:HG22	33:f:93:ASN:C	2.27	0.59
36:i:148:ASN:ND2	39:l:73:GLU:OE2	2.34	0.59
2:2:878:A:OP1	39:l:80:ARG:NH1	2.33	0.59
7:F:45:ALA:O	7:F:46:ASP:OD1	2.21	0.59
46:s:67:LEU:HD22	46:s:78:TYR:CE1	2.38	0.59
55:B:42:TYR:HA	55:B:45:LYS:HE3	1.83	0.59
18:Q:38:VAL:HG13	18:Q:54:VAL:HB	1.84	0.59
2:2:754:C:O5'	46:s:72:ARG:NH1	2.36	0.58
1:1:2062:A:H61	55:B:61:ALA:HA	1.67	0.58
17:P:50:ARG:O	17:P:54:LYS:NZ	2.35	0.58
36:i:11:LEU:HD11	36:i:45:ARG:NH1	2.18	0.58
54:z:46:G:H22	54:z:55:5MU:HN3	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1754:A:O2'	16:O:103:ARG:NH2	2.35	0.58
1:1:1901:A:OP2	4:C:253:LYS:NZ	2.29	0.58
21:T:36:VAL:CG1	21:T:39:ILE:HD12	2.33	0.58
5:D:25:THR:OG1	5:D:191:GLY:O	2.20	0.58
15:N:28:VAL:HG12	15:N:93:ASP:O	2.03	0.58
29:b:13:SER:HA	29:b:49:TYR:CD1	2.38	0.58
40:m:62:ASP:C	40:m:63:LEU:HD12	2.28	0.58
51:x:82:GLN:O	51:x:85:LYS:HG3	2.03	0.58
1:1:2343:U:HO2'	1:1:2373:G:HO2'	1.51	0.58
37:j:69:GLU:OE1	37:j:69:GLU:N	2.37	0.58
38:k:15:ASP:OD1	38:k:20:SER:N	2.35	0.58
39:l:74:SER:OG	39:l:130:ALA:HB3	2.03	0.58
27:Z:51:VAL:HG23	27:Z:52:ALA:H	1.67	0.58
28:a:52:ARG:NH2	28:a:54:VAL:HG12	2.19	0.58
33:f:129:LEU:HD23	33:f:129:LEU:H	1.69	0.58
38:k:47:LEU:HD23	38:k:58:GLU:HB3	1.86	0.58
37:j:42:TRP:HZ2	37:j:61:LEU:HD22	1.69	0.58
1:1:1063:G:N7	1:1:1064:C:N4	2.52	0.58
1:1:2646:C:OP2	1:1:2732:G:O2'	2.22	0.58
26:Y:47:MET:O	26:Y:51:VAL:HG22	2.04	0.58
34:g:51:SER:OG	34:g:71:ALA:HB3	2.04	0.58
2:2:1320:C:N3	50:w:36:ARG:NH1	2.52	0.58
7:F:153:ASP:OD1	7:F:154:ILE:N	2.37	0.58
47:t:18:GLN:OE1	47:t:35:ARG:NE	2.28	0.58
1:1:210:C:OP1	30:c:29:GLN:NE2	2.37	0.58
1:1:2133:G:C2	1:1:2158:A:N1	2.72	0.58
2:2:890:G:O2'	2:2:906:A:N6	2.37	0.58
3:3:66:A:O4'	3:3:108:A:N6	2.37	0.58
52:y:4:ILE:HD12	52:y:19:PHE:HD1	1.68	0.58
1:1:2128:G:H21	1:1:2174:C:H5'	1.69	0.57
1:1:2249:U:N3	1:1:2253:G:OP2	2.35	0.57
36:i:57:PRO:HA	36:i:60:ILE:HG12	1.86	0.57
55:B:60:LYS:HG3	55:B:64:ALA:HB3	1.84	0.57
2:2:406:G:H5'	35:h:5:LEU:HD22	1.86	0.57
2:2:841:C:H2'	2:2:843:U:H5'	1.85	0.57
38:k:140:ASP:OD1	38:k:143:ARG:NH1	2.37	0.57
5:D:17:GLU:OE1	5:D:17:GLU:N	2.35	0.57
8:G:46:ALA:O	8:G:47:ASP:OD1	2.23	0.57
10:I:19:ASP:OD1	10:I:58:ASN:ND2	2.34	0.57
26:Y:45:ARG:NH1	26:Y:59:GLU:OE1	2.33	0.57
34:g:20:SER:OG	34:g:40:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:62:MET:HG2	37:j:64:VAL:HG23	1.85	0.57
1:1:2134:A:N6	1:1:2157:G:H1'	2.19	0.57
2:2:80:A:H2'	2:2:81:A:C8	2.39	0.57
21:T:36:VAL:HG11	21:T:39:ILE:HD12	1.85	0.57
43:p:16:VAL:HG23	43:p:16:VAL:O	2.04	0.57
2:2:1222:G:OP2	2:2:1322:C:N4	2.34	0.57
54:z:49:G:C2	54:z:52:A:N1	2.72	0.57
1:1:776:G:N7	1:1:793:A:O2'	2.33	0.57
1:1:955:PSU:HN3	1:1:962:G:H1	1.52	0.57
2:2:1279:G:O2'	2:2:1282:C:N4	2.38	0.57
36:i:111:MET:HA	36:i:114:VAL:HG12	1.85	0.57
44:q:11:ASP:OD1	44:q:46:SER:OG	2.20	0.57
12:K:124:GLY:C	12:K:125:LEU:HD12	2.30	0.57
33:f:129:LEU:HD11	33:f:134:ALA:CA	2.33	0.57
33:f:207:ILE:HA	33:f:210:VAL:HG22	1.87	0.57
1:1:491:G:O6	19:R:49:LYS:NZ	2.31	0.57
1:1:1078:U:O2'	1:1:1088:A:OP1	2.22	0.57
9:H:4:ILE:HD12	9:H:17:ASP:C	2.30	0.57
8:G:85:LYS:HB3	8:G:133:LEU:HD11	1.86	0.57
15:N:2:ASP:N	15:N:2:ASP:OD1	2.38	0.57
38:k:22:LEU:HD21	38:k:66:LEU:CD2	2.34	0.57
1:1:2266:A:N6	1:1:2273:A:OP2	2.38	0.56
2:2:811:C:O2'	2:2:901:A:N1	2.38	0.56
33:f:185:ALA:HB3	33:f:196:VAL:HG11	1.86	0.56
55:B:9:VAL:HG12	55:B:21:ILE:CG1	2.33	0.56
55:B:45:LYS:HD3	55:B:49:GLN:NE2	2.20	0.56
1:1:2159:G:H2'	1:1:2160:C:C6	2.40	0.56
9:H:54:LEU:O	9:H:57:LYS:HG2	2.04	0.56
40:m:106:ARG:NH1	40:m:107:ASP:O	2.38	0.56
1:1:2127:G:H5''	1:1:2127:G:C8	2.40	0.56
1:1:2676:C:OP1	11:J:31:ARG:NH2	2.38	0.56
2:2:404:G:O6	35:h:2:ALA:N	2.39	0.56
9:H:79:THR:HG23	9:H:79:THR:O	2.05	0.56
19:R:86:MET:SD	19:R:87:PRO:HD2	2.46	0.56
41:n:88:MET:HE2	41:n:100:ILE:HD13	1.88	0.56
50:w:50:ALA:HB1	50:w:57:HIS:HB3	1.86	0.56
51:x:59:ASP:OD1	51:x:59:ASP:N	2.38	0.56
6:E:1:MET:HB3	6:E:14:VAL:HG23	1.87	0.56
21:T:72:ILE:HD12	21:T:83:VAL:HG21	1.87	0.56
44:q:104:THR:HG22	44:q:105:ASN:OD1	2.05	0.56
15:N:15:ARG:NH2	15:N:95:SER:OG	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:18:ALA:O	23:V:20:ARG:NH1	2.32	0.56
27:Z:4:ASP:OD1	27:Z:5:ILE:HG23	2.05	0.56
7:F:95:ARG:HH12	27:Z:1:MET:HE1	1.69	0.56
18:Q:52:PRO:O	18:Q:53:PHE:CG	2.59	0.56
1:1:1066:U:H2'	1:1:1067:A:H2'	1.88	0.56
34:g:47:LEU:HD11	34:g:87:LEU:HD11	1.87	0.56
1:1:2194:U:H2'	1:1:2195:U:C6	2.41	0.56
2:2:544:G:OP1	35:h:56:ARG:NH2	2.31	0.56
2:2:1422:G:H4'	11:J:48:PRO:HB3	1.88	0.56
7:F:117:LEU:N	7:F:177:PHE:O	2.37	0.56
9:H:4:ILE:HD12	9:H:17:ASP:O	2.06	0.56
15:N:70:ALA:O	15:N:74:VAL:HG23	2.06	0.56
33:f:118:GLU:O	33:f:122:GLN:HG3	2.06	0.56
33:f:128:LYS:HD2	33:f:128:LYS:O	2.06	0.56
34:g:36:ASP:OD1	34:g:59:ARG:NH2	2.39	0.56
1:1:534:U:O2'	17:P:49:ASP:OD2	2.14	0.55
1:1:2519:U:O4'	1:1:2542:A:N6	2.39	0.55
1:1:2316:G:H2'	1:1:2317:A:H8	1.70	0.55
2:2:1179:A:OP2	40:m:99:ARG:NH2	2.39	0.55
15:N:50:ALA:O	15:N:81:ARG:NH2	2.40	0.55
22:U:9:ARG:HG2	22:U:41:GLU:CG	2.36	0.55
36:i:156:LYS:HG2	39:l:71:VAL:HG13	1.87	0.55
1:1:65:U:O2'	1:1:456:C:N3	2.32	0.55
3:3:74:U:O2	22:U:29:ILE:HD13	2.06	0.55
41:n:28:THR:HG22	41:n:87:LEU:HD11	1.88	0.55
43:p:4:VAL:O	43:p:8:VAL:HG23	2.06	0.55
52:y:31:GLU:OE2	52:y:34:ARG:NH2	2.38	0.55
1:1:2102:G:C6	1:1:2187:U:N3	2.74	0.55
1:1:2126:A:H2	1:1:2162:G:H1'	1.71	0.55
2:2:1328:C:O2'	44:q:29:ARG:NH1	2.33	0.55
6:E:189:THR:HG22	6:E:191:ASP:H	1.70	0.55
52:y:16:LEU:HD23	52:y:20:LYS:HE2	1.88	0.55
1:1:2061:G:H21	55:B:69:SER:HA	1.72	0.55
1:1:2182:U:O2'	1:1:2183:A:O5'	2.25	0.55
2:2:1100:C:N4	2:2:1103:C:OP1	2.40	0.55
26:Y:6:LYS:HB2	26:Y:58:GLU:HB3	1.87	0.55
6:E:6:LYS:O	6:E:9:GLN:NE2	2.39	0.55
12:K:132:ARG:HG3	12:K:142:ILE:HD12	1.88	0.55
16:O:14:LYS:HE2	16:O:77:HIS:HA	1.89	0.55
28:a:26:THR:HG23	28:a:27:SER:H	1.71	0.55
45:r:50:THR:HG22	50:w:13:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:x:31:PHE:O	51:x:35:VAL:HG23	2.05	0.55
1:1:247:G:OP2	1:1:249:C:N4	2.37	0.55
1:1:545:U:O2'	1:1:546:U:O3'	2.22	0.55
1:1:818:G:N1	1:1:1188:U:OP2	2.36	0.55
9:H:81:ALA:HA	9:H:147:VAL:HG23	1.89	0.55
13:L:78:LEU:O	23:V:5:LYS:NZ	2.36	0.55
38:k:60:GLU:O	38:k:64:VAL:HG23	2.06	0.55
54:z:19:G:O2'	54:z:20:5MU:OP1	2.22	0.55
1:1:2585:U:H1'	55:B:70:LEU:HD13	1.89	0.55
1:1:2681:C:OP2	5:D:114:LYS:NZ	2.36	0.55
12:K:55:MET:SD	12:K:59:ARG:NH2	2.80	0.55
1:1:887:A:O2'	1:1:888:C:O5'	2.22	0.55
1:1:2128:G:C2	1:1:2173:A:O2'	2.60	0.55
18:Q:34:GLU:HG2	18:Q:60:LYS:HG2	1.89	0.55
19:R:85:ILE:HG23	19:R:85:ILE:O	2.05	0.55
33:f:31:ILE:HD13	33:f:39:HIS:ND1	2.22	0.55
2:2:412:A:H62	2:2:431:A:H61	1.55	0.55
1:1:599:A:O2'	1:1:600:G:H5'	2.07	0.54
2:2:1132:C:H2'	2:2:1133:G:C8	2.42	0.54
14:M:54:LEU:HD11	14:M:62:ASN:HD22	1.72	0.54
18:Q:52:PRO:HD2	18:Q:53:PHE:H	1.72	0.54
40:m:130:ARG:NH1	54:z:34:U:OP2	2.40	0.54
27:Z:16:CYS:SG	27:Z:17:SER:N	2.81	0.54
1:1:643:A:N1	1:1:2369:A:O2'	2.38	0.54
42:o:18:ASP:OD2	42:o:37:ARG:NE	2.35	0.54
2:2:1176:A:H2'	2:2:1177:G:C8	2.42	0.54
4:C:107:PRO:HD2	4:C:110:LEU:HD22	1.89	0.54
41:n:15:HIS:HA	41:n:18:ILE:HG22	1.88	0.54
44:q:100:GLN:OE1	44:q:100:GLN:N	2.40	0.54
46:s:64:ARG:HH12	46:s:89:ARG:HB3	1.72	0.54
4:C:69:ARG:NH2	4:C:127:GLY:O	2.38	0.54
19:R:91:GLY:HA3	55:B:53:PHE:HB3	1.90	0.54
1:1:2667:C:N3	8:G:110:SER:OG	2.35	0.54
2:2:1004:A:H2'	2:2:1005:A:O4'	2.07	0.54
36:i:165:LEU:HD12	39:l:114:ARG:HD2	1.90	0.54
43:p:56:ARG:NE	43:p:62:GLU:OE1	2.37	0.54
46:s:21:ASP:O	46:s:22:THR:HG22	2.08	0.54
2:2:346:G:OP1	16:O:39:ARG:NH2	2.40	0.54
50:w:36:ARG:NH2	50:w:75:ALA:O	2.40	0.54
1:1:1419:A:O2'	1:1:1421:G:N7	2.30	0.54
2:2:983:A:OP1	45:r:6:MET:HE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:69:PHE:HB3	33:f:80:VAL:CG2	2.37	0.54
38:k:71:PRO:O	38:k:96:ARG:HG2	2.08	0.54
1:1:896:A:H2	1:1:897:C:H41	1.54	0.54
2:2:1043:G:H2'	2:2:1044:A:C8	2.43	0.54
55:B:13:ASN:OD1	55:B:16:LYS:N	2.37	0.54
36:i:151:GLU:OE1	36:i:151:GLU:N	2.38	0.53
47:t:55:ASP:OD1	47:t:56:ARG:N	2.41	0.53
1:1:1392:A:N6	20:S:18:GLU:OE1	2.40	0.53
1:1:1607:C:O2	1:1:1607:C:C2'	2.55	0.53
2:2:1261:A:N6	2:2:1274:A:O2'	2.37	0.53
19:R:34:ASP:OD1	19:R:35:ILE:N	2.40	0.53
23:V:26:PHE:N	23:V:29:GLU:OE1	2.38	0.53
2:2:203:G:N2	2:2:204:G:O6	2.40	0.53
2:2:1417:G:O2'	2:2:1483:A:N6	2.41	0.53
12:K:57:LEU:HD22	31:d:54:ASP:HB3	1.91	0.53
34:g:155:GLY:O	34:g:196:ILE:HG12	2.09	0.53
50:w:64:ASP:O	50:w:67:VAL:HG23	2.08	0.53
2:2:90:C:H2'	2:2:91:U:C6	2.43	0.53
2:2:1168:U:HO2'	2:2:1169:A:P	2.30	0.53
7:F:95:ARG:NH1	27:Z:1:MET:HE1	2.24	0.53
55:B:5:MET:HE3	55:B:6:THR:HG23	1.89	0.53
1:1:895:U:H2'	1:1:896:A:C4	2.44	0.53
1:1:1074:G:H2'	1:1:1075:C:C6	2.44	0.53
1:1:1915:3TD:H2'	1:1:1916:A:O4'	2.08	0.53
1:1:2148:G:H2'	1:1:2149:U:C6	2.43	0.53
28:a:26:THR:HG23	28:a:27:SER:N	2.22	0.53
37:j:9:MET:HG2	37:j:59:TYR:CE1	2.44	0.53
1:1:1020:A:N1	1:1:1141:U:O2'	2.25	0.53
9:H:15:LEU:HD23	9:H:15:LEU:C	2.32	0.53
55:B:47:GLU:O	55:B:51:VAL:HG23	2.09	0.53
1:1:573:U:O2'	1:1:575:A:OP1	2.22	0.53
1:1:2113:U:O4	1:1:2114:A:N6	2.42	0.53
1:1:2189:U:C2	1:1:2190:G:C8	2.96	0.53
1:1:2820:A:OP2	14:M:2:ARG:NH2	2.41	0.53
2:2:1241:G:OP1	38:k:35:LYS:NZ	2.41	0.53
4:C:125:LYS:HG2	4:C:128:ASN:OD1	2.08	0.53
25:X:32:ALA:HB2	25:X:37:LEU:HD23	1.91	0.53
45:r:80:SER:O	45:r:84:VAL:HG23	2.08	0.53
48:u:48:ASP:CG	48:u:75:LEU:HD21	2.34	0.53
1:1:1914:C:H2'	1:1:1915:3TD:O4	2.08	0.53
5:D:1:MET:HE2	5:D:100:LEU:CD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:38:MET:HE3	7:F:87:CYS:SG	2.49	0.53
19:R:13:SER:O	19:R:17:VAL:HG23	2.08	0.53
54:z:49:G:N3	54:z:52:A:C6	2.77	0.53
1:1:463:G:N2	1:1:465:G:H3'	2.23	0.53
1:1:587:C:OP2	12:K:21:ARG:NH2	2.38	0.53
1:1:621:A:C8	1:1:621:A:C5'	2.86	0.53
1:1:1019:U:OP1	1:1:1035:U:O2'	2.21	0.53
1:1:1798:U:OP2	4:C:271:ARG:NH2	2.42	0.53
2:2:108:G:H5'	2:2:109:A:H5''	1.90	0.53
20:S:72:GLN:NE2	55:B:30:VAL:O	2.39	0.53
51:x:28:MET:HE1	51:x:67:ILE:HG21	1.91	0.53
1:1:1328:A:H2'	1:1:1330:C:C5	2.44	0.53
1:1:2061:G:N2	55:B:69:SER:HA	2.23	0.53
7:F:140:GLU:OE1	27:Z:28:VAL:HG23	2.09	0.53
38:k:24:ALA:HA	38:k:27:VAL:HG22	1.90	0.53
55:B:9:VAL:HG11	55:B:12:PHE:HD1	1.74	0.53
1:1:995:C:O2	10:I:3:THR:OG1	2.21	0.52
1:1:1278:C:O2'	14:M:27:SER:OG	2.25	0.52
9:H:83:LYS:O	9:H:91:PHE:CE2	2.62	0.52
21:T:38:GLY:N	21:T:62:GLU:OE2	2.41	0.52
36:i:136:VAL:O	36:i:140:THR:HG23	2.10	0.52
2:2:1377:A:OP1	38:k:92:ARG:NH1	2.42	0.52
5:D:1:MET:HE2	5:D:100:LEU:HD21	1.90	0.52
19:R:31:GLN:O	19:R:34:ASP:OD1	2.27	0.52
55:B:42:TYR:CD1	55:B:42:TYR:C	2.88	0.52
55:B:53:PHE:C	55:B:55:ILE:H	2.16	0.52
1:1:2131:U:H4'	1:1:2133:G:N7	2.25	0.52
9:H:70:GLU:HG2	9:H:138:VAL:CG1	2.39	0.52
13:L:53:MET:HG3	13:L:63:ILE:HD13	1.92	0.52
1:1:714:U:OP2	46:s:89:ARG:NH1	2.42	0.52
14:M:24:MET:SD	14:M:44:LEU:HD22	2.49	0.52
36:i:11:LEU:HD11	36:i:45:ARG:HH12	1.73	0.52
36:i:46:VAL:HG22	36:i:118:ALA:HA	1.91	0.52
51:x:37:ALA:O	51:x:40:GLU:HG3	2.09	0.52
52:y:8:GLU:N	52:y:8:GLU:OE1	2.40	0.52
1:1:887:A:HO2'	1:1:888:C:P	2.32	0.52
7:F:149:VAL:HG23	7:F:149:VAL:O	2.09	0.52
19:R:23:LEU:HD22	28:a:24:ALA:HB2	1.91	0.52
19:R:73:LYS:HB2	19:R:106:VAL:HB	1.92	0.52
54:z:68:G:C5	54:z:69:5MU:H1'	2.45	0.52
1:1:1378:A:O2'	1:1:1380:G:N7	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1356:G:H2'	2:2:1357:A:C8	2.45	0.52
5:D:151:THR:CG2	5:D:152:PRO:HD3	2.22	0.52
34:g:87:LEU:O	34:g:91:VAL:HG23	2.09	0.52
55:B:39:ASN:HA	55:B:42:TYR:CE2	2.45	0.52
55:B:42:TYR:O	55:B:45:LYS:HB3	2.10	0.52
1:1:2795:C:H2'	1:1:2796:U:C6	2.45	0.52
2:2:1527:U:OP2	52:y:42:THR:HG22	2.10	0.52
26:Y:25:LEU:HD23	26:Y:25:LEU:C	2.34	0.52
34:g:7:PRO:HA	34:g:10:ILE:HG22	1.90	0.52
1:1:355:U:H2'	1:1:356:G:H8	1.74	0.52
1:1:402:A:H2'	1:1:403:U:C5'	2.39	0.52
1:1:2113:U:N3	1:1:2114:A:N7	2.57	0.52
1:1:2305:U:O3'	7:F:133:ARG:NH1	2.43	0.52
2:2:1062:U:H2'	2:2:1063:C:C6	2.45	0.52
19:R:91:GLY:HA3	55:B:53:PHE:CB	2.40	0.52
28:a:9:THR:HG23	28:a:12:LYS:H	1.73	0.52
33:f:14:VAL:HG13	33:f:213:TYR:OH	2.10	0.52
33:f:85:LEU:C	33:f:85:LEU:HD12	2.35	0.52
33:f:130:THR:O	33:f:133:GLU:N	2.43	0.52
38:k:115:SER:O	38:k:119:ARG:HD3	2.09	0.52
40:m:44:ALA:HA	40:m:47:VAL:HG22	1.91	0.52
55:B:45:LYS:NZ	55:B:46:ASP:OD1	2.40	0.52
26:Y:40:ASP:OD1	26:Y:45:ARG:NE	2.42	0.52
33:f:27:MET:HE1	33:f:187:VAL:HG11	1.90	0.52
45:r:54:ASP:HA	45:r:59:ARG:HD3	1.92	0.52
2:2:81:A:N6	2:2:87:C:C4	2.78	0.52
2:2:1119:C:OP2	40:m:11:ARG:NH1	2.43	0.52
2:2:1181:G:O2'	2:2:1182:G:N7	2.37	0.52
8:G:105:LEU:HD13	8:G:107:LEU:HD11	1.91	0.52
9:H:91:PHE:CD1	9:H:92:GLY:N	2.78	0.52
37:j:3:HIS:CD2	37:j:95:ALA:HB2	2.45	0.51
43:p:24:LEU:HD23	43:p:27:CYS:O	2.10	0.51
1:1:307:G:N1	1:1:310:A:OP2	2.37	0.51
1:1:1584:U:H5'	1:1:1585:C:C6	2.45	0.51
9:H:96:THR:HG22	9:H:117:LEU:HD11	1.92	0.51
1:1:1056:G:O2'	1:1:1103:A:N6	2.43	0.51
2:2:1126:U:O4	41:n:9:ARG:NH1	2.43	0.51
22:U:56:PHE:CE1	22:U:61:LEU:HD21	2.45	0.51
1:1:2362:C:OP1	31:d:40:ARG:NE	2.41	0.51
2:2:552:U:H2'	2:2:553:A:H8	1.75	0.51
9:H:77:THR:HA	9:H:143:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1607:C:N4	1:1:1621:U:H2'	2.25	0.51
2:2:844:G:N1	2:2:846:G:H1'	2.25	0.51
9:H:41:LYS:O	9:H:45:GLU:OE1	2.28	0.51
9:H:84:ALA:O	9:H:148:ALA:HB2	2.11	0.51
33:f:127:ASP:O	33:f:128:LYS:HB3	2.10	0.51
38:k:40:GLU:OE1	40:m:41:ARG:NH2	2.40	0.51
41:n:17:LEU:CD2	41:n:96:VAL:HG23	2.41	0.51
42:o:60:PRO:HD3	42:o:91:PRO:HB2	1.91	0.51
52:y:3:VAL:HG23	52:y:3:VAL:O	2.09	0.51
54:z:38:G:H2'	54:z:39:5MU:O4'	2.11	0.51
1:1:244:A:OP2	31:d:8:ARG:NH2	2.40	0.51
9:H:68:ARG:C	9:H:68:ARG:HD2	2.36	0.51
18:Q:52:PRO:CD	18:Q:53:PHE:H	2.24	0.51
39:l:74:SER:HG	39:l:130:ALA:HB3	1.74	0.51
1:1:276:U:O2'	1:1:277:G:N7	2.29	0.51
1:1:2584:U:H2'	1:1:2585:U:C2	2.46	0.51
9:H:103:VAL:O	9:H:106:ALA:C	2.54	0.51
54:z:49:G:N2	54:z:52:A:C2	2.78	0.51
1:1:856:G:H2'	1:1:857:G:C8	2.45	0.51
1:1:2134:A:C5	1:1:2158:A:H2	2.29	0.51
1:1:2175:C:H2'	1:1:2176:A:C8	2.46	0.51
3:3:1:U:O2'	3:3:2:G:H8	1.93	0.51
4:C:4:VAL:O	4:C:4:VAL:HG23	2.11	0.51
21:T:15:THR:OG1	21:T:69:ASN:OD1	2.29	0.51
27:Z:59:ARG:O	27:Z:63:ARG:HG3	2.11	0.51
1:1:2199:A:OP1	24:W:37:ARG:NH1	2.44	0.51
2:2:1006:G:C6	2:2:1024:G:C2	2.99	0.51
36:i:120:VAL:HG11	36:i:123:VAL:HG13	1.92	0.51
37:j:99:ALA:HB1	37:j:103:VAL:HG11	1.91	0.51
2:2:261:U:N3	2:2:264:C:OP2	2.31	0.51
2:2:1060:U:H5''	41:n:53:ILE:HD12	1.93	0.51
2:2:1152:A:P	41:n:72:ARG:HH22	2.34	0.51
2:2:1319:A:O2'	2:2:1323:G:N7	2.35	0.51
2:2:1328:C:H5''	44:q:28:THR:HG21	1.92	0.51
34:g:42:TYR:CE2	34:g:90:VAL:HG21	2.46	0.51
36:i:120:VAL:HG11	36:i:123:VAL:CG1	2.41	0.51
45:r:46:LEU:HD12	50:w:13:LEU:HB3	1.93	0.51
1:1:84:A:N1	1:1:98:G:O2'	2.42	0.50
1:1:402:A:C2'	1:1:403:U:H5'	2.40	0.50
1:1:870:U:OP1	13:L:6:ARG:NH1	2.41	0.50
1:1:2314:A:H1'	7:F:155:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:90:C:H2'	2:2:91:U:H6	1.76	0.50
2:2:713:G:H2'	2:2:714:G:C8	2.46	0.50
36:i:150:PRO:HA	36:i:153:VAL:HG22	1.93	0.50
55:B:8:ILE:HG13	55:B:25:ASP:HB2	1.93	0.50
55:B:45:LYS:HD2	55:B:46:ASP:N	2.27	0.50
1:1:2387:U:OP1	23:V:55:ARG:NH2	2.37	0.50
2:2:1242:G:H2'	2:2:1243:C:H5''	1.93	0.50
6:E:150:THR:HG22	6:E:152:GLU:H	1.76	0.50
33:f:50:PHE:CE2	33:f:54:LEU:HD11	2.46	0.50
36:i:133:PRO:HA	36:i:136:VAL:HG12	1.92	0.50
44:q:83:LEU:HD21	50:w:65:GLU:CB	2.41	0.50
55:B:34:PHE:HA	55:B:37:ILE:HD12	1.93	0.50
1:1:570:G:H2'	1:1:2030:6MZ:N7	2.26	0.50
1:1:1061:U:H4'	1:1:1070:A:O4'	2.11	0.50
1:1:2122:U:H2'	1:1:2123:G:C8	2.46	0.50
2:2:1007:U:H2'	2:2:1008:U:H6	1.76	0.50
33:f:130:THR:HG23	33:f:133:GLU:CB	2.42	0.50
39:l:55:THR:HG23	39:l:56:LYS:H	1.77	0.50
7:F:135:GLN:CG	7:F:141:ILE:HD13	2.40	0.50
18:Q:52:PRO:O	18:Q:53:PHE:CD2	2.64	0.50
39:l:30:SER:O	39:l:34:VAL:HG23	2.11	0.50
41:n:42:LEU:HB2	41:n:71:LEU:HB3	1.94	0.50
1:1:370:G:O2'	1:1:424:G:OP1	2.26	0.50
1:1:2192:U:H2'	1:1:2193:G:O4'	2.11	0.50
6:E:118:LEU:HD11	6:E:188:MET:SD	2.51	0.50
40:m:7:TYR:HH	40:m:9:THR:HG1	1.57	0.50
1:1:1534:U:O2'	1:1:1537:G:O6	2.29	0.50
1:1:1936:A:OP2	1:1:1962:5MC:N4	2.37	0.50
2:2:1305:G:HO2'	2:2:1306:A:H8	1.55	0.50
10:I:114:LEU:HG	10:I:118:MET:HE3	1.92	0.50
2:2:202:G:O2'	2:2:468:A:H8	1.94	0.50
54:z:50:C:O2'	54:z:51:A:OP1	2.29	0.50
1:1:2305:U:H5''	7:F:131:GLY:HA3	1.93	0.50
5:D:3:GLY:HA3	5:D:204:LYS:HG2	1.93	0.50
37:j:37:HIS:NE2	37:j:65:GLU:HB2	2.27	0.50
44:q:9:ILE:CG2	44:q:18:ALA:HB1	2.38	0.50
44:q:16:VAL:HG23	44:q:17:ILE:HD12	1.94	0.50
55:B:45:LYS:HD3	55:B:49:GLN:CD	2.36	0.50
1:1:85:G:OP2	21:T:7:ARG:HB2	2.11	0.50
1:1:1870:C:O2'	1:1:1871:A:O4'	2.28	0.50
9:H:124:THR:HG23	9:H:128:HIS:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:6:ARG:NH1	20:S:37:ASP:OD1	2.45	0.50
31:d:26:HIS:CE1	31:d:48:ALA:HB2	2.47	0.50
33:f:72:THR:HG22	33:f:93:ASN:O	2.12	0.50
33:f:161:LEU:HD13	33:f:181:ILE:HG21	1.94	0.50
35:h:95:GLU:HA	35:h:100:ASN:HD22	1.77	0.50
42:o:47:ALA:HB1	42:o:62:ALA:HB1	1.94	0.50
1:1:891:G:O2'	1:1:892:A:P	2.70	0.49
1:1:996:A:OP2	17:P:93:LYS:NZ	2.41	0.49
2:2:280:C:N4	48:u:41:THR:OG1	2.45	0.49
39:l:87:LYS:HG3	39:l:125:ILE:HD11	1.92	0.49
48:u:59:VAL:HG12	48:u:60:GLU:N	2.27	0.49
54:z:19:G:C4'	54:z:20:5MU:OP2	2.60	0.49
1:1:2402:U:O2'	1:1:2403:C:H5''	2.12	0.49
2:2:496:A:H2'	2:2:496:A:N3	2.27	0.49
8:G:54:PRO:HG2	8:G:62:TRP:CE2	2.48	0.49
9:H:88:GLY:C	9:H:90:LEU:H	2.20	0.49
1:1:170:U:H2'	1:1:171:U:C6	2.47	0.49
1:1:601:C:H2'	1:1:602:A:O4'	2.12	0.49
2:2:770:C:O2'	2:2:899:C:N3	2.42	0.49
2:2:1145:A:C2'	2:2:1146:A:OP2	2.60	0.49
27:Z:45:THR:O	27:Z:49:ARG:HG2	2.13	0.49
1:1:1062:G:C6	1:1:1077:A:N6	2.80	0.49
1:1:1173:U:H4'	1:1:1174:U:H5'	1.92	0.49
4:C:144:VAL:HB	4:C:154:LEU:HB2	1.94	0.49
7:F:38:MET:HE2	7:F:57:LEU:HB2	1.94	0.49
13:L:47:GLU:OE2	13:L:50:ARG:NH1	2.45	0.49
2:2:438:U:H3	2:2:496:A:H62	1.59	0.49
2:2:1013:G:N2	2:2:1016:A:OP2	2.41	0.49
2:2:1530:G:H2'	2:2:1531:A:H8	1.77	0.49
23:V:59:LEU:HD12	23:V:80:ILE:HD12	1.93	0.49
55:B:56:GLU:CD	55:B:56:GLU:N	2.69	0.49
1:1:1079:C:H2'	1:1:1080:A:C8	2.48	0.49
2:2:946:A:H2'	2:2:947:G:C8	2.46	0.49
2:2:1406:U:C6	2:2:1407:5MC:HM53	2.48	0.49
9:H:88:GLY:O	9:H:90:LEU:N	2.42	0.49
10:I:31:GLU:OE2	10:I:35:ARG:NE	2.46	0.49
13:L:53:MET:O	13:L:57:VAL:HG22	2.12	0.49
15:N:27:VAL:CG2	15:N:40:ILE:HD12	2.41	0.49
1:1:811:U:O4	12:K:21:ARG:NH1	2.46	0.49
1:1:2052:A:C8	5:D:146:ILE:HD11	2.48	0.49
1:1:2150:C:H2'	1:1:2151:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:25:LEU:HD23	26:Y:25:LEU:O	2.13	0.49
33:f:137:ARG:O	33:f:140:GLU:HG2	2.12	0.49
34:g:32:ASN:OD1	34:g:59:ARG:NH1	2.46	0.49
1:1:635:C:H2'	1:1:636:G:O4'	2.13	0.49
1:1:645:C:H2'	1:1:647:G:C8	2.48	0.49
1:1:2127:G:H21	1:1:2173:A:C1'	2.25	0.49
15:N:33:ARG:O	15:N:65:THR:OG1	2.18	0.49
30:c:12:ARG:HG2	30:c:44:VAL:HG11	1.94	0.49
33:f:62:SER:HA	33:f:224:GLY:O	2.12	0.49
36:i:113:ALA:O	36:i:117:VAL:HG22	2.13	0.49
54:z:14:A:H2'	54:z:15:A:O4'	2.13	0.49
54:z:23:A:OP2	54:z:24:C:C5	2.65	0.49
1:1:1469:A:H2'	1:1:1470:A:C8	2.48	0.49
1:1:1604:C:O2'	1:1:1610:A:N1	2.40	0.49
1:1:2195:U:O2'	1:1:2196:C:H5'	2.13	0.49
5:D:34:VAL:HB	5:D:92:VAL:O	2.12	0.49
33:f:126:PHE:O	33:f:129:LEU:HD22	2.13	0.49
51:x:44:LYS:HE3	51:x:83:ILE:O	2.13	0.49
1:1:323:C:H2'	6:E:163:ASN:OD1	2.13	0.49
1:1:700:G:O2'	1:1:1632:A:N3	2.39	0.49
1:1:989:G:OP2	26:Y:12:SER:OG	2.31	0.49
1:1:1779:U:H5	1:1:1784:A:N7	2.11	0.49
1:1:2308:G:O6	1:1:2311:A:N7	2.45	0.49
1:1:2314:A:O4'	7:F:155:THR:HG21	2.12	0.49
17:P:106:PHE:O	17:P:110:VAL:HG23	2.13	0.49
1:1:993:G:OP1	17:P:50:ARG:NE	2.46	0.48
1:1:2182:U:O2'	1:1:2183:A:C8	2.61	0.48
1:1:2294:G:OP1	15:N:10:ARG:HD3	2.13	0.48
11:J:7:MET:HE3	11:J:18:ARG:HG3	1.93	0.48
20:S:53:VAL:HG23	20:S:91:GLN:OE1	2.13	0.48
44:q:33:ILE:HD11	44:q:63:PHE:HE2	1.78	0.48
1:1:137:U:C2'	1:1:138:U:H5'	2.43	0.48
1:1:2314:A:C1'	7:F:155:THR:HG21	2.43	0.48
2:2:672:U:H2'	2:2:673:A:C8	2.49	0.48
3:3:48:U:OP1	15:N:30:ARG:NH2	2.44	0.48
30:c:42:LEU:HD23	30:c:43:THR:HG23	1.96	0.48
34:g:155:GLY:HA2	34:g:163:ALA:HB1	1.95	0.48
37:j:9:MET:HE3	37:j:59:TYR:CE1	2.48	0.48
1:1:137:U:H2'	1:1:138:U:H5'	1.94	0.48
1:1:2123:G:C2	1:1:2176:A:C2	3.01	0.48
1:1:2145:C:O2	1:1:2145:C:O2'	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:766:A:OP2	2:2:812:G:N2	2.46	0.48
1:1:2118:U:O4	1:1:2143:C:O2'	2.27	0.48
2:2:1009:U:O2	2:2:1021:A:C2	2.66	0.48
2:2:1391:U:H2'	2:2:1392:G:C8	2.48	0.48
9:H:81:ALA:HA	9:H:147:VAL:CG2	2.43	0.48
34:g:123:GLN:HB3	34:g:128:VAL:HG21	1.95	0.48
43:p:99:ARG:NE	43:p:104:CYS:SG	2.85	0.48
54:z:71:5MU:H2'	54:z:72:C:C6	2.49	0.48
1:1:1156:A:C8	17:P:51:ARG:HG2	2.49	0.48
1:1:1818:U:O2'	4:C:153:GLN:O	2.18	0.48
1:1:2168:G:H2'	1:1:2169:A:C8	2.48	0.48
1:1:2849:U:N3	1:1:2867:G:O4'	2.46	0.48
8:G:101:ASN:HB2	8:G:117:LEU:HB2	1.96	0.48
38:k:69:VAL:HG12	38:k:135:VAL:HG12	1.96	0.48
48:u:15:ASP:OD1	48:u:55:ILE:HD11	2.13	0.48
1:1:639:U:H2'	1:1:640:C:C6	2.48	0.48
1:1:721:A:H2'	1:1:722:A:C8	2.49	0.48
1:1:1077:A:H61	1:1:1088:A:C2'	2.26	0.48
1:1:2591:C:H2'	1:1:2592:G:C8	2.48	0.48
1:1:2636:C:O2'	5:D:45:TYR:OH	2.30	0.48
2:2:496:A:O2'	2:2:497:G:C8	2.65	0.48
3:3:13:G:N2	3:3:16:G:N3	2.60	0.48
9:H:85:GLY:O	9:H:90:LEU:HB2	2.13	0.48
39:l:55:THR:HG23	39:l:56:LYS:N	2.29	0.48
41:n:90:LEU:HD23	41:n:91:ASP:N	2.28	0.48
44:q:11:ASP:CG	44:q:46:SER:HG	2.20	0.48
48:u:25:ILE:HD11	48:u:61:ILE:HD11	1.95	0.48
48:u:58:VAL:HB	48:u:79:VAL:O	2.13	0.48
1:1:1105:U:H2'	1:1:1106:G:H8	1.79	0.48
1:1:1590:A:H2'	1:1:1591:A:C8	2.48	0.48
1:1:1607:C:O2	1:1:1607:C:O2'	2.28	0.48
1:1:1980:G:O2'	1:1:1982:U:OP2	2.28	0.48
1:1:2425:A:H5''	1:1:2427:C:O4'	2.14	0.48
2:2:187:G:N2	2:2:190:A:OP2	2.46	0.48
7:F:135:GLN:HG3	7:F:141:ILE:HD13	1.94	0.48
13:L:14:LYS:O	13:L:71:LYS:NZ	2.32	0.48
1:1:372:G:O2'	1:1:400:G:O6	2.19	0.48
1:1:2131:U:C4'	1:1:2133:G:N7	2.77	0.48
9:H:94:ILE:HG13	9:H:94:ILE:O	2.13	0.48
54:z:76:5MU:OP2	54:z:76:5MU:H6	1.97	0.48
1:1:784:G:O2'	1:1:785:G:O5'	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1077:A:C2	1:1:1088:A:C2	3.02	0.48
1:1:2050:C:H2'	1:1:2051:A:O4'	2.14	0.48
1:1:2102:G:C2	1:1:2188:U:C2	3.01	0.48
1:1:2108:A:C2	1:1:2181:U:O2	2.66	0.48
1:1:2148:G:C2	1:1:2149:U:O4	2.66	0.48
1:1:2291:U:H2'	1:1:2292:U:C6	2.49	0.48
2:2:73:C:H2'	2:2:74:A:H5'	1.94	0.48
2:2:459:A:H2'	2:2:460:A:C8	2.49	0.48
2:2:632:U:H5''	2:2:633:G:C8	2.48	0.48
2:2:1377:A:C5	38:k:7:ILE:HD13	2.49	0.48
17:P:74:ILE:HD11	17:P:78:LYS:HB3	1.95	0.48
34:g:7:PRO:O	34:g:11:ARG:HD3	2.14	0.48
1:1:714:U:P	46:s:89:ARG:NH1	2.87	0.48
1:1:2103:C:N4	1:1:2186:G:O6	2.46	0.48
1:1:2314:A:OP1	7:F:88:LYS:NZ	2.39	0.48
2:2:269:C:H2'	2:2:270:A:C8	2.49	0.48
2:2:1239:A:H62	2:2:1299:A:N6	2.11	0.48
20:S:31:VAL:HG22	20:S:84:TYR:CD1	2.49	0.48
33:f:67:ILE:N	33:f:89:GLN:OE1	2.33	0.48
37:j:74:LEU:HG	37:j:78:PHE:CE2	2.49	0.48
38:k:65:ALA:O	38:k:69:VAL:HG22	2.14	0.48
41:n:39:PRO:HA	41:n:74:VAL:HG22	1.96	0.48
46:s:21:ASP:OD1	46:s:22:THR:N	2.45	0.48
55:B:53:PHE:N	55:B:53:PHE:CD1	2.81	0.48
1:1:2109:U:O2	1:1:2180:U:O2	2.31	0.47
1:1:2125:G:H22	1:1:2171:A:P	2.37	0.47
2:2:392:C:OP1	47:t:8:ARG:NH2	2.47	0.47
2:2:559:A:H4'	2:2:560:A:H3'	1.96	0.47
2:2:677:U:H3	2:2:713:G:H22	1.62	0.47
2:2:1458:G:OP1	51:x:30:THR:OG1	2.27	0.47
7:F:122:PHE:O	7:F:123:ASP:OD1	2.32	0.47
27:Z:44:PHE:CD2	27:Z:45:THR:HG23	2.49	0.47
33:f:97:LEU:H	33:f:100:MET:HE3	1.79	0.47
36:i:39:VAL:HG12	36:i:40:GLY:N	2.29	0.47
54:z:49:G:H1'	54:z:52:A:H61	1.79	0.47
1:1:1664:A:C2	11:J:1:MET:HE1	2.47	0.47
1:1:2160:C:H6	1:1:2160:C:O5'	1.96	0.47
2:2:580:C:H2'	2:2:581:G:O4'	2.14	0.47
6:E:8:ALA:HB3	6:E:122:GLU:OE2	2.14	0.47
9:H:58:LEU:HA	9:H:61:VAL:HG22	1.96	0.47
33:f:4:VAL:HG11	33:f:212:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:140:ASN:OD1	34:g:143:ARG:NH2	2.40	0.47
54:z:15:A:H3'	54:z:16:U:C5'	2.45	0.47
1:1:2328:A:H2'	1:1:2329:U:C6	2.49	0.47
2:2:978:A:C2	2:2:1319:A:C4	3.02	0.47
13:L:21:ALA:HB2	13:L:97:GLN:HB2	1.96	0.47
27:Z:4:ASP:OD1	27:Z:5:ILE:N	2.47	0.47
37:j:42:TRP:CZ2	37:j:61:LEU:HD22	2.48	0.47
39:l:48:ASP:OD1	39:l:49:PHE:N	2.47	0.47
1:1:931:U:O4	1:1:1166:G:N2	2.47	0.47
1:1:2148:G:H2'	1:1:2149:U:C5	2.49	0.47
9:H:56:ALA:O	9:H:60:GLU:CD	2.57	0.47
21:T:33:LYS:HB3	21:T:64:ALA:HB1	1.97	0.47
35:h:174:ASP:OD2	35:h:177:LYS:HB2	2.14	0.47
37:j:42:TRP:HB2	37:j:59:TYR:HB2	1.96	0.47
41:n:59:LYS:HE2	41:n:62:ARG:NH2	2.30	0.47
1:1:636:G:N7	12:K:109:LYS:HE2	2.29	0.47
2:2:279:A:H5''	2:2:280:C:H3'	1.95	0.47
19:R:82:MET:HG3	19:R:98:LYS:HB2	1.95	0.47
28:a:40:ARG:HG3	28:a:41:HIS:ND1	2.29	0.47
43:p:68:GLY:O	43:p:99:ARG:NH1	2.46	0.47
1:1:458:G:O2'	1:1:469:G:O6	2.30	0.47
2:2:475:C:H2'	2:2:476:U:H6	1.79	0.47
2:2:492:C:H2'	2:2:493:A:C8	2.50	0.47
2:2:579:A:H2'	2:2:580:C:C6	2.49	0.47
10:I:49:ASP:OD1	10:I:121:LYS:NZ	2.32	0.47
34:g:73:PRO:HA	34:g:76:VAL:HG22	1.96	0.47
1:1:400:G:N7	24:W:57:ARG:NH1	2.63	0.47
1:1:548:G:H3'	1:1:549:G:O4'	2.14	0.47
1:1:2512:C:H6	1:1:2512:C:H5''	1.79	0.47
1:1:2591:C:H2'	1:1:2592:G:H8	1.80	0.47
1:1:2900:A:H2'	1:1:2901:C:C6	2.50	0.47
2:2:945:G:C2	2:2:946:A:C8	3.02	0.47
2:2:1314:C:OP2	50:w:4:SER:OG	2.26	0.47
4:C:262:ARG:O	4:C:265:LYS:NZ	2.47	0.47
6:E:152:GLU:CD	6:E:153:LEU:N	2.72	0.47
7:F:119:ALA:HB1	7:F:167:ARG:HE	1.80	0.47
8:G:155:GLU:HG2	8:G:157:TYR:H	1.79	0.47
23:V:18:ALA:O	23:V:20:ARG:HD2	2.15	0.47
41:n:80:THR:HG1	41:n:83:THR:HG1	1.53	0.47
45:r:47:LYS:O	45:r:50:THR:OG1	2.24	0.47
54:z:49:G:O6	54:z:53:G:O6	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:z:69:5MU:O2	54:z:69:5MU:H3'	2.14	0.47
55:B:64:ALA:O	55:B:67:VAL:HG12	2.15	0.47
1:1:281:C:H2'	1:1:282:A:H8	1.79	0.47
1:1:848:C:H2'	1:1:849:A:C8	2.50	0.47
1:1:2099:U:N3	1:1:2100:G:N7	2.63	0.47
1:1:2756:U:OP2	32:e:19:ARG:NE	2.36	0.47
1:1:2902:C:H2'	1:1:2903:U:C4'	2.45	0.47
14:M:56:LYS:NZ	14:M:94:TYR:OH	2.39	0.47
15:N:52:SER:OG	15:N:54:VAL:HG12	2.15	0.47
20:S:14:PRO:HD3	25:X:30:MET:SD	2.54	0.47
21:T:7:ARG:O	21:T:25:VAL:HB	2.14	0.47
21:T:99:ASN:C	21:T:99:ASN:OD1	2.58	0.47
46:s:67:LEU:HD22	46:s:78:TYR:HE1	1.78	0.47
1:1:2359:C:O2'	31:d:54:ASP:OD2	2.29	0.47
2:2:83:C:O2'	2:2:86:G:O6	2.30	0.47
2:2:1100:C:OP2	33:f:95:ARG:HD3	2.15	0.47
6:E:48:THR:O	6:E:52:VAL:HG23	2.14	0.47
43:p:48:ALA:C	43:p:49:LEU:HD12	2.40	0.47
43:p:72:HIS:HB2	43:p:74:LEU:HD23	1.95	0.47
51:x:55:GLN:O	51:x:59:ASP:OD1	2.33	0.47
1:1:1827:U:OP2	4:C:221:ARG:NE	2.48	0.47
10:I:89:PHE:O	10:I:93:ILE:HG12	2.14	0.47
11:J:76:VAL:HG12	16:O:73:VAL:HB	1.97	0.47
33:f:116:ASP:OD1	33:f:117:LEU:N	2.47	0.47
33:f:120:GLN:O	33:f:126:PHE:HB2	2.14	0.47
44:q:40:ALA:O	44:q:43:VAL:HG22	2.15	0.47
47:t:76:LYS:O	47:t:80:LYS:HG2	2.14	0.47
55:B:9:VAL:HG23	55:B:9:VAL:O	2.14	0.47
1:1:11:C:H2'	1:1:12:U:H5'	1.97	0.46
1:1:287:G:H2'	1:1:288:U:C6	2.49	0.46
33:f:117:LEU:HD11	33:f:137:ARG:HD2	1.97	0.46
34:g:180:ALA:HB1	34:g:203:PHE:CE1	2.50	0.46
37:j:17:GLN:OE1	37:j:17:GLN:N	2.47	0.46
55:B:27:SER:O	55:B:30:VAL:HB	2.15	0.46
1:1:1172:C:H5''	1:1:1173:U:C4	2.51	0.46
1:1:1266:G:O2'	1:1:2012:G:O6	2.26	0.46
1:1:2120:G:C2	1:1:2179:C:C2	3.02	0.46
1:1:2376:A:N3	15:N:111:ARG:NH1	2.63	0.46
2:2:194:C:O4'	51:x:59:ASP:OD2	2.33	0.46
2:2:1316:G:N1	2:2:1319:A:OP2	2.47	0.46
6:E:77:ILE:HG22	6:E:77:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:113:MET:SD	11:J:114:LYS:N	2.88	0.46
14:M:47:VAL:O	14:M:51:LEU:HD23	2.15	0.46
39:l:10:MET:HG3	39:l:27:MET:HE1	1.98	0.46
44:q:33:ILE:HD11	44:q:63:PHE:CE2	2.50	0.46
54:z:57:5MU:C2	54:z:68:G:H1'	2.51	0.46
2:2:1135:U:O2	2:2:1138:G:N1	2.45	0.46
3:3:42:C:OP1	7:F:64:LYS:NZ	2.40	0.46
7:F:153:ASP:OD1	7:F:153:ASP:C	2.57	0.46
41:n:51:VAL:HB	45:r:81:ARG:HB2	1.98	0.46
1:1:510:C:C2'	1:1:511:U:H5'	2.45	0.46
1:1:2128:G:H2'	1:1:2129:C:O4'	2.15	0.46
1:1:2189:U:C2	1:1:2190:G:N7	2.84	0.46
1:1:2902:C:H2'	1:1:2903:U:H5''	1.96	0.46
2:2:938:A:N3	2:2:1376:U:O2'	2.40	0.46
4:C:225:MET:SD	4:C:230:HIS:HB2	2.55	0.46
7:F:141:ILE:HG23	7:F:146:VAL:HG11	1.96	0.46
9:H:104:THR:HG23	9:H:109:GLU:HA	1.97	0.46
20:S:33:LYS:HG3	20:S:80:TRP:CE3	2.50	0.46
33:f:133:GLU:OE2	33:f:137:ARG:NE	2.48	0.46
1:1:1315:C:O2'	1:1:1392:A:N3	2.48	0.46
1:1:1939:5MU:OP1	1:1:2604:U:O2'	2.33	0.46
1:1:2051:A:N6	1:1:2614:A:O2'	2.46	0.46
1:1:2902:C:C3'	1:1:2903:U:H5''	2.45	0.46
13:L:47:GLU:OE2	13:L:51:ARG:NE	2.44	0.46
35:h:58:LYS:NZ	35:h:69:GLU:OE1	2.42	0.46
36:i:142:ASP:HA	36:i:145:GLU:HG2	1.97	0.46
42:o:96:THR:HG23	42:o:97:ILE:N	2.31	0.46
44:q:46:SER:C	44:q:47:GLU:HG3	2.40	0.46
50:w:63:THR:HG22	50:w:64:ASP:N	2.31	0.46
51:x:54:MET:SD	51:x:58:VAL:HG21	2.56	0.46
54:z:23:A:OP2	54:z:23:A:N3	2.47	0.46
55:B:26:GLY:H	55:B:30:VAL:HG11	1.79	0.46
1:1:1796:U:H2'	1:1:1797:G:H8	1.81	0.46
1:1:2130:U:H4'	1:1:2158:A:N6	2.31	0.46
1:1:2189:U:H1'	1:1:2190:G:C8	2.50	0.46
1:1:2195:U:H2'	1:1:2196:C:H6	1.81	0.46
2:2:255:G:OP1	48:u:71:LYS:NZ	2.44	0.46
2:2:516:PSU:H4'	2:2:517:G:OP1	2.15	0.46
19:R:10:ALA:HB3	19:R:101:SER:HB2	1.96	0.46
26:Y:23:THR:HG23	26:Y:47:MET:CG	2.45	0.46
35:h:3:ARG:HD2	35:h:115:ARG:HE	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:174:ASP:OD1	35:h:179:GLU:HG3	2.16	0.46
36:i:111:MET:HG2	36:i:115:LEU:HD12	1.97	0.46
38:k:78:ARG:HE	38:k:80:VAL:HG11	1.79	0.46
41:n:57:VAL:O	41:n:57:VAL:HG13	2.16	0.46
18:Q:45:GLU:OE1	18:Q:45:GLU:O	2.33	0.46
35:h:106:GLY:HA3	35:h:162:ALA:HB2	1.98	0.46
45:r:50:THR:HG22	50:w:13:LEU:CD1	2.46	0.46
54:z:49:G:N3	54:z:52:A:N1	2.64	0.46
1:1:125:A:C5	30:c:10:LEU:HD13	2.51	0.46
1:1:781:A:OP1	4:C:217:ARG:NH2	2.39	0.46
2:2:664:G:H22	2:2:741:G:H1	1.64	0.46
2:2:1168:U:H3'	2:2:1169:A:H5'	1.98	0.46
4:C:120:VAL:HG11	9:H:91:PHE:O	2.16	0.46
4:C:258:ARG:NH2	4:C:263:THR:OG1	2.49	0.46
34:g:166:GLU:N	34:g:166:GLU:OE2	2.49	0.46
38:k:66:LEU:O	38:k:70:ARG:HG3	2.16	0.46
41:n:14:ASP:CG	41:n:17:LEU:HB3	2.41	0.46
42:o:31:ILE:HG12	42:o:46:THR:HG22	1.97	0.46
54:z:20:5MU:O2'	54:z:21:A:OP1	2.29	0.46
1:1:1447:C:O2'	1:1:1544:A:N3	2.44	0.46
1:1:2127:G:H21	1:1:2173:A:H1'	1.80	0.46
2:2:992:U:O4	2:2:1044:A:OP2	2.34	0.46
19:R:83:LYS:HG2	19:R:97:LEU:HD13	1.97	0.46
1:1:1141:U:H4'	1:1:1142:A:O4'	2.17	0.46
1:1:2161:C:O2'	1:1:2173:A:OP2	2.34	0.46
8:G:60:ASP:OD1	8:G:60:ASP:N	2.49	0.46
24:W:71:LEU:HD22	24:W:76:GLU:OE1	2.17	0.46
36:i:99:ALA:HB1	36:i:103:THR:HG21	1.97	0.46
37:j:18:VAL:HB	37:j:19:PRO:HD3	1.98	0.46
39:l:13:ARG:NH1	39:l:27:MET:HA	2.31	0.46
1:1:1364:G:N7	24:W:2:SER:OG	2.48	0.45
2:2:675:A:H1'	42:o:118:HIS:CD2	2.51	0.45
20:S:72:GLN:HG3	55:B:33:HIS:HB3	1.98	0.45
35:h:170:TRP:CD2	35:h:186:PRO:HB3	2.51	0.45
39:l:7:ILE:O	39:l:11:LEU:HG	2.16	0.45
2:2:515:G:H3'	2:2:516:PSU:O4	2.16	0.45
2:2:779:C:H2'	2:2:780:A:O4'	2.16	0.45
2:2:1061:G:OP2	34:g:2:GLY:O	2.35	0.45
2:2:1183:U:O2'	2:2:1185:G:OP2	2.34	0.45
33:f:93:ASN:OD1	33:f:94:HIS:N	2.49	0.45
48:u:60:GLU:O	48:u:76:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:z:49:G:C2	54:z:52:A:C2	3.04	0.45
1:1:92:U:O2	55:B:10:LYS:CE	2.65	0.45
1:1:2104:C:H5	1:1:2186:G:N2	2.15	0.45
1:1:2233:U:H2'	1:1:2234:G:C8	2.51	0.45
13:L:110:GLU:O	13:L:114:ARG:HG2	2.16	0.45
22:U:21:ARG:HE	22:U:87:GLN:HA	1.80	0.45
33:f:113:ARG:O	33:f:116:ASP:OD1	2.34	0.45
38:k:40:GLU:OE1	40:m:41:ARG:NH1	2.46	0.45
38:k:137:LYS:O	38:k:141:VAL:HG23	2.16	0.45
44:q:29:ARG:O	44:q:33:ILE:HG12	2.16	0.45
45:r:10:GLU:O	45:r:14:VAL:HG23	2.16	0.45
46:s:21:ASP:O	46:s:23:GLY:N	2.49	0.45
1:1:1060:U:H1'	1:1:1062:G:O5'	2.16	0.45
1:1:1064:C:O2'	1:1:1065:U:O5'	2.33	0.45
1:1:1071:G:H1'	1:1:1089:A:H2'	1.98	0.45
1:1:1244:A:O2'	6:E:29:HIS:NE2	2.37	0.45
1:1:1432:G:H2'	1:1:1433:A:C8	2.52	0.45
1:1:1614:A:P	1:1:1614:A:H8	2.40	0.45
1:1:2126:A:H61	1:1:2163:A:H5'	1.81	0.45
1:1:2133:G:N2	1:1:2158:A:C4	2.84	0.45
1:1:2728:U:O2'	1:1:2729:G:H8	1.99	0.45
8:G:10:VAL:CA	8:G:49:THR:HG22	2.46	0.45
54:z:34:U:H5	54:z:37:G:OP2	1.99	0.45
2:2:521:G:N7	43:p:50:ARG:NH2	2.64	0.45
2:2:848:C:OP1	33:f:37:LYS:NZ	2.36	0.45
19:R:25:ARG:NH1	19:R:74:ILE:O	2.49	0.45
34:g:51:SER:HB2	34:g:115:LEU:HD22	1.97	0.45
36:i:153:VAL:HG23	36:i:164:ILE:HD13	1.98	0.45
36:i:156:LYS:NZ	39:l:73:GLU:OE2	2.50	0.45
48:u:19:LYS:HA	48:u:48:ASP:O	2.15	0.45
2:2:1498:UR3:O5'	2:2:1498:UR3:H6	2.16	0.45
7:F:47:LYS:HE2	7:F:47:LYS:HA	1.98	0.45
33:f:23:TRP:CZ3	33:f:25:PRO:HA	2.51	0.45
34:g:181:ASP:OD2	34:g:204:LYS:HD2	2.16	0.45
45:r:42:TRP:O	45:r:46:LEU:HD23	2.17	0.45
55:B:61:ALA:N	55:B:62:PRO:CD	2.80	0.45
1:1:2364:C:H2'	1:1:2365:G:O4'	2.17	0.45
1:1:2808:G:O2'	1:1:2890:G:O6	2.32	0.45
18:Q:69:GLY:O	18:Q:90:ARG:NE	2.42	0.45
33:f:129:LEU:HD23	33:f:129:LEU:N	2.32	0.45
37:j:21:MET:HG2	37:j:24:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:n:102:LEU:C	41:n:102:LEU:HD23	2.41	0.45
54:z:15:A:H3'	54:z:16:U:H5''	1.99	0.45
1:1:2747:G:O6	1:1:2755:C:H5''	2.17	0.45
2:2:205:A:H2'	2:2:206:C:C6	2.52	0.45
2:2:451:A:H4'	2:2:452:A:O4'	2.16	0.45
2:2:477:C:H2'	2:2:478:A:C8	2.52	0.45
5:D:153:GLY:O	5:D:154:LYS:HB3	2.16	0.45
55:B:9:VAL:HG12	55:B:21:ILE:HD11	1.99	0.45
1:1:280:U:O4	1:1:361:G:N2	2.49	0.45
1:1:1954:G:O2'	1:1:1956:U:O4	2.23	0.45
1:1:2570:G:H2'	1:1:2571:U:O4'	2.16	0.45
2:2:235:C:H2'	2:2:236:A:C8	2.52	0.45
2:2:427:U:OP1	35:h:13:ARG:NH1	2.48	0.45
2:2:1168:U:O2'	2:2:1169:A:C5'	2.64	0.45
6:E:22:ASP:OD1	6:E:23:PHE:N	2.49	0.45
19:R:85:ILE:HD13	55:B:46:ASP:OD1	2.17	0.45
34:g:123:GLN:HB3	34:g:128:VAL:CG2	2.46	0.45
38:k:5:ARG:NH1	38:k:7:ILE:HA	2.32	0.45
38:k:135:VAL:O	38:k:139:GLU:HG2	2.17	0.45
41:n:22:THR:O	41:n:26:VAL:HG23	2.17	0.45
47:t:69:ASP:OD1	47:t:69:ASP:N	2.43	0.45
1:1:549:G:H2'	1:1:550:C:C6	2.52	0.45
1:1:1043:C:H2'	1:1:1044:C:O4'	2.17	0.45
20:S:11:LEU:HD22	20:S:32:LEU:HD13	1.99	0.45
25:X:42:LEU:O	25:X:46:VAL:HG23	2.16	0.45
33:f:10:LEU:HD23	33:f:10:LEU:C	2.42	0.45
36:i:39:VAL:HG12	36:i:40:GLY:H	1.82	0.45
52:y:6:VAL:HG13	52:y:6:VAL:O	2.17	0.45
55:B:9:VAL:HA	55:B:21:ILE:CG1	2.47	0.45
1:1:653:U:H5	1:1:654:A:H62	1.65	0.44
1:1:1722:A:N6	1:1:1738:G:H1'	2.32	0.44
2:2:1518:MA6:H103	2:2:1519:MA6:H102	1.98	0.44
25:X:49:ASP:O	25:X:53:VAL:HG23	2.17	0.44
1:1:1322:A:C5	1:1:1323:C:C5	3.05	0.44
1:1:2297:A:N1	1:1:2321:U:H5	2.14	0.44
2:2:552:U:H2'	2:2:553:A:C8	2.51	0.44
2:2:1317:C:OP1	45:r:24:ARG:NH2	2.39	0.44
2:2:1355:G:H2'	2:2:1356:G:H8	1.82	0.44
7:F:17:MET:SD	7:F:22:TYR:HB2	2.58	0.44
40:m:41:ARG:O	40:m:45:ARG:HG3	2.17	0.44
1:1:886:A:C2'	1:1:887:A:O5'	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2885:G:O6	28:a:40:ARG:NH2	2.50	0.44
2:2:857:C:H2'	2:2:858:G:O4'	2.18	0.44
9:H:40:THR:O	9:H:44:ILE:HG12	2.18	0.44
9:H:130:VAL:HG23	9:H:130:VAL:O	2.17	0.44
33:f:207:ILE:O	33:f:210:VAL:HG22	2.17	0.44
54:z:46:G:N3	54:z:46:G:H2'	2.32	0.44
1:1:1062:G:H2'	1:1:1063:G:C8	2.52	0.44
1:1:2133:G:N3	1:1:2158:A:C6	2.85	0.44
2:2:1414:U:H2'	2:2:1415:G:H8	1.81	0.44
9:H:3:VAL:HG22	9:H:36:ALA:HB1	2.00	0.44
21:T:98:SER:O	21:T:99:ASN:OD1	2.35	0.44
33:f:27:MET:HE1	33:f:187:VAL:HG12	1.98	0.44
36:i:120:VAL:CG1	36:i:123:VAL:HG13	2.47	0.44
1:1:2101:A:H2'	1:1:2102:G:O4'	2.17	0.44
1:1:2106:U:O2	1:1:2184:A:C2	2.71	0.44
2:2:714:G:H2'	2:2:715:A:C8	2.53	0.44
2:2:1530:G:H2'	2:2:1531:A:C8	2.52	0.44
4:C:118:SER:OG	4:C:119:GLY:N	2.49	0.44
7:F:123:ASP:OD2	7:F:127:ASN:HB2	2.17	0.44
8:G:16:ASP:HB3	8:G:27:LYS:HB2	1.99	0.44
35:h:124:MET:HE3	35:h:146:ARG:HB2	1.98	0.44
1:1:353:C:H6	1:1:353:C:H5''	1.82	0.44
1:1:714:U:OP2	46:s:88:ARG:NH1	2.38	0.44
1:1:754:U:H4'	1:1:1618:6MZ:H2	1.99	0.44
1:1:2121:G:H2'	1:1:2122:U:C6	2.53	0.44
7:F:59:ALA:O	27:Z:27:THR:OG1	2.28	0.44
27:Z:35:ASP:C	27:Z:35:ASP:OD1	2.60	0.44
42:o:109:ASN:OD1	52:y:5:LYS:HG2	2.18	0.44
1:1:373:U:H2'	1:1:374:A:H8	1.81	0.44
1:1:1321:A:C2	55:B:31:PHE:CG	3.06	0.44
2:2:689:C:OP1	42:o:29:ASN:ND2	2.45	0.44
2:2:1004:A:C8	2:2:1025:U:H1'	2.52	0.44
2:2:1071:C:H2'	2:2:1072:G:H8	1.83	0.44
9:H:115:VAL:HG12	9:H:117:LEU:CD1	2.48	0.44
12:K:29:LYS:HG3	12:K:30:THR:HG23	1.98	0.44
31:d:32:ILE:O	31:d:32:ILE:HG22	2.18	0.44
51:x:36:TYR:CE2	51:x:79:LEU:HD21	2.52	0.44
55:B:9:VAL:HB	55:B:11:TRP:O	2.18	0.44
1:1:1871:A:H1'	1:1:1872:A:C8	2.52	0.44
1:1:2822:G:O2'	1:1:2824:C:OP2	2.32	0.44
2:2:22:G:O2'	2:2:913:A:N1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:86:G:O2'	2:2:87:C:O4'	2.35	0.44
2:2:685:G:N1	2:2:704:A:OP2	2.41	0.44
7:F:140:GLU:CD	27:Z:28:VAL:HG23	2.42	0.44
12:K:82:LEU:O	12:K:85:VAL:HG22	2.18	0.44
33:f:130:THR:HG23	33:f:133:GLU:HB3	2.00	0.44
45:r:15:ALA:HA	45:r:18:ASP:OD2	2.18	0.44
54:z:49:G:O6	54:z:53:G:C6	2.71	0.44
54:z:53:G:C8	54:z:53:G:OP2	2.71	0.44
1:1:45:G:H5''	1:1:46:G:H5'	2.00	0.44
1:1:538:A:H5''	10:I:7:LYS:HE2	2.00	0.44
1:1:1076:C:H2'	1:1:1077:A:H8	1.82	0.44
1:1:2581:G:N2	1:1:2581:G:OP2	2.50	0.44
1:1:2684:U:O4'	11:J:70:ARG:NH1	2.51	0.44
2:2:153:C:N3	2:2:169:C:N4	2.65	0.44
2:2:999:C:N3	2:2:1042:A:N6	2.66	0.44
2:2:1168:U:O2'	2:2:1169:A:P	2.75	0.44
6:E:7:ASP:OD1	6:E:7:ASP:N	2.49	0.44
9:H:58:LEU:O	9:H:62:LEU:HD23	2.18	0.44
25:X:44:LYS:O	25:X:48:ARG:HD2	2.18	0.44
33:f:133:GLU:O	33:f:137:ARG:HG2	2.18	0.44
33:f:163:VAL:HG22	33:f:185:ALA:HB2	2.00	0.44
34:g:47:LEU:N	34:g:47:LEU:CD1	2.80	0.44
55:B:10:LYS:NZ	55:B:22:THR:OG1	2.49	0.44
1:1:2102:G:N1	1:1:2187:U:N3	2.66	0.43
1:1:2142:A:H3'	1:1:2143:C:C6	2.53	0.43
1:1:2766:A:C5	1:1:2767:C:C5	3.05	0.43
2:2:608:A:H2'	2:2:609:A:O4'	2.18	0.43
2:2:1241:G:H2'	2:2:1242:G:H8	1.81	0.43
2:2:1523:G:OP1	42:o:128:ARG:NH1	2.41	0.43
3:3:49:C:H2'	3:3:50:A:C8	2.53	0.43
7:F:7:TYR:O	7:F:10:ASP:OD1	2.36	0.43
7:F:74:VAL:CG2	7:F:79:ILE:HD11	2.48	0.43
17:P:74:ILE:HG13	17:P:78:LYS:HD3	2.00	0.43
19:R:81:SER:HB3	19:R:97:LEU:HD12	2.00	0.43
23:V:56:ASP:OD1	23:V:58:THR:OG1	2.35	0.43
36:i:13:GLU:HG2	36:i:39:VAL:HG13	1.99	0.43
40:m:58:VAL:HG13	40:m:59:GLU:N	2.32	0.43
42:o:96:THR:CG2	42:o:97:ILE:N	2.81	0.43
1:1:388:G:N7	1:1:390:U:H2'	2.32	0.43
1:1:895:U:O2'	1:1:896:A:C1'	2.66	0.43
2:2:1077:G:N2	2:2:1080:A:OP2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1168:U:C3'	2:2:1169:A:H5'	2.49	0.43
10:I:37:ARG:HD2	10:I:118:MET:HE1	2.00	0.43
11:J:41:ILE:HD11	11:J:86:LEU:HD22	1.99	0.43
33:f:161:LEU:CD1	33:f:181:ILE:HG21	2.48	0.43
47:t:19:VAL:HG22	47:t:37:GLY:C	2.42	0.43
48:u:9:GLN:HA	48:u:59:VAL:O	2.18	0.43
52:y:39:GLU:HG2	52:y:44:GLU:OE2	2.18	0.43
1:1:2350:C:OP2	31:d:45:ARG:NH2	2.48	0.43
1:1:2561:U:O3'	11:J:40:LYS:NZ	2.46	0.43
2:2:246:A:C2	2:2:282:A:C5	3.06	0.43
4:C:4:VAL:CG2	4:C:18:LYS:HB2	2.48	0.43
12:K:92:LEU:O	12:K:96:LYS:HG3	2.18	0.43
27:Z:13:THR:HB	27:Z:31:ASP:OD1	2.18	0.43
27:Z:46:GLY:O	27:Z:50:ASP:OD2	2.36	0.43
35:h:102:VAL:HB	35:h:114:ALA:HB1	1.99	0.43
36:i:57:PRO:HA	36:i:60:ILE:CG1	2.48	0.43
40:m:7:TYR:OH	40:m:9:THR:OG1	2.33	0.43
50:w:22:ALA:HA	50:w:27:ASP:OD1	2.18	0.43
1:1:2300:C:O2'	1:1:2301:C:H5'	2.19	0.43
2:2:1218:C:H2'	2:2:1219:A:C8	2.54	0.43
3:3:8:C:O3'	15:N:25:ARG:NH1	2.40	0.43
6:E:176:ASP:OD1	6:E:176:ASP:N	2.51	0.43
7:F:78:LYS:CG	7:F:78:LYS:O	2.66	0.43
9:H:51:ARG:HA	9:H:54:LEU:HB3	2.00	0.43
19:R:80:PRO:O	19:R:100:THR:OG1	2.35	0.43
33:f:50:PHE:CZ	33:f:54:LEU:HD11	2.54	0.43
34:g:160:ALA:HB3	34:g:164:ARG:HH22	1.84	0.43
1:1:161:A:OP2	1:1:162:U:O2'	2.30	0.43
1:1:414:C:H2'	1:1:415:A:H8	1.84	0.43
1:1:460:A:P	30:c:41:ARG:HH22	2.40	0.43
1:1:494:G:H4'	19:R:6:LYS:HB2	2.00	0.43
1:1:1094:U:N3	1:1:1097:U:OP2	2.47	0.43
1:1:1357:C:H2'	1:1:1358:G:O4'	2.18	0.43
26:Y:17:LEU:HD12	26:Y:20:HIS:CE1	2.53	0.43
44:q:2:ALA:O	44:q:9:ILE:N	2.49	0.43
55:B:48:GLY:O	55:B:51:VAL:HB	2.17	0.43
1:1:278:A:C6	1:1:362:A:C8	3.06	0.43
1:1:279:A:N6	1:1:361:G:H1'	2.34	0.43
1:1:285:G:C6	1:1:356:G:C6	3.07	0.43
1:1:1342:A:O2'	1:1:1344:U:OP2	2.25	0.43
1:1:2171:A:O2'	1:1:2173:A:OP1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:753:A:OP1	46:s:73:LYS:NZ	2.47	0.43
4:C:174:LEU:O	4:C:181:MET:HA	2.19	0.43
7:F:167:ARG:HG3	7:F:177:PHE:CE2	2.54	0.43
10:I:7:LYS:HB2	10:I:10:THR:HG22	2.01	0.43
33:f:184:PHE:HE1	33:f:198:PHE:CD2	2.37	0.43
35:h:95:GLU:HA	35:h:100:ASN:ND2	2.34	0.43
37:j:88:MET:HE1	49:v:61:ARG:HG2	1.99	0.43
45:r:48:LEU:HD12	45:r:51:LEU:HD12	2.01	0.43
52:y:9:ASN:OD1	52:y:9:ASN:O	2.36	0.43
54:z:49:G:N1	54:z:51:A:N1	2.66	0.43
1:1:12:U:H2'	1:1:13:A:H5'	1.99	0.43
1:1:2102:G:C6	1:1:2187:U:C4	3.05	0.43
1:1:2119:A:N1	1:1:2169:A:H2'	2.33	0.43
1:1:2698:U:H2'	1:1:2699:C:C6	2.53	0.43
2:2:439:U:O2	35:h:120:HIS:CD2	2.71	0.43
2:2:1006:G:H22	2:2:1023:U:H2'	1.83	0.43
9:H:4:ILE:HA	9:H:17:ASP:O	2.19	0.43
9:H:95:GLY:O	9:H:98:ASP:OD1	2.36	0.43
14:M:38:LEU:HB3	14:M:39:PRO:HD3	2.00	0.43
23:V:65:GLY:HA2	23:V:85:GLU:HB3	2.00	0.43
36:i:74:VAL:HG12	36:i:76:LEU:HD12	2.00	0.43
39:l:93:PRO:O	39:l:117:ARG:NH2	2.51	0.43
43:p:55:VAL:HG21	43:p:80:ILE:HD11	2.00	0.43
44:q:81:MET:HE2	44:q:91:HIS:HB3	2.00	0.43
55:B:9:VAL:O	55:B:9:VAL:CG2	2.67	0.43
55:B:53:PHE:N	55:B:53:PHE:HD1	2.17	0.43
1:1:615:U:O4	6:E:39:ALA:HB2	2.19	0.43
1:1:1722:A:H2'	1:1:1723:G:H8	1.82	0.43
1:1:2092:U:N3	1:1:2226:C:OP2	2.46	0.43
1:1:2193:G:C6	1:1:2194:U:C4	3.06	0.43
2:2:999:C:H2'	2:2:1000:A:H8	1.84	0.43
2:2:1106:G:H5''	34:g:172:ARG:HB3	2.00	0.43
2:2:1323:G:H2'	2:2:1324:A:C8	2.54	0.43
2:2:1417:G:C6	2:2:1482:G:C6	3.07	0.43
3:3:15:A:O4'	3:3:109:A:C8	2.72	0.43
4:C:41:GLY:O	4:C:43:ARG:NH1	2.52	0.43
7:F:5:HIS:NE2	7:F:9:LYS:HD2	2.34	0.43
9:H:21:VAL:HG21	9:H:26:ALA:HB2	2.01	0.43
23:V:30:SER:OG	23:V:85:GLU:OE2	2.33	0.43
39:l:5:ASP:CG	39:l:77:ARG:HH12	2.27	0.43
50:w:3:ARG:NH1	50:w:9:PRO:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B:45:LYS:HE3	55:B:45:LYS:HB3	1.86	0.43
1:1:613:A:O4'	1:1:614:A:C8	2.72	0.43
1:1:1962:5MC:O2'	1:1:1964:G:OP2	2.33	0.43
1:1:2313:C:H2'	1:1:2314:A:C8	2.54	0.43
4:C:120:VAL:HG13	4:C:134:ASN:OD1	2.19	0.43
9:H:8:LYS:HA	9:H:14:SER:HA	2.00	0.43
34:g:8:ASN:O	34:g:12:LEU:HG	2.19	0.43
34:g:69:HIS:HA	34:g:104:ALA:O	2.19	0.43
41:n:35:GLN:HB3	41:n:78:GLU:OE1	2.19	0.43
52:y:28:VAL:HG23	52:y:29:LEU:N	2.34	0.43
1:1:807:U:OP1	12:K:36:LYS:HE2	2.19	0.43
1:1:1197:G:H2'	1:1:1198:U:H6	1.84	0.43
1:1:1722:A:O2'	1:1:1723:G:H5'	2.19	0.43
1:1:2116:G:N1	1:1:2162:G:OP2	2.46	0.43
1:1:2305:U:O2	7:F:151:GLY:HA3	2.19	0.43
1:1:2822:G:OP1	5:D:164:GLN:NE2	2.51	0.43
2:2:715:A:H2'	2:2:716:A:C8	2.54	0.43
2:2:868:C:H2'	2:2:869:G:O4'	2.19	0.43
6:E:152:GLU:OE1	6:E:153:LEU:C	2.62	0.43
7:F:38:MET:HG2	7:F:151:GLY:O	2.19	0.43
33:f:184:PHE:HD1	33:f:198:PHE:HB2	1.84	0.43
33:f:218:ALA:HA	33:f:221:VAL:HG22	2.00	0.43
50:w:36:ARG:NH2	50:w:72:GLY:O	2.51	0.43
55:B:30:VAL:O	55:B:33:HIS:HB2	2.19	0.43
55:B:60:LYS:HG2	55:B:60:LYS:O	2.19	0.43
1:1:445:C:O2'	1:1:449:A:N3	2.47	0.42
1:1:601:C:O5'	1:1:601:C:H6	2.01	0.42
1:1:732:C:H2'	1:1:733:G:O4'	2.19	0.42
1:1:2141:G:N2	1:1:2151:U:O2	2.52	0.42
2:2:209:U:H3'	2:2:210:C:O2	2.20	0.42
2:2:1145:A:O2'	2:2:1146:A:H5''	2.19	0.42
5:D:4:LEU:HD23	5:D:29:VAL:HG11	1.99	0.42
5:D:104:VAL:HG12	5:D:105:LYS:N	2.34	0.42
9:H:56:ALA:O	9:H:60:GLU:OE1	2.36	0.42
28:a:55:ILE:HG12	28:a:56:ALA:O	2.19	0.42
33:f:213:TYR:O	33:f:217:VAL:HG23	2.19	0.42
36:i:137:VAL:O	36:i:141:ILE:HG12	2.18	0.42
1:1:201:C:OP1	24:W:18:ARG:NH1	2.50	0.42
1:1:613:A:H4'	1:1:614:A:OP1	2.19	0.42
1:1:2125:G:H21	1:1:2174:C:N4	2.18	0.42
1:1:2129:C:OP2	1:1:2130:U:C5	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2580:PSU:OP1	5:D:137:SER:OG	2.27	0.42
1:1:2880:C:O3'	14:M:90:ARG:NH2	2.52	0.42
2:2:41:G:H2'	2:2:42:G:H8	1.83	0.42
2:2:463:U:H5'	2:2:464:U:OP2	2.19	0.42
2:2:475:C:H2'	2:2:476:U:C6	2.54	0.42
9:H:89:LYS:O	9:H:91:PHE:N	2.52	0.42
13:L:27:SER:N	13:L:104:GLU:OE2	2.52	0.42
21:T:7:ARG:O	21:T:25:VAL:O	2.37	0.42
31:d:40:ARG:O	31:d:44:LEU:HG	2.19	0.42
35:h:172:GLU:HB2	35:h:183:LYS:HD2	2.00	0.42
36:i:115:LEU:HD13	36:i:123:VAL:HG21	2.00	0.42
55:B:45:LYS:O	55:B:46:ASP:C	2.62	0.42
1:1:142:A:H2'	1:1:143:C:C6	2.55	0.42
1:1:645:C:H2'	1:1:647:G:N7	2.34	0.42
1:1:1630:A:N6	1:1:1637:A:N6	2.67	0.42
1:1:1799:G:H8	4:C:180:GLU:OE1	2.03	0.42
1:1:2097:A:H2'	1:1:2098:U:C6	2.54	0.42
1:1:2170:A:C2	1:1:2171:A:C4	3.07	0.42
1:1:2301:C:H2'	1:1:2302:U:H6	1.85	0.42
2:2:297:G:N2	2:2:300:A:OP2	2.48	0.42
2:2:489:C:H2'	2:2:490:C:H6	1.85	0.42
2:2:563:A:N3	43:p:12:ARG:NH1	2.67	0.42
4:C:130:LEU:O	4:C:135:ILE:HD11	2.18	0.42
15:N:93:ASP:OD1	15:N:95:SER:N	2.48	0.42
38:k:113:ASP:O	38:k:119:ARG:HD2	2.18	0.42
41:n:83:THR:O	41:n:87:LEU:HD13	2.18	0.42
45:r:14:VAL:O	45:r:18:ASP:OD2	2.37	0.42
48:u:68:SER:OG	48:u:69:LYS:N	2.51	0.42
49:v:21:ILE:HD12	49:v:54:GLN:HB2	2.00	0.42
54:z:71:5MU:H2'	54:z:72:C:H6	1.83	0.42
1:1:143:C:O2	1:1:143:C:H2'	2.18	0.42
1:1:469:G:O6	30:c:37:LYS:HE2	2.18	0.42
1:1:720:U:H2'	1:1:721:A:C8	2.54	0.42
1:1:1607:C:C4'	1:1:1608:A:H5'	2.34	0.42
1:1:2102:G:H3'	1:1:2103:C:C6	2.54	0.42
1:1:2246:G:H2'	1:1:2247:A:C8	2.54	0.42
9:H:90:LEU:HD21	9:H:123:ARG:HG2	2.01	0.42
9:H:100:ALA:HA	9:H:103:VAL:HG22	2.00	0.42
29:b:10:LYS:HD3	29:b:53:LYS:O	2.18	0.42
31:d:55:LEU:HA	31:d:58:VAL:HG12	2.00	0.42
33:f:27:MET:HG3	33:f:189:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:113:ASP:OD2	38:k:122:ASN:ND2	2.49	0.42
41:n:84:VAL:HG13	41:n:85:ASP:N	2.33	0.42
52:y:31:GLU:OE2	52:y:35:ARG:NE	2.49	0.42
1:1:2114:A:N7	1:1:2167:U:H4'	2.34	0.42
1:1:2188:U:O4	1:1:2189:U:C5	2.73	0.42
1:1:2450:A:N6	1:1:2501:C:O2	2.52	0.42
2:2:1522:U:H5''	42:o:128:ARG:NH2	2.35	0.42
6:E:129:PRO:HB3	6:E:156:ASN:HA	2.02	0.42
14:M:80:PHE:N	14:M:80:PHE:HD1	2.17	0.42
24:W:51:VAL:HG22	24:W:52:SER:O	2.19	0.42
27:Z:57:VAL:HG22	50:w:67:VAL:HG21	2.00	0.42
33:f:116:ASP:O	33:f:120:GLN:HG3	2.20	0.42
33:f:122:GLN:CD	33:f:123:ASP:N	2.77	0.42
34:g:11:ARG:NH2	34:g:177:THR:O	2.52	0.42
41:n:91:ASP:C	41:n:92:LEU:HD22	2.45	0.42
44:q:116:ILE:O	44:q:116:ILE:HG13	2.20	0.42
48:u:17:MET:HG3	48:u:20:SER:HB2	2.01	0.42
55:B:53:PHE:O	55:B:55:ILE:N	2.47	0.42
1:1:357:C:C2	1:1:358:U:C5	3.07	0.42
1:1:620:G:H4'	1:1:621:A:H5'	1.98	0.42
1:1:1231:U:H2'	1:1:1232:G:H8	1.85	0.42
1:1:2511:U:O4	1:1:2575:C:N3	2.52	0.42
1:1:2839:G:N2	14:M:91:ALA:O	2.46	0.42
9:H:96:THR:CG2	9:H:117:LEU:HD11	2.49	0.42
21:T:52:LEU:O	21:T:53:ASN:OD1	2.36	0.42
37:j:9:MET:HE3	37:j:59:TYR:HE1	1.85	0.42
50:w:29:LYS:O	50:w:31:LEU:HD12	2.20	0.42
54:z:70:C:O2	54:z:70:C:H2'	2.19	0.42
1:1:5:A:H2'	1:1:6:A:C8	2.55	0.42
1:1:279:A:C6	1:1:362:A:H5'	2.55	0.42
1:1:603:A:O5'	1:1:655:A:N6	2.43	0.42
1:1:1563:U:H2'	1:1:1564:C:C6	2.55	0.42
1:1:2514:U:H2'	1:1:2515:C:C6	2.55	0.42
2:2:1064:G:O2'	2:2:1190:G:N2	2.53	0.42
4:C:108:LYS:HA	4:C:196:GLY:HA2	2.00	0.42
14:M:65:LEU:O	14:M:69:ARG:HG3	2.19	0.42
21:T:45:HIS:O	21:T:47:LYS:HD2	2.20	0.42
30:c:31:LEU:HD22	30:c:42:LEU:CD2	2.49	0.42
33:f:91:PHE:CE1	33:f:150:GLY:HA2	2.55	0.42
37:j:99:ALA:HB1	37:j:103:VAL:CG1	2.50	0.42
54:z:69:5MU:O2	54:z:69:5MU:C3'	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1:G:H2'	1:1:2:G:H8	1.85	0.42
1:1:270:A:H5'	1:1:271:G:H5''	2.01	0.42
1:1:358:U:C2	1:1:359:G:C8	3.08	0.42
1:1:882:G:H2'	1:1:883:G:H5'	2.02	0.42
1:1:1077:A:H61	1:1:1088:A:H2'	1.85	0.42
1:1:2183:A:H2'	1:1:2184:A:C8	2.55	0.42
2:2:82:G:H1	2:2:86:G:H22	1.68	0.42
2:2:501:C:OP2	43:p:121:ARG:NH1	2.52	0.42
2:2:1412:C:H2'	2:2:1413:A:C8	2.54	0.42
3:3:49:C:H2'	3:3:50:A:H8	1.85	0.42
4:C:65:VAL:HG11	4:C:105:LEU:CD1	2.50	0.42
8:G:80:THR:HG23	8:G:81:GLU:HG3	2.01	0.42
8:G:83:PHE:CB	8:G:141:ILE:HD13	2.50	0.42
33:f:5:SER:HG	33:f:8:ASP:CG	2.27	0.42
33:f:66:LYS:HB2	33:f:158:PRO:HA	2.01	0.42
33:f:101:LEU:HB3	33:f:179:LEU:CD1	2.48	0.42
37:j:9:MET:HG2	37:j:59:TYR:CD1	2.54	0.42
37:j:100:SER:O	37:j:103:VAL:HG12	2.19	0.42
52:y:13:ASP:OD1	52:y:13:ASP:N	2.53	0.42
54:z:39:5MU:H2'	54:z:40:5MU:O4'	2.19	0.42
1:1:1365:A:OP1	24:W:3:ARG:NH2	2.44	0.42
1:1:2148:G:H2'	1:1:2149:U:H6	1.84	0.42
1:1:2301:C:H2'	1:1:2302:U:C6	2.54	0.42
1:1:2751:G:H5'	1:1:2752:C:C5	2.54	0.42
2:2:514:C:H2'	2:2:515:G:H8	1.84	0.42
2:2:1220:G:P	45:r:53:ARG:HH12	2.42	0.42
2:2:1391:U:H2'	2:2:1392:G:H8	1.85	0.42
4:C:161:TYR:HB3	4:C:194:GLU:HG2	2.01	0.42
9:H:124:THR:CG2	9:H:128:HIS:CE1	3.02	0.42
14:M:80:PHE:N	14:M:80:PHE:CD1	2.87	0.42
16:O:33:VAL:HG22	16:O:38:LYS:HG2	2.01	0.42
21:T:74:ASN:ND2	21:T:81:ASP:OD2	2.50	0.42
24:W:6:GLN:O	24:W:74:ARG:NH2	2.53	0.42
34:g:118:ASP:OD1	34:g:119:SER:N	2.53	0.42
54:z:71:5MU:OP2	54:z:71:5MU:H6	2.02	0.42
1:1:116:C:H2'	1:1:117:G:O4'	2.20	0.42
1:1:563:A:C2'	17:P:37:GLN:HE21	2.33	0.42
1:1:885:C:N4	1:1:892:A:N6	2.68	0.42
1:1:1680:U:H2'	1:1:1681:G:O4'	2.19	0.42
1:1:2081:U:H2'	1:1:2082:A:H8	1.85	0.42
2:2:556:C:H2'	2:2:557:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:138:GLY:N	4:C:164:ILE:O	2.51	0.42
5:D:105:LYS:O	5:D:177:VAL:HG12	2.20	0.42
7:F:8:TYR:HB2	7:F:173:PHE:HZ	1.85	0.42
9:H:84:ALA:O	9:H:148:ALA:CB	2.67	0.42
19:R:91:GLY:CA	55:B:53:PHE:CD2	3.00	0.42
24:W:43:GLU:OE1	24:W:45:ARG:NE	2.52	0.42
31:d:31:HIS:N	31:d:31:HIS:CD2	2.88	0.42
33:f:124:GLY:O	33:f:125:THR:OG1	2.28	0.42
33:f:217:VAL:O	33:f:221:VAL:HG13	2.20	0.42
35:h:140:ASN:N	35:h:182:PHE:O	2.53	0.42
37:j:45:ARG:HD3	37:j:59:TYR:CE2	2.54	0.42
1:1:12:U:H2'	1:1:12:U:O2	2.20	0.41
1:1:810:U:N3	12:K:29:LYS:O	2.53	0.41
1:1:2313:C:O4'	7:F:37:ASN:ND2	2.53	0.41
1:1:2571:U:C2'	5:D:151:THR:HG21	2.49	0.41
2:2:71:A:C2	2:2:100:G:C8	3.07	0.41
2:2:214:C:H2'	2:2:215:C:H6	1.84	0.41
2:2:1425:U:H2'	2:2:1426:G:H8	1.84	0.41
7:F:10:ASP:OD1	7:F:11:GLU:N	2.53	0.41
7:F:78:LYS:O	7:F:78:LYS:HG3	2.20	0.41
12:K:127:VAL:HG12	12:K:128:THR:O	2.20	0.41
18:Q:27:ILE:O	18:Q:66:HIS:NE2	2.40	0.41
50:w:18:LYS:HB3	50:w:31:LEU:HD23	2.02	0.41
1:1:57:C:H2'	1:1:58:G:O4'	2.20	0.41
1:1:1827:U:H2'	1:1:1828:G:O4'	2.20	0.41
1:1:2169:A:H8	1:1:2169:A:O5'	2.03	0.41
1:1:2236:U:H2'	1:1:2237:G:O4'	2.20	0.41
2:2:1041:G:C2	2:2:1042:A:C5	3.08	0.41
9:H:115:VAL:O	9:H:116:ARG:NH2	2.53	0.41
9:H:125:THR:O	9:H:125:THR:HG23	2.19	0.41
19:R:34:ASP:OD1	19:R:35:ILE:HG13	2.21	0.41
21:T:48:PRO:HG3	21:T:55:PRO:O	2.19	0.41
21:T:53:ASN:OD1	21:T:53:ASN:O	2.38	0.41
26:Y:13:ALA:O	26:Y:21:LYS:HE2	2.20	0.41
33:f:117:LEU:HB3	33:f:141:LEU:HD13	2.01	0.41
33:f:120:GLN:HB3	33:f:126:PHE:HB2	2.02	0.41
33:f:206:ALA:O	33:f:210:VAL:HG13	2.20	0.41
39:l:55:THR:HG23	39:l:56:LYS:HG2	2.01	0.41
48:u:8:LEU:HD22	48:u:25:ILE:HD13	2.03	0.41
1:1:1955:U:C5	1:1:2552:OMU:H1'	2.55	0.41
1:1:2103:C:C4	1:1:2186:G:N1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:769:G:H4'	2:2:1513:A:H4'	2.03	0.41
22:U:43:ASP:OD1	22:U:44:HIS:N	2.53	0.41
34:g:73:PRO:O	34:g:76:VAL:HG22	2.20	0.41
37:j:75:GLU:OE2	37:j:89:VAL:HG11	2.21	0.41
38:k:69:VAL:HG23	38:k:100:ALA:HB1	2.02	0.41
41:n:86:ALA:O	41:n:89:ARG:HG2	2.20	0.41
48:u:25:ILE:HD12	48:u:44:LEU:HD12	2.02	0.41
49:v:73:ARG:O	49:v:75:GLN:OE1	2.38	0.41
54:z:16:U:C4'	54:z:17:U:OP1	2.69	0.41
54:z:68:G:C8	54:z:69:5MU:H6	2.38	0.41
1:1:275:C:N3	1:1:362:A:N6	2.69	0.41
1:1:588:U:O4	1:1:670:A:H1'	2.21	0.41
1:1:630:G:N2	1:1:633:A:OP2	2.42	0.41
1:1:1754:A:O3'	16:O:103:ARG:NH2	2.41	0.41
2:2:949:A:N7	44:q:105:ASN:ND2	2.69	0.41
5:D:13:ARG:HD2	5:D:21:SER:OG	2.20	0.41
9:H:103:VAL:O	9:H:106:ALA:O	2.38	0.41
10:I:57:LEU:HD23	10:I:125:TYR:HB2	2.02	0.41
19:R:93:ALA:HB2	55:B:49:GLN:OE1	2.19	0.41
41:n:71:LEU:O	41:n:72:ARG:NH1	2.41	0.41
42:o:70:CYS:O	42:o:74:VAL:HG22	2.21	0.41
1:1:620:G:H4'	1:1:621:A:O5'	2.20	0.41
1:1:1064:C:O2'	1:1:1065:U:C6	2.68	0.41
1:1:2146:C:H4'	1:1:2147:A:OP1	2.21	0.41
1:1:2278:A:OP2	23:V:12:ASN:OD1	2.37	0.41
2:2:203:G:H2'	2:2:204:G:C8	2.56	0.41
6:E:97:ASN:ND2	6:E:100:MET:SD	2.91	0.41
10:I:76:HIS:O	10:I:84:ILE:HD12	2.20	0.41
27:Z:42:PRO:HB2	27:Z:46:GLY:HA3	2.02	0.41
37:j:38:ARG:NH2	37:j:63:ASN:OD1	2.54	0.41
46:s:25:THR:HG23	46:s:66:LEU:HD22	2.02	0.41
1:1:248:G:H5'	1:1:250:G:N7	2.35	0.41
1:1:901:C:H2'	1:1:902:C:O4'	2.21	0.41
1:1:910:A:N3	1:1:2264:C:O2'	2.46	0.41
1:1:2500:U:O2'	1:1:2504:PSU:OP1	2.32	0.41
2:2:136:C:O2'	47:t:64:GLY:O	2.33	0.41
2:2:1242:G:H3'	2:2:1243:C:H5''	2.03	0.41
8:G:52:PHE:CE2	8:G:69:ARG:HA	2.56	0.41
15:N:4:LYS:HD2	15:N:7:ARG:HH12	1.86	0.41
33:f:85:LEU:HD12	33:f:86:SER:N	2.36	0.41
41:n:36:VAL:O	41:n:36:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:y:49:LYS:O	52:y:53:VAL:HG23	2.21	0.41
55:B:53:PHE:C	55:B:55:ILE:N	2.78	0.41
1:1:172:A:H2'	1:1:173:A:C8	2.55	0.41
1:1:593:U:H2'	1:1:594:U:C6	2.55	0.41
1:1:641:U:O2'	1:1:2350:C:OP1	2.37	0.41
1:1:1248:G:OP1	6:E:44:ARG:NH2	2.53	0.41
1:1:2313:C:H2'	1:1:2314:A:H8	1.86	0.41
1:1:2503:2MA:O2'	1:1:2505:G:OP2	2.39	0.41
1:1:2847:U:H2'	1:1:2848:G:O4'	2.20	0.41
2:2:463:U:H3'	2:2:464:U:C6	2.55	0.41
2:2:555:U:H2'	2:2:556:C:C6	2.56	0.41
2:2:1355:G:H2'	2:2:1356:G:C8	2.55	0.41
5:D:64:GLU:HG2	5:D:68:PHE:HE2	1.85	0.41
9:H:42:LYS:CD	9:H:42:LYS:C	2.94	0.41
9:H:51:ARG:HG3	9:H:54:LEU:HD23	2.02	0.41
13:L:47:GLU:OE1	13:L:51:ARG:NE	2.54	0.41
21:T:41:LEU:HD13	21:T:60:GLU:OE2	2.21	0.41
38:k:84:THR:O	38:k:84:THR:HG23	2.21	0.41
44:q:16:VAL:HG13	44:q:34:LEU:CD1	2.51	0.41
54:z:48:C:C4	54:z:49:G:O6	2.73	0.41
55:B:36:ALA:HA	55:B:39:ASN:HB3	2.02	0.41
1:1:11:C:H6	1:1:11:C:O5'	2.04	0.41
1:1:92:U:O2	55:B:10:LYS:HE2	2.20	0.41
1:1:644:A:H2'	1:1:645:C:O4'	2.21	0.41
1:1:1055:G:N1	1:1:1105:U:N3	2.68	0.41
1:1:1370:C:H2'	1:1:1371:G:O4'	2.21	0.41
2:2:69:G:H2'	2:2:70:U:C6	2.55	0.41
2:2:439:U:O2	2:2:439:U:O4'	2.37	0.41
9:H:38:PRO:O	9:H:40:THR:N	2.51	0.41
9:H:81:ALA:HA	9:H:147:VAL:O	2.21	0.41
15:N:29:HIS:HB3	15:N:36:TYR:HB2	2.03	0.41
16:O:91:ALA:HB3	16:O:111:LYS:HG3	2.01	0.41
23:V:59:LEU:HD13	23:V:80:ILE:HD12	2.02	0.41
55:B:46:ASP:C	55:B:50:LYS:HZ3	2.29	0.41
1:1:321:U:O3'	6:E:162:ARG:NH1	2.49	0.41
1:1:357:C:H2'	1:1:358:U:H6	1.86	0.41
1:1:414:C:H2'	1:1:415:A:C8	2.56	0.41
1:1:1048:A:C5	1:1:1049:C:C5	3.09	0.41
1:1:1172:C:H2'	1:1:1173:U:C2	2.55	0.41
1:1:1198:U:H2'	1:1:1199:U:C6	2.56	0.41
1:1:1358:G:C8	1:1:1371:G:O6	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1438:U:H2'	1:1:1439:A:H8	1.85	0.41
1:1:1452:G:H2'	1:1:1457:U:O4	2.21	0.41
1:1:1534:U:O2	1:1:1538:G:C6	2.74	0.41
1:1:2030:6MZ:H2	1:1:2499:C:H5''	2.02	0.41
1:1:2102:G:C2	1:1:2103:C:C2	3.09	0.41
1:1:2133:G:N3	1:1:2158:A:C2	2.89	0.41
1:1:2900:A:H2'	1:1:2901:C:H6	1.84	0.41
1:1:2902:C:H3'	1:1:2903:U:H5''	2.03	0.41
2:2:41:G:H2'	2:2:42:G:C8	2.55	0.41
2:2:83:C:H2'	2:2:85:U:C4	2.55	0.41
2:2:204:G:H1'	2:2:465:A:C2	2.55	0.41
2:2:411:A:P	35:h:26:ARG:HH12	2.44	0.41
2:2:692:U:H1'	2:2:695:A:N7	2.36	0.41
9:H:3:VAL:HG23	9:H:37:VAL:C	2.46	0.41
9:H:94:ILE:HA	9:H:98:ASP:OD2	2.21	0.41
13:L:20:LEU:HD23	13:L:20:LEU:HA	1.96	0.41
33:f:87:CYS:CB	33:f:221:VAL:HG21	2.51	0.41
33:f:221:VAL:HG23	33:f:222:ARG:N	2.36	0.41
34:g:130:PHE:O	34:g:134:MET:HG3	2.21	0.41
44:q:46:SER:O	44:q:47:GLU:HG3	2.21	0.41
44:q:104:THR:HG22	44:q:105:ASN:CG	2.45	0.41
48:u:8:LEU:O	48:u:60:GLU:HA	2.21	0.41
55:B:6:THR:O	55:B:7:GLY:C	2.63	0.41
55:B:8:ILE:HG13	55:B:25:ASP:CB	2.51	0.41
1:1:558:U:H2'	1:1:559:G:C8	2.56	0.41
1:1:1584:U:H4'	1:1:1585:C:H5''	2.03	0.41
1:1:1746:A:H2'	1:1:1747:U:C6	2.56	0.41
1:1:2133:G:C2	1:1:2158:A:C2	3.09	0.41
1:1:2350:C:H2'	1:1:2351:G:O4'	2.21	0.41
2:2:718:A:H4'	42:o:119:ASN:OD1	2.20	0.41
2:2:842:U:C2'	2:2:844:G:H21	2.34	0.41
2:2:1026:G:H2'	2:2:1026:G:N3	2.36	0.41
2:2:1060:U:C5	34:g:2:GLY:CA	3.04	0.41
5:D:121:THR:HB	5:D:127:PHE:CD2	2.56	0.41
8:G:54:PRO:HB3	8:G:61:GLY:HA3	2.03	0.41
9:H:3:VAL:HG12	9:H:19:VAL:O	2.21	0.41
33:f:120:GLN:C	33:f:126:PHE:HB2	2.46	0.41
33:f:125:THR:C	33:f:127:ASP:H	2.28	0.41
43:p:54:ARG:HD2	43:p:62:GLU:HG3	2.02	0.41
44:q:52:GLN:O	44:q:56:LEU:HG	2.20	0.41
51:x:56:PRO:O	51:x:59:ASP:OD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B:39:ASN:O	55:B:43:LYS:HG3	2.21	0.41
1:1:411:G:OP2	1:1:2406:A:O2'	2.35	0.40
1:1:1078:U:C2'	1:1:1088:A:OP1	2.69	0.40
1:1:2170:A:C2	1:1:2171:A:C5	3.09	0.40
2:2:362:G:N2	2:2:365:U:OP2	2.48	0.40
2:2:1356:G:H2'	2:2:1357:A:H8	1.83	0.40
9:H:87:GLU:HG3	37:j:17:GLN:HG2	2.01	0.40
16:O:78:SER:OG	16:O:80:VAL:HG12	2.21	0.40
21:T:52:LEU:O	21:T:52:LEU:HD23	2.20	0.40
29:b:10:LYS:HE3	29:b:20:PHE:CG	2.57	0.40
31:d:55:LEU:O	31:d:58:VAL:HG12	2.21	0.40
40:m:39:PHE:O	40:m:45:ARG:NE	2.52	0.40
1:1:657:U:H2'	1:1:658:U:C6	2.57	0.40
1:1:1483:G:C6	1:1:1507:C:N3	2.89	0.40
1:1:1866:A:C6	1:1:1876:A:N7	2.89	0.40
1:1:2128:G:C4	1:1:2173:A:O2'	2.74	0.40
2:2:213:G:C8	2:2:214:C:C5	3.10	0.40
2:2:456:A:C6	2:2:457:G:C5	3.09	0.40
3:3:2:G:H2'	3:3:3:C:C6	2.56	0.40
11:J:24:VAL:HG13	11:J:33:ALA:HB2	2.03	0.40
19:R:85:ILE:O	19:R:85:ILE:CG2	2.69	0.40
36:i:56:VAL:HB	36:i:57:PRO:HD3	2.03	0.40
40:m:15:SER:OG	40:m:78:ALA:HB2	2.21	0.40
43:p:66:TYR:HB2	43:p:93:VAL:HG11	2.03	0.40
45:r:46:LEU:HD12	50:w:13:LEU:CB	2.51	0.40
46:s:40:GLN:OE1	46:s:40:GLN:HA	2.21	0.40
54:z:19:G:C1'	54:z:20:5MU:OP2	2.69	0.40
54:z:31:G:H2'	54:z:32:A:C8	2.57	0.40
1:1:281:C:H2'	1:1:282:A:C8	2.56	0.40
1:1:1055:G:H1'	1:1:1085:A:C2	2.55	0.40
1:1:2140:G:O6	1:1:2152:G:C8	2.75	0.40
1:1:2394:C:OP1	31:d:30:ARG:NH2	2.54	0.40
2:2:81:A:N1	2:2:88:U:O4	2.54	0.40
2:2:842:U:H2'	2:2:844:G:H21	1.86	0.40
2:2:1242:G:C3'	2:2:1243:C:H5''	2.51	0.40
2:2:1359:C:OP2	45:r:75:ARG:NE	2.54	0.40
3:3:48:U:P	15:N:30:ARG:HH22	2.44	0.40
7:F:122:PHE:HB2	7:F:163:ASP:OD2	2.20	0.40
9:H:115:VAL:HG12	9:H:117:LEU:HD11	2.03	0.40
20:S:10:VAL:HG13	20:S:38:ALA:CB	2.51	0.40
34:g:105:GLU:OE1	34:g:107:ARG:NE	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:i:56:VAL:O	36:i:60:ILE:HG12	2.21	0.40
37:j:4:TYR:CD2	37:j:71:ILE:HG13	2.57	0.40
52:y:4:ILE:CD1	52:y:19:PHE:HA	2.52	0.40
52:y:62:ARG:NH2	52:y:63:GLU:OE2	2.54	0.40
53:4:3:U:O2	53:4:3:U:O4'	2.39	0.40
1:1:157:C:H2'	1:1:158:U:O4'	2.22	0.40
1:1:993:G:OP1	17:P:50:ARG:NH2	2.53	0.40
1:1:1429:G:H2'	1:1:1430:G:H8	1.87	0.40
1:1:1589:U:O2'	1:1:1590:A:H8	2.04	0.40
1:1:1916:A:H61	2:2:1408:A:HO2'	1.68	0.40
1:1:2094:A:P	9:H:22:LYS:HD2	2.61	0.40
1:1:2184:A:H2'	1:1:2185:U:C6	2.56	0.40
1:1:2788:C:H2'	1:1:2789:C:C6	2.55	0.40
2:2:1400:C:O4'	53:4:6:A:C6	2.75	0.40
5:D:105:LYS:C	5:D:177:VAL:HG12	2.46	0.40
9:H:124:THR:HG23	9:H:124:THR:O	2.21	0.40
23:V:10:THR:C	23:V:12:ASN:H	2.30	0.40
24:W:12:PRO:HB3	24:W:30:LEU:HD23	2.04	0.40
33:f:114:LEU:HD23	33:f:114:LEU:C	2.45	0.40
34:g:77:ILE:HG12	34:g:84:VAL:HG21	2.04	0.40
1:1:2:G:H2'	1:1:3:U:C6	2.57	0.40
1:1:720:U:H2'	1:1:721:A:H8	1.85	0.40
1:1:1883:U:H2'	1:1:1884:G:O4'	2.22	0.40
1:1:2505:G:H1'	55:B:68:THR:HG22	2.03	0.40
2:2:1005:A:OP2	2:2:1005:A:H8	2.05	0.40
8:G:73:ASN:O	8:G:77:ILE:HG12	2.22	0.40
8:G:76:VAL:O	8:G:80:THR:HG22	2.21	0.40
11:J:7:MET:SD	11:J:20:MET:HB2	2.61	0.40
15:N:7:ARG:NH1	15:N:7:ARG:HB3	2.37	0.40
17:P:89:GLU:O	18:Q:11:GLN:NE2	2.46	0.40
19:R:91:GLY:HA3	55:B:53:PHE:CG	2.56	0.40
25:X:9:LYS:O	25:X:60:LYS:HE2	2.22	0.40
33:f:58:ASN:OD1	33:f:224:GLY:HA3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	269/271 (99%)	257 (96%)	12 (4%)	0	100	100
5	D	207/209 (99%)	201 (97%)	3 (1%)	3 (1%)	9	30
6	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
7	F	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	21	51
8	G	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
9	H	147/149 (99%)	136 (92%)	9 (6%)	2 (1%)	9	30
10	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	J	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
12	K	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
13	L	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
14	M	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
15	N	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
16	O	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
17	P	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
18	Q	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	6	22
19	R	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
20	S	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
21	T	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
22	U	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
23	V	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	9	32
24	W	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
25	X	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	Z	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
28	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	b	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
30	c	44/46 (96%)	44 (100%)	0	0	100	100
31	d	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
32	e	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
33	f	223/225 (99%)	212 (95%)	11 (5%)	0	100	100
34	g	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
35	h	203/205 (99%)	199 (98%)	4 (2%)	0	100	100
36	i	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
37	j	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
38	k	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
39	l	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
40	m	125/127 (98%)	118 (94%)	7 (6%)	0	100	100
41	n	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
42	o	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
43	p	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
44	q	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
45	r	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
46	s	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
47	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
48	u	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
49	v	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
50	w	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
51	x	84/86 (98%)	84 (100%)	0	0	100	100
52	y	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
55	B	64/66 (97%)	46 (72%)	17 (27%)	1 (2%)	7	27
All	All	5677/5778 (98%)	5462 (96%)	205 (4%)	10 (0%)	44	72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	152	PRO
5	D	153	GLY
5	D	154	LYS

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Mol	Chain	Res	Type
9	H	90	LEU
18	Q	52	PRO
18	Q	53	PHE
23	V	11	ARG
55	B	54	THR
9	H	89	LYS
7	F	124	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	216/216 (100%)	216 (100%)	0	100	100
5	D	164/164 (100%)	163 (99%)	1 (1%)	78	93
6	E	165/165 (100%)	165 (100%)	0	100	100
7	F	148/148 (100%)	148 (100%)	0	100	100
8	G	136/136 (100%)	135 (99%)	1 (1%)	76	92
9	H	114/114 (100%)	113 (99%)	1 (1%)	70	90
10	I	116/116 (100%)	116 (100%)	0	100	100
11	J	104/104 (100%)	104 (100%)	0	100	100
12	K	103/103 (100%)	103 (100%)	0	100	100
13	L	109/109 (100%)	109 (100%)	0	100	100
14	M	99/99 (100%)	99 (100%)	0	100	100
15	N	86/86 (100%)	86 (100%)	0	100	100
16	O	99/99 (100%)	99 (100%)	0	100	100
17	P	89/89 (100%)	89 (100%)	0	100	100
18	Q	84/84 (100%)	84 (100%)	0	100	100
19	R	93/93 (100%)	93 (100%)	0	100	100
20	S	81/81 (100%)	81 (100%)	0	100	100
21	T	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	U	78/78 (100%)	78 (100%)	0	100	100
23	V	60/60 (100%)	60 (100%)	0	100	100
24	W	67/67 (100%)	67 (100%)	0	100	100
25	X	54/54 (100%)	54 (100%)	0	100	100
26	Y	48/48 (100%)	48 (100%)	0	100	100
27	Z	59/59 (100%)	59 (100%)	0	100	100
28	a	47/47 (100%)	47 (100%)	0	100	100
29	b	47/47 (100%)	47 (100%)	0	100	100
30	c	38/38 (100%)	38 (100%)	0	100	100
31	d	51/51 (100%)	50 (98%)	1 (2%)	48	78
32	e	34/34 (100%)	34 (100%)	0	100	100
33	f	187/187 (100%)	187 (100%)	0	100	100
34	g	171/171 (100%)	171 (100%)	0	100	100
35	h	172/172 (100%)	172 (100%)	0	100	100
36	i	119/119 (100%)	119 (100%)	0	100	100
37	j	91/91 (100%)	91 (100%)	0	100	100
38	k	124/124 (100%)	124 (100%)	0	100	100
39	l	104/104 (100%)	104 (100%)	0	100	100
40	m	105/105 (100%)	105 (100%)	0	100	100
41	n	86/86 (100%)	86 (100%)	0	100	100
42	o	90/90 (100%)	90 (100%)	0	100	100
43	p	102/102 (100%)	102 (100%)	0	100	100
44	q	94/94 (100%)	94 (100%)	0	100	100
45	r	83/83 (100%)	83 (100%)	0	100	100
46	s	76/76 (100%)	75 (99%)	1 (1%)	61	86
47	t	65/65 (100%)	65 (100%)	0	100	100
48	u	74/74 (100%)	74 (100%)	0	100	100
49	v	57/57 (100%)	57 (100%)	0	100	100
50	w	72/72 (100%)	72 (100%)	0	100	100
51	x	65/65 (100%)	64 (98%)	1 (2%)	57	84
52	y	60/60 (100%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	B	52/52 (100%)	47 (90%)	5 (10%)	8	26
All	All	4722/4722 (100%)	4711 (100%)	11 (0%)	85	96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	151	THR
8	G	47	ASP
9	H	122	LEU
31	d	31	HIS
46	s	89	ARG
51	x	57	ILE
55	B	42	TYR
55	B	52	SER
55	B	53	PHE
55	B	54	THR
55	B	56	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	70	ASN
4	C	134	ASN
4	C	226	ASN
6	E	92	HIS
6	E	136	GLN
8	G	104	ASN
9	H	43	ASN
9	H	119	ASN
10	I	136	GLN
11	J	9	ASN
12	K	35	HIS
13	L	60	GLN
14	M	9	GLN
14	M	31	HIS
14	M	73	ASN
15	N	98	GLN
16	O	56	HIS
24	W	36	HIS
29	b	26	ASN
31	d	31	HIS

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Mol	Chain	Res	Type
32	e	35	GLN
36	i	121	HIS
37	j	94	HIS
40	m	37	GLN
40	m	110	GLN
45	r	4	GLN
47	t	79	ASN
51	x	52	ASN
51	x	61	GLN
51	x	82	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2903 (99%)	498 (17%)	14 (0%)
2	2	1532/1534 (99%)	254 (16%)	3 (0%)
3	3	119/120 (99%)	16 (13%)	0
53	4	5/6 (83%)	0	1 (20%)
54	z	84/85 (98%)	31 (36%)	0
All	All	4642/4648 (99%)	799 (17%)	18 (0%)

All (799) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	51	G
1	1	71	A
1	1	74	A
1	1	75	G
1	1	84	A
1	1	85	G
1	1	101	A
1	1	102	U
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U

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Mol	Chain	Res	Type
1	1	122	G
1	1	125	A
1	1	138	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A
1	1	221	A
1	1	222	A
1	1	225	C
1	1	248	G
1	1	249	C
1	1	264	C
1	1	265	A
1	1	266	G
1	1	272	A
1	1	273	G
1	1	275	C
1	1	276	U
1	1	285	G
1	1	311	A
1	1	329	G
1	1	330	A
1	1	343	C
1	1	353	C
1	1	361	G
1	1	371	A
1	1	372	G
1	1	383	C
1	1	386	G
1	1	396	G
1	1	399	U
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G

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Mol	Chain	Res	Type
1	1	435	C
1	1	457	A
1	1	467	G
1	1	481	G
1	1	489	G
1	1	491	G
1	1	505	A
1	1	509	C
1	1	513	A
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	573	U
1	1	575	A
1	1	603	A
1	1	612	G
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	621	A
1	1	622	G
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G
1	1	654	A
1	1	655	A
1	1	670	A
1	1	685	A
1	1	686	U
1	1	702	U
1	1	709	U
1	1	710	U
1	1	717	C

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Mol	Chain	Res	Type
1	1	726	G
1	1	730	A
1	1	747	5MU
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	792	A
1	1	800	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	866	A
1	1	869	G
1	1	878	A
1	1	880	G
1	1	882	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U
1	1	896	A
1	1	897	C
1	1	898	C
1	1	907	G
1	1	910	A
1	1	931	U
1	1	932	U
1	1	941	A

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Mol	Chain	Res	Type
1	1	946	C
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1096	A
1	1	1101	U
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U

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Mol	Chain	Res	Type
1	1	1122	G
1	1	1128	G
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1139	G
1	1	1142	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1171	G
1	1	1173	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1182	G
1	1	1186	G
1	1	1206	G
1	1	1212	G
1	1	1218	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1250	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1300	G
1	1	1301	A
1	1	1321	A
1	1	1329	U
1	1	1341	G
1	1	1345	C
1	1	1352	U
1	1	1365	A

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Mol	Chain	Res	Type
1	1	1368	G
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1408	G
1	1	1411	U
1	1	1417	C
1	1	1419	A
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1460	U
1	1	1468	U
1	1	1476	U
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1494	A
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1532	A
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1583	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1607	C

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Mol	Chain	Res	Type
1	1	1608	A
1	1	1618	6MZ
1	1	1634	A
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1756	G
1	1	1764	C
1	1	1773	A
1	1	1782	U
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1835	2MG
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1865	U
1	1	1868	C
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1896	G
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1914	C
1	1	1923	U

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Mol	Chain	Res	Type
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A
1	1	1938	A
1	1	1955	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2030	6MZ
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2093	G
1	1	2095	A
1	1	2100	G
1	1	2102	G
1	1	2107	G
1	1	2110	G
1	1	2112	G
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A

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Mol	Chain	Res	Type
1	1	2121	G
1	1	2122	U
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2140	G
1	1	2142	A
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2168	G
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2178	C
1	1	2183	A
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2211	A
1	1	2225	A
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2278	A

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Mol	Chain	Res	Type
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2305	U
1	1	2309	A
1	1	2319	G
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G
1	1	2476	A
1	1	2478	A
1	1	2480	C
1	1	2491	U
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU

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Mol	Chain	Res	Type
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2586	U
1	1	2602	A
1	1	2609	U
1	1	2613	U
1	1	2629	U
1	1	2646	C
1	1	2663	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2725	A
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2757	A
1	1	2765	A
1	1	2777	G
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2794	C
1	1	2796	U
1	1	2797	U
1	1	2799	A

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Mol	Chain	Res	Type
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2825	G
1	1	2833	U
1	1	2835	A
1	1	2836	U
1	1	2861	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2898	U
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	66	A
2	2	68	G
2	2	69	G
2	2	70	U
2	2	72	A
2	2	73	C
2	2	74	A
2	2	75	G
2	2	76	G
2	2	79	G
2	2	81	A

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Mol	Chain	Res	Type
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	92	U
2	2	120	A
2	2	121	U
2	2	130	A
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A
2	2	160	A
2	2	163	C
2	2	164	G
2	2	177	G
2	2	181	A
2	2	182	A
2	2	197	A
2	2	204	G
2	2	210	C
2	2	211	G
2	2	212	G
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	266	G
2	2	267	C
2	2	279	A
2	2	289	G
2	2	306	A
2	2	319	G
2	2	321	A
2	2	328	C
2	2	332	G
2	2	347	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	372	C

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Mol	Chain	Res	Type
2	2	384	G
2	2	392	C
2	2	398	U
2	2	406	G
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	436	C
2	2	439	U
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	476	U
2	2	478	A
2	2	479	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	496	A
2	2	499	A
2	2	510	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	521	G
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	533	A
2	2	547	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A

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Mol	Chain	Res	Type
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	633	G
2	2	650	G
2	2	653	U
2	2	660	C
2	2	665	A
2	2	700	G
2	2	701	U
2	2	702	A
2	2	703	G
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	753	A
2	2	755	G
2	2	777	A
2	2	787	A
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
2	2	821	G
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	843	U
2	2	844	G
2	2	845	A
2	2	846	G
2	2	884	U
2	2	887	G
2	2	914	A
2	2	934	C

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Mol	Chain	Res	Type
2	2	935	A
2	2	960	U
2	2	965	U
2	2	966	2MG
2	2	967	5MC
2	2	969	A
2	2	971	G
2	2	972	C
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	979	C
2	2	982	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1004	A
2	2	1009	U
2	2	1019	A
2	2	1022	A
2	2	1025	U
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1034	G
2	2	1043	G
2	2	1046	A
2	2	1065	U
2	2	1085	U
2	2	1089	G
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1104	G
2	2	1108	G
2	2	1124	G
2	2	1125	U
2	2	1132	C
2	2	1136	C

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Mol	Chain	Res	Type
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1169	A
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1212	U
2	2	1213	A
2	2	1215	G
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1243	C
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G
2	2	1299	A
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C

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Mol	Chain	Res	Type
2	2	1336	C
2	2	1340	A
2	2	1346	A
2	2	1353	G
2	2	1363	A
2	2	1370	G
2	2	1379	G
2	2	1381	U
2	2	1419	G
2	2	1441	A
2	2	1446	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1519	MA6
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	13	G
3	3	24	G
3	3	31	C
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
54	z	8	5MU
54	z	9	G
54	z	10	G
54	z	14	A
54	z	16	U

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Mol	Chain	Res	Type
54	z	17	U
54	z	18	G
54	z	19	G
54	z	20	5MU
54	z	21	A
54	z	22	G
54	z	23	A
54	z	24	C
54	z	46	G
54	z	49	G
54	z	50	C
54	z	51	A
54	z	53	G
54	z	54	G
54	z	56	G
54	z	57	5MU
54	z	64	5MU
54	z	65	C
54	z	67	A
54	z	68	G
54	z	69	5MU
54	z	70	C
54	z	71	5MU
54	z	76	5MU
54	z	82	A
54	z	85	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	125	A
1	1	404	A
1	1	613	A
1	1	621	A
1	1	784	G
1	1	887	A
1	1	891	G
1	1	894	U
1	1	1379	U
1	1	1475	G
1	1	1608	A
1	1	2146	C

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Mol	Chain	Res	Type
1	1	2189	U
1	1	2756	U
2	2	516	PSU
2	2	1109	C
2	2	1145	A
53	4	3	U

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

46 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$
1	3TD	1	1915	1	18,22,23	4.07	7 (38%)	22,32,35	1.58	2 (9%)
1	PSU	1	1917	1	18,21,22	1.06	1 (5%)	22,30,33	1.88	5 (22%)
1	5MU	1	747	1	19,22,23	4.63	7 (36%)	28,32,35	3.73	10 (35%)
2	4OC	2	1402	2	20,23,24	2.93	8 (40%)	26,32,35	0.94	0
54	5MU	z	76	54	19,22,23	1.45	5 (26%)	28,32,35	2.21	7 (25%)
54	5MU	z	64	54	19,22,23	1.44	6 (31%)	28,32,35	2.38	10 (35%)
1	2MA	1	2503	1,56	22,25,26	3.68	9 (40%)	33,37,40	2.40	9 (27%)
1	5MU	1	1939	1,56	19,22,23	4.61	7 (36%)	28,32,35	3.72	9 (32%)
2	5MC	2	1407	2	18,22,23	3.34	7 (38%)	26,32,35	0.85	1 (3%)
1	OMU	1	2552	1	19,22,23	2.87	8 (42%)	26,31,34	1.64	5 (19%)
2	5MC	2	967	2	18,22,23	3.44	7 (38%)	26,32,35	1.03	2 (7%)
43	0TD	p	89	43	7,9,10	1.51	1 (14%)	6,11,13	1.91	2 (33%)
1	PSU	1	2504	1	18,21,22	0.98	2 (11%)	22,30,33	1.82	4 (18%)
1	OMC	1	2498	1,56	19,22,23	2.73	7 (36%)	26,31,34	0.86	0
54	5MU	z	63	54	19,22,23	1.46	6 (31%)	28,32,35	2.18	8 (28%)
54	5MU	z	39	54	19,22,23	1.44	6 (31%)	28,32,35	2.20	9 (32%)
1	OMG	1	2251	1,54	23,26,27	2.17	7 (30%)	33,38,41	1.71	8 (24%)
54	5MU	z	8	54	19,22,23	4.71	7 (36%)	28,32,35	3.68	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	5MU	z	69	54	19,22,23	1.41	6 (31%)	28,32,35	1.92	7 (25%)
2	UR3	2	1498	56,2	19,22,23	2.63	6 (31%)	26,32,35	1.07	2 (7%)
1	PSU	1	2605	1	18,21,22	0.98	2 (11%)	22,30,33	1.96	5 (22%)
2	2MG	2	1516	2	23,26,27	2.68	9 (39%)	32,38,41	2.08	10 (31%)
54	5MU	z	71	54	19,22,23	1.44	6 (31%)	28,32,35	2.15	8 (28%)
54	5MU	z	55	54	19,22,23	4.79	7 (36%)	28,32,35	3.58	9 (32%)
1	PSU	1	955	1,56	18,21,22	0.99	2 (11%)	22,30,33	1.93	5 (22%)
1	2MG	1	1835	1	23,26,27	2.68	8 (34%)	32,38,41	2.10	8 (25%)
1	G7M	1	2069	1	23,26,27	2.56	9 (39%)	35,39,42	2.21	11 (31%)
2	MA6	2	1519	2	23,26,27	1.47	4 (17%)	34,38,41	3.28	11 (32%)
54	5MU	z	20	56,54	19,22,23	4.94	7 (36%)	28,32,35	3.63	10 (35%)
54	5MU	z	42	2,54	19,22,23	4.58	7 (36%)	28,32,35	3.73	10 (35%)
1	2MG	1	2445	1	23,26,27	2.62	8 (34%)	32,38,41	2.00	9 (28%)
1	1MG	1	745	1	22,26,27	2.86	7 (31%)	33,39,42	2.16	7 (21%)
54	5MU	z	40	54	19,22,23	1.39	5 (26%)	28,32,35	2.29	12 (42%)
2	2MG	2	966	2	23,26,27	2.79	7 (30%)	32,38,41	2.11	7 (21%)
1	PSU	1	2580	1,56	18,21,22	1.01	1 (5%)	22,30,33	1.95	6 (27%)
2	PSU	2	516	56,2	18,21,22	0.98	1 (5%)	22,30,33	1.85	4 (18%)
54	5MU	z	57	54	19,22,23	4.71	7 (36%)	28,32,35	3.64	10 (35%)
1	6MZ	1	2030	1	22,25,26	2.52	6 (27%)	30,36,39	3.29	12 (40%)
1	6MZ	1	1618	1	22,25,26	2.37	5 (22%)	30,36,39	3.29	11 (36%)
1	PSU	1	1911	1	18,21,22	0.98	1 (5%)	22,30,33	1.87	5 (22%)
2	2MG	2	1207	2	23,26,27	2.68	9 (39%)	32,38,41	2.08	10 (31%)
1	5MC	1	1962	1	18,22,23	3.29	7 (38%)	26,32,35	1.13	3 (11%)
2	MA6	2	1518	2	23,26,27	1.45	4 (17%)	34,38,41	3.15	11 (32%)
1	PSU	1	746	1,56	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
2	G7M	2	527	2	23,26,27	2.65	8 (34%)	35,39,42	2.26	10 (28%)
1	PSU	1	2457	1	18,21,22	1.02	1 (5%)	22,30,33	1.98	5 (22%)

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
1	3TD	1	1915	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
54	5MU	z	76	54	-	0/7/25/26	0/2/2/2
54	5MU	z	64	54	-	4/7/25/26	0/2/2/2
1	2MA	1	2503	1,56	-	2/7/25/26	0/3/3/3
1	5MU	1	1939	1,56	-	0/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
2	5MC	2	967	2	-	2/7/25/26	0/2/2/2
43	0TD	p	89	43	-	2/7/12/14	-
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	OMC	1	2498	1,56	-	0/9/27/28	0/2/2/2
54	5MU	z	63	54	-	0/7/25/26	0/2/2/2
54	5MU	z	39	54	-	3/7/25/26	0/2/2/2
1	OMG	1	2251	1,54	-	0/9/27/28	0/3/3/3
54	5MU	z	8	54	-	2/7/25/26	0/2/2/2
54	5MU	z	69	54	-	5/7/25/26	0/2/2/2
2	UR3	2	1498	56,2	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
54	5MU	z	71	54	-	3/7/25/26	0/2/2/2
54	5MU	z	55	54	-	0/7/25/26	0/2/2/2
1	PSU	1	955	1,56	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/9/27/28	0/3/3/3
1	G7M	1	2069	1	-	1/7/25/26	0/3/3/3
2	MA6	2	1519	2	-	2/11/29/30	0/3/3/3
54	5MU	z	20	56,54	-	2/7/25/26	0/2/2/2
54	5MU	z	42	2,54	-	0/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
1	1MG	1	745	1	-	0/7/25/26	0/3/3/3
54	5MU	z	40	54	-	2/7/25/26	0/2/2/2
2	2MG	2	966	2	-	0/9/27/28	0/3/3/3
1	PSU	1	2580	1,56	-	0/7/25/26	0/2/2/2
2	PSU	2	516	56,2	-	2/7/25/26	0/2/2/2
54	5MU	z	57	54	-	0/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	2/9/27/28	0/3/3/3
1	6MZ	1	1618	1	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	0/9/27/28	0/3/3/3
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/11/29/30	0/3/3/3
1	PSU	1	746	1,56	-	1/7/25/26	0/2/2/2
2	G7M	2	527	2	-	3/7/25/26	0/3/3/3
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2

All (259) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	11.83	1.49	1.35
1	1	2503	2MA	C4-N3	11.34	1.48	1.34
54	z	20	5MU	C2-N1	11.28	1.56	1.38
54	z	57	5MU	C2-N1	11.11	1.56	1.38
54	z	55	5MU	C2-N1	11.07	1.56	1.38
54	z	20	5MU	C6-N1	10.90	1.56	1.38
1	1	747	5MU	C2-N1	10.77	1.55	1.38
54	z	42	5MU	C2-N1	10.75	1.55	1.38
54	z	8	5MU	C2-N1	10.73	1.55	1.38
1	1	1939	5MU	C2-N1	10.62	1.55	1.38
54	z	20	5MU	C4-C5	10.30	1.61	1.44
54	z	55	5MU	C6-N1	10.27	1.55	1.38
54	z	8	5MU	C6-N1	10.20	1.55	1.38
54	z	57	5MU	C6-N1	10.03	1.55	1.38
54	z	55	5MU	C4-C5	9.84	1.61	1.44
1	1	747	5MU	C6-N1	9.78	1.54	1.38
1	1	1939	5MU	C6-N1	9.74	1.54	1.38
1	1	2030	6MZ	C6-N6	9.69	1.44	1.34
54	z	42	5MU	C6-N1	9.60	1.54	1.38
54	z	8	5MU	C4-C5	9.48	1.60	1.44
1	1	1939	5MU	C4-C5	9.42	1.60	1.44
1	1	1618	6MZ	C6-N6	9.30	1.44	1.34
1	1	747	5MU	C4-C5	9.27	1.60	1.44
54	z	57	5MU	C4-C5	9.27	1.60	1.44
1	1	1915	3TD	C2-N1	8.95	1.48	1.37
54	z	42	5MU	C4-C5	8.91	1.59	1.44
2	2	1407	5MC	C6-C5	8.79	1.49	1.34
2	2	967	5MC	C6-C5	8.55	1.48	1.34
1	1	745	1MG	C2-N2	8.37	1.49	1.34
1	1	1962	5MC	C6-C5	8.09	1.47	1.34
54	z	42	5MU	C4-N3	-7.76	1.24	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	747	5MU	C4-N3	-7.67	1.24	1.38
54	z	57	5MU	C4-N3	-7.63	1.24	1.38
2	2	966	2MG	C2-N3	7.57	1.46	1.31
1	1	1939	5MU	C4-N3	-7.57	1.24	1.38
54	z	8	5MU	C4-N3	-7.40	1.25	1.38
54	z	55	5MU	C4-N3	-7.37	1.25	1.38
1	1	1835	2MG	C2-N3	7.26	1.45	1.31
2	2	1207	2MG	C2-N3	7.10	1.45	1.31
54	z	20	5MU	C4-N3	-7.03	1.25	1.38
2	2	1516	2MG	C2-N3	7.02	1.45	1.31
1	1	2445	2MG	C2-N3	6.87	1.45	1.31
54	z	20	5MU	C6-C5	6.60	1.45	1.34
2	2	1402	4OC	C4-N3	6.48	1.44	1.32
1	1	2552	OMU	C2-N1	6.45	1.48	1.38
2	2	967	5MC	C4-N3	6.38	1.44	1.34
1	1	2552	OMU	C2-N3	6.37	1.49	1.38
1	1	2503	2MA	C2-N3	6.33	1.45	1.34
2	2	1498	UR3	C6-C5	6.31	1.49	1.35
1	1	1962	5MC	C4-N3	6.31	1.44	1.34
2	2	966	2MG	C4-N3	6.24	1.49	1.34
54	z	55	5MU	C6-C5	6.22	1.44	1.34
2	2	527	G7M	C5-N7	-6.16	1.32	1.39
2	2	527	G7M	C4-N3	6.14	1.48	1.34
1	1	2069	G7M	C5-N7	-6.13	1.32	1.39
1	1	2503	2MA	C6-N1	6.03	1.43	1.35
2	2	967	5MC	C2-N3	5.98	1.48	1.36
54	z	8	5MU	C6-C5	5.97	1.44	1.34
2	2	1207	2MG	C4-N3	5.97	1.48	1.34
2	2	1498	UR3	C2-N1	5.97	1.47	1.38
1	1	1835	2MG	C4-N3	5.94	1.48	1.34
54	z	57	5MU	C6-C5	5.93	1.44	1.34
2	2	1402	4OC	C6-C5	5.84	1.48	1.35
1	1	2498	OMC	C2-N3	5.83	1.48	1.36
2	2	1407	5MC	C4-N3	5.82	1.44	1.34
2	2	1516	2MG	C4-N3	5.81	1.48	1.34
1	1	745	1MG	C4-N3	5.80	1.48	1.34
1	1	1962	5MC	C2-N3	5.79	1.48	1.36
1	1	1915	3TD	C6-N1	5.73	1.45	1.36
2	2	1402	4OC	C2-N3	5.68	1.47	1.36
1	1	2445	2MG	C4-N3	5.67	1.47	1.34
1	1	2069	G7M	C4-N3	5.57	1.47	1.34
1	1	747	5MU	C6-C5	5.57	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2251	OMG	C4-N3	5.55	1.47	1.34
2	2	1407	5MC	C2-N3	5.54	1.47	1.36
1	1	2498	OMC	C6-C5	5.51	1.47	1.35
1	1	1939	5MU	C6-C5	5.50	1.43	1.34
1	1	2552	OMU	C6-C5	5.47	1.47	1.35
1	1	2503	2MA	C2-N1	5.46	1.43	1.34
54	z	42	5MU	C6-C5	5.45	1.43	1.34
2	2	527	G7M	C2-N3	5.30	1.45	1.33
2	2	966	2MG	C2-N2	5.14	1.44	1.33
2	2	1498	UR3	C2-N3	5.11	1.48	1.39
1	1	745	1MG	C2-N3	5.10	1.43	1.34
1	1	2251	OMG	C2-N3	4.92	1.45	1.33
2	2	1207	2MG	C2-N2	4.87	1.44	1.33
1	1	1835	2MG	C2-N2	4.77	1.44	1.33
2	2	1516	2MG	C2-N2	4.72	1.43	1.33
1	1	1915	3TD	C2-N3	4.66	1.48	1.38
1	1	2498	OMC	C4-N3	4.60	1.43	1.34
1	1	2069	G7M	C2-N3	4.58	1.44	1.33
1	1	2445	2MG	C2-N2	4.56	1.43	1.33
2	2	1516	2MG	C2-N1	4.46	1.43	1.36
2	2	966	2MG	C2-N1	4.39	1.43	1.36
2	2	527	G7M	C2-N2	4.39	1.44	1.34
1	1	2498	OMC	C4-N4	4.32	1.44	1.33
2	2	1207	2MG	C2-N1	4.29	1.43	1.36
1	1	2503	2MA	C5-C6	4.27	1.52	1.41
2	2	967	5MC	C4-N4	4.22	1.45	1.34
2	2	1402	4OC	C4-N4	4.20	1.44	1.35
2	2	967	5MC	C2-N1	4.11	1.48	1.40
1	1	1835	2MG	C2-N1	4.09	1.43	1.36
2	2	1407	5MC	C4-N4	4.07	1.44	1.34
2	2	1407	5MC	C6-N1	4.07	1.45	1.38
2	2	967	5MC	C6-N1	4.04	1.44	1.38
1	1	1962	5MC	C2-N1	4.03	1.48	1.40
1	1	2069	G7M	C2-N2	4.01	1.43	1.34
1	1	1962	5MC	C4-N4	3.96	1.44	1.34
1	1	745	1MG	C5-N7	-3.93	1.31	1.39
1	1	2498	OMC	C2-N1	3.91	1.48	1.40
1	1	2445	2MG	C2-N1	3.90	1.43	1.36
2	2	1402	4OC	C2-N1	3.90	1.48	1.40
1	1	745	1MG	O6-C6	-3.80	1.15	1.23
1	1	1962	5MC	C6-N1	3.78	1.44	1.38
1	1	2552	OMU	C4-N3	3.78	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2503	2MA	C6-N6	-3.76	1.24	1.34
1	1	2030	6MZ	C5-N7	-3.66	1.32	1.39
2	2	1407	5MC	C2-N1	3.62	1.47	1.40
1	1	2445	2MG	C5-N7	-3.50	1.32	1.39
2	2	1519	MA6	C5-C4	-3.48	1.32	1.39
1	1	1835	2MG	C5-N7	-3.47	1.32	1.39
2	2	966	2MG	C5-N7	-3.32	1.32	1.39
2	2	527	G7M	C5-C6	3.32	1.52	1.43
2	2	1402	4OC	C5-C4	3.32	1.47	1.40
1	1	2069	G7M	C5-C6	3.27	1.52	1.43
2	2	1518	MA6	C6-N6	3.24	1.46	1.36
1	1	2251	OMG	C5-N7	-3.23	1.32	1.39
2	2	1518	MA6	C5-C4	-3.22	1.33	1.39
1	1	2030	6MZ	C5-C4	-3.21	1.33	1.39
2	2	1516	2MG	C5-N7	-3.20	1.32	1.39
1	1	747	5MU	O4-C4	-3.18	1.17	1.23
54	z	42	5MU	O4-C4	-3.15	1.17	1.23
2	2	1519	MA6	C6-N6	3.15	1.46	1.36
54	z	8	5MU	O4-C4	-3.08	1.17	1.23
2	2	1207	2MG	C5-N7	-3.06	1.33	1.39
1	1	2251	OMG	C2-N2	3.02	1.41	1.34
1	1	2251	OMG	O6-C6	-3.00	1.17	1.23
1	1	1917	PSU	C6-C5	2.99	1.38	1.35
1	1	745	1MG	C5-C6	2.99	1.53	1.45
1	1	1618	6MZ	C5-N7	-2.99	1.33	1.39
54	z	57	5MU	O4-C4	-2.98	1.17	1.23
2	2	1407	5MC	O2-C2	-2.97	1.18	1.23
1	1	1939	5MU	O4-C4	-2.97	1.17	1.23
1	1	1618	6MZ	C5-C4	-2.96	1.33	1.39
2	2	1402	4OC	O2-C2	-2.94	1.18	1.23
1	1	2552	OMU	O4-C4	-2.94	1.18	1.24
2	2	967	5MC	O2-C2	-2.90	1.18	1.23
1	1	1962	5MC	O2-C2	-2.86	1.18	1.23
1	1	746	PSU	C6-C5	2.86	1.38	1.35
54	z	20	5MU	O4-C4	-2.86	1.18	1.23
1	1	2498	OMC	O2-C2	-2.82	1.18	1.23
1	1	2503	2MA	C4-N9	-2.82	1.31	1.37
54	z	55	5MU	O4-C4	-2.80	1.18	1.23
54	z	69	5MU	C4-N3	-2.80	1.33	1.38
54	z	64	5MU	C4-N3	-2.79	1.33	1.38
1	1	2069	G7M	C4-N9	-2.78	1.30	1.38
54	z	39	5MU	C4-N3	-2.76	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2445	2MG	O6-C6	-2.76	1.18	1.23
1	1	2069	G7M	O6-C6	-2.75	1.18	1.23
2	2	1498	UR3	C6-N1	2.75	1.44	1.38
54	z	8	5MU	O2-C2	-2.74	1.18	1.23
2	2	1518	MA6	C5-N7	-2.74	1.33	1.39
54	z	39	5MU	C6-C5	2.73	1.39	1.34
2	2	527	G7M	O6-C6	-2.72	1.18	1.23
54	z	69	5MU	C6-C5	2.72	1.39	1.34
1	1	2030	6MZ	C8-N9	-2.71	1.32	1.37
54	z	63	5MU	C4-N3	-2.71	1.33	1.38
2	2	1402	4OC	C6-N1	2.70	1.44	1.38
54	z	76	5MU	C4-N3	-2.67	1.33	1.38
54	z	71	5MU	C6-C5	2.66	1.39	1.34
1	1	1911	PSU	C6-C5	2.66	1.38	1.35
1	1	1939	5MU	O2-C2	-2.65	1.18	1.23
54	z	42	5MU	O2-C2	-2.64	1.18	1.23
2	2	516	PSU	C6-C5	2.63	1.38	1.35
1	1	1835	2MG	O6-C6	-2.63	1.18	1.23
2	2	1207	2MG	O6-C6	-2.61	1.18	1.23
54	z	63	5MU	C6-C5	2.61	1.38	1.34
1	1	2580	PSU	C6-C5	2.61	1.38	1.35
2	2	966	2MG	O6-C6	-2.61	1.18	1.23
1	1	2503	2MA	C5-N7	-2.60	1.34	1.39
54	z	57	5MU	O2-C2	-2.60	1.18	1.23
54	z	71	5MU	C4-N3	-2.59	1.34	1.38
54	z	76	5MU	C6-C5	2.58	1.38	1.34
2	2	1519	MA6	C5-N7	-2.58	1.34	1.39
2	2	1519	MA6	C8-N9	-2.57	1.32	1.37
1	1	747	5MU	O2-C2	-2.56	1.18	1.23
1	1	1915	3TD	O2-C2	-2.55	1.18	1.23
1	1	2552	OMU	O2-C2	-2.55	1.18	1.23
54	z	40	5MU	C4-N3	-2.54	1.34	1.38
54	z	63	5MU	C4-C5	2.53	1.49	1.44
1	1	2457	PSU	C6-C5	2.53	1.38	1.35
2	2	1518	MA6	C8-N9	-2.52	1.33	1.37
54	z	64	5MU	C2-N1	2.51	1.42	1.38
54	z	64	5MU	C6-N1	-2.51	1.33	1.38
2	2	1516	2MG	O6-C6	-2.50	1.18	1.23
1	1	2251	OMG	C4-N9	-2.50	1.31	1.38
1	1	2445	2MG	C4-N9	-2.49	1.31	1.38
1	1	2504	PSU	C6-C5	2.49	1.38	1.35
2	2	527	G7M	C2-N1	2.48	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1618	6MZ	C6-N1	-2.48	1.31	1.35
1	1	2498	OMC	C6-N1	2.48	1.44	1.38
54	z	71	5MU	C4-C5	2.47	1.48	1.44
1	1	2552	OMU	C6-N1	2.47	1.44	1.38
54	z	40	5MU	C6-C5	2.45	1.38	1.34
54	z	55	5MU	O2-C2	-2.45	1.18	1.23
54	z	76	5MU	C4-C5	2.45	1.48	1.44
54	z	40	5MU	C6-N1	-2.45	1.33	1.38
2	2	1516	2MG	C4-N9	-2.44	1.31	1.38
1	1	745	1MG	C4-N9	-2.44	1.31	1.38
54	z	39	5MU	C2-N1	2.44	1.42	1.38
1	1	1915	3TD	C4-N3	2.44	1.45	1.40
54	z	76	5MU	C2-N1	2.43	1.42	1.38
54	z	40	5MU	C4-C5	2.42	1.48	1.44
2	2	1516	2MG	C5-C6	2.42	1.53	1.44
2	2	1207	2MG	C5-C6	2.40	1.53	1.44
54	z	76	5MU	C6-N1	-2.38	1.34	1.38
2	2	966	2MG	C5-C6	2.36	1.53	1.44
1	1	1835	2MG	C5-C6	2.36	1.53	1.44
1	1	1915	3TD	O4-C4	-2.36	1.18	1.23
2	2	1207	2MG	C4-N9	-2.34	1.32	1.38
2	2	1498	UR3	C3U-N3	-2.34	1.42	1.47
1	1	2030	6MZ	C6-N1	-2.34	1.31	1.35
54	z	64	5MU	C6-C5	2.34	1.38	1.34
54	z	20	5MU	O2-C2	-2.33	1.18	1.23
54	z	71	5MU	C6-N1	-2.31	1.34	1.38
54	z	39	5MU	C4-C5	2.29	1.48	1.44
54	z	63	5MU	C6-N1	-2.28	1.34	1.38
1	1	2605	PSU	C6-C5	2.26	1.38	1.35
54	z	71	5MU	C2-N1	2.24	1.42	1.38
54	z	64	5MU	C4-C5	2.22	1.48	1.44
54	z	69	5MU	C4-C5	2.22	1.48	1.44
54	z	39	5MU	C6-N1	-2.21	1.34	1.38
1	1	2069	G7M	C2-N1	2.20	1.43	1.37
1	1	955	PSU	C6-C5	2.20	1.37	1.35
1	1	2030	6MZ	C5-C6	-2.19	1.36	1.41
54	z	69	5MU	C6-N1	-2.19	1.34	1.38
54	z	40	5MU	C2-N1	2.19	1.42	1.38
54	z	69	5MU	C2-N1	2.19	1.42	1.38
1	1	2251	OMG	C5-C6	2.18	1.52	1.44
54	z	63	5MU	C2-N1	2.18	1.41	1.38
1	1	2445	2MG	C5-C6	2.16	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1618	6MZ	C8-N9	-2.16	1.33	1.37
1	1	2552	OMU	C5-C4	2.16	1.48	1.43
54	z	63	5MU	C2-N3	-2.15	1.34	1.38
2	2	1516	2MG	C6-N1	2.14	1.42	1.38
2	2	1498	UR3	O2-C2	-2.11	1.18	1.22
2	2	1207	2MG	C6-N1	2.10	1.42	1.38
54	z	64	5MU	C2-N3	-2.10	1.34	1.38
43	p	89	0TD	CSB-SB	-2.10	1.75	1.79
1	1	1835	2MG	C4-N9	-2.09	1.32	1.38
1	1	2503	2MA	C8-N7	2.06	1.35	1.31
1	1	2069	G7M	C6-N1	2.06	1.42	1.38
1	1	955	PSU	C4-C5	-2.05	1.38	1.44
1	1	2504	PSU	C4-C5	-2.05	1.38	1.44
54	z	71	5MU	C2-N3	-2.05	1.34	1.38
2	2	527	G7M	C4-N9	-2.05	1.32	1.38
54	z	39	5MU	C2-N3	-2.03	1.34	1.38
54	z	69	5MU	C2-N3	-2.03	1.34	1.38
1	1	2605	PSU	C4-C5	-2.02	1.38	1.44

All (323) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1519	MA6	N1-C6-N6	-13.02	102.84	117.08
54	z	8	5MU	C5-C4-N3	12.58	126.05	115.31
2	2	1518	MA6	N1-C6-N6	-12.51	103.40	117.08
54	z	20	5MU	C5-C4-N3	12.49	125.97	115.31
1	1	747	5MU	C5-C4-N3	12.27	125.78	115.31
54	z	42	5MU	C5-C4-N3	12.23	125.75	115.31
54	z	57	5MU	C5-C4-N3	12.17	125.70	115.31
54	z	55	5MU	C5-C4-N3	12.12	125.65	115.31
1	1	1939	5MU	C5-C4-N3	12.04	125.58	115.31
54	z	42	5MU	C5-C6-N1	-10.12	112.93	123.34
54	z	57	5MU	C5-C6-N1	-9.78	113.28	123.34
1	1	1939	5MU	C5-C6-N1	-9.72	113.34	123.34
1	1	747	5MU	C5-C6-N1	-9.63	113.43	123.34
54	z	55	5MU	C5-C6-N1	-9.42	113.64	123.34
54	z	8	5MU	C5-C6-N1	-9.17	113.90	123.34
54	z	20	5MU	C5-C6-N1	-8.84	114.24	123.34
1	1	1618	6MZ	C1'-N9-C8	8.69	146.77	127.14
1	1	1618	6MZ	C4-N9-C1'	-8.54	106.24	126.59
1	1	2030	6MZ	C4-N9-C1'	-8.14	107.19	126.59
1	1	2030	6MZ	C1'-N9-C8	8.01	145.22	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2030	6MZ	C5-C4-N3	-6.85	117.81	126.75
1	1	1618	6MZ	C5-C4-N3	-6.58	118.17	126.75
1	1	2503	2MA	C1'-N9-C8	-6.58	112.28	127.14
2	2	1518	MA6	C5-C6-N6	6.40	136.44	125.30
2	2	1519	MA6	C5-C6-N6	6.34	136.34	125.30
1	1	745	1MG	C1'-N9-C4	-6.18	108.15	126.50
1	1	1835	2MG	C2-N3-C4	6.13	119.64	112.04
1	1	2069	G7M	CN7-N7-C5	6.10	134.35	126.77
2	2	966	2MG	C2-N3-C4	6.02	119.50	112.04
1	1	2030	6MZ	C4-C5-C6	5.99	121.45	116.81
2	2	1516	2MG	C2-N3-C4	5.83	119.27	112.04
2	2	1207	2MG	C2-N3-C4	5.80	119.23	112.04
54	z	42	5MU	O4-C4-C5	-5.79	118.19	124.90
1	1	2503	2MA	N9-C8-N7	-5.75	106.04	113.91
1	1	745	1MG	C1'-N9-C8	5.75	143.05	126.70
54	z	8	5MU	O4-C4-C5	-5.67	118.33	124.90
2	2	527	G7M	CN7-N7-C5	5.59	133.72	126.77
2	2	1519	MA6	N1-C2-N3	-5.53	119.95	128.60
54	z	42	5MU	C4-N3-C2	-5.53	120.20	127.35
1	1	747	5MU	O4-C4-C5	-5.52	118.51	124.90
1	1	2445	2MG	C2-N3-C4	5.50	118.86	112.04
1	1	747	5MU	C4-N3-C2	-5.49	120.24	127.35
1	1	1835	2MG	C5-C4-N3	-5.45	119.62	128.46
1	1	2069	G7M	CN7-N7-C8	-5.42	116.47	124.84
54	z	76	5MU	C4-N3-C2	-5.40	120.36	127.35
2	2	966	2MG	C5-C4-N3	-5.38	119.73	128.46
2	2	1519	MA6	C5-C4-N3	-5.37	119.75	126.75
54	z	57	5MU	C4-N3-C2	-5.36	120.41	127.35
1	1	1939	5MU	C4-N3-C2	-5.35	120.43	127.35
1	1	2457	PSU	C4-N3-C2	-5.33	118.66	126.34
54	z	57	5MU	O4-C4-C5	-5.32	118.73	124.90
1	1	1618	6MZ	N1-C2-N3	-5.28	120.35	128.60
54	z	8	5MU	C4-N3-C2	-5.22	120.60	127.35
54	z	64	5MU	C4-N3-C2	-5.21	120.61	127.35
54	z	63	5MU	C4-N3-C2	-5.21	120.61	127.35
54	z	71	5MU	C4-N3-C2	-5.19	120.64	127.35
1	1	1939	5MU	O4-C4-C5	-5.18	118.90	124.90
1	1	745	1MG	C5-C4-N3	-5.12	120.15	128.46
2	2	1518	MA6	N1-C2-N3	-5.12	120.59	128.60
54	z	39	5MU	N3-C2-N1	5.11	121.68	114.89
1	1	2605	PSU	C4-N3-C2	-5.10	119.00	126.34
54	z	40	5MU	C4-N3-C2	-5.05	120.82	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1518	MA6	C5-C4-N3	-5.04	120.18	126.75
1	1	2030	6MZ	N3-C4-N9	4.99	135.31	127.08
1	1	2457	PSU	N1-C2-N3	4.98	120.77	115.13
54	z	39	5MU	C4-N3-C2	-4.97	120.92	127.35
54	z	20	5MU	C4-N3-C2	-4.96	120.93	127.35
54	z	55	5MU	C4-N3-C2	-4.96	120.93	127.35
54	z	76	5MU	N3-C2-N1	4.95	121.47	114.89
1	1	2580	PSU	C4-N3-C2	-4.91	119.26	126.34
1	1	955	PSU	C4-N3-C2	-4.91	119.27	126.34
1	1	1911	PSU	C4-N3-C2	-4.90	119.27	126.34
1	1	1915	3TD	N1-C2-N3	4.90	120.01	116.14
2	2	516	PSU	C4-N3-C2	-4.89	119.29	126.34
54	z	69	5MU	N3-C2-N1	4.88	121.37	114.89
54	z	64	5MU	N3-C2-N1	4.88	121.37	114.89
54	z	20	5MU	O4-C4-C5	-4.87	119.25	124.90
54	z	57	5MU	N3-C2-N1	4.87	121.35	114.89
1	1	2552	OMU	C4-N3-C2	-4.86	120.17	126.58
2	2	1516	2MG	C5-C4-N3	-4.85	120.59	128.46
54	z	71	5MU	N3-C2-N1	4.85	121.33	114.89
1	1	2605	PSU	N1-C2-N3	4.84	120.62	115.13
1	1	2504	PSU	C4-N3-C2	-4.83	119.38	126.34
1	1	1917	PSU	C4-N3-C2	-4.80	119.42	126.34
1	1	2580	PSU	N1-C2-N3	4.78	120.55	115.13
1	1	1939	5MU	N3-C2-N1	4.78	121.24	114.89
1	1	2445	2MG	C5-C4-N3	-4.78	120.70	128.46
1	1	746	PSU	C4-N3-C2	-4.77	119.46	126.34
54	z	40	5MU	N3-C2-N1	4.75	121.20	114.89
1	1	1939	5MU	C5M-C5-C6	-4.74	116.51	122.85
1	1	2503	2MA	C4-N9-C8	4.74	110.87	105.73
1	1	2251	OMG	C5-C4-N3	-4.72	120.80	128.46
54	z	20	5MU	C5M-C5-C4	4.71	123.95	118.77
1	1	747	5MU	N3-C2-N1	4.70	121.13	114.89
54	z	63	5MU	C5-C4-N3	4.70	119.32	115.31
2	2	1207	2MG	C5-C4-N3	-4.69	120.85	128.46
54	z	63	5MU	N3-C2-N1	4.68	121.10	114.89
54	z	76	5MU	C5-C4-N3	4.67	119.30	115.31
1	1	955	PSU	N1-C2-N3	4.67	120.42	115.13
1	1	1917	PSU	N1-C2-N3	4.66	120.42	115.13
54	z	42	5MU	N3-C2-N1	4.66	121.07	114.89
1	1	1911	PSU	N1-C2-N3	4.63	120.38	115.13
1	1	2030	6MZ	N1-C2-N3	-4.62	121.38	128.60
1	1	1939	5MU	C5M-C5-C4	4.62	123.85	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	527	G7M	CN7-N7-C8	-4.61	117.73	124.84
54	z	55	5MU	O4-C4-C5	-4.57	119.60	124.90
54	z	8	5MU	N3-C2-N1	4.57	120.95	114.89
54	z	69	5MU	C4-N3-C2	-4.56	121.44	127.35
1	1	1835	2MG	C2-N1-C6	-4.56	119.23	124.48
54	z	20	5MU	N3-C2-N1	4.54	120.91	114.89
1	1	746	PSU	N1-C2-N3	4.51	120.24	115.13
54	z	71	5MU	C5-C4-N3	4.49	119.14	115.31
2	2	1516	2MG	C2-N1-C6	-4.47	119.34	124.48
2	2	966	2MG	C2-N1-C6	-4.46	119.34	124.48
54	z	55	5MU	N3-C2-N1	4.40	120.73	114.89
1	1	2504	PSU	N1-C2-N3	4.40	120.11	115.13
2	2	1519	MA6	N9-C8-N7	-4.35	107.96	113.91
1	1	2503	2MA	C5-C4-N3	-4.34	122.31	127.19
1	1	2503	2MA	C4-N9-C1'	4.29	136.81	126.59
1	1	747	5MU	C5M-C5-C6	-4.27	117.14	122.85
54	z	64	5MU	C5-C4-N3	4.27	118.96	115.31
2	2	1207	2MG	C2-N1-C6	-4.26	119.57	124.48
2	2	527	G7M	C5-C4-N3	-4.25	120.00	128.15
2	2	516	PSU	N1-C2-N3	4.23	119.93	115.13
1	1	2445	2MG	C2-N1-C6	-4.23	119.62	124.48
1	1	1618	6MZ	N3-C4-N9	4.17	133.95	127.08
54	z	40	5MU	C5-C4-N3	4.15	118.85	115.31
54	z	63	5MU	C5-C6-N1	-4.15	119.07	123.34
2	2	527	G7M	C1'-N9-C8	-4.14	112.77	126.74
54	z	39	5MU	C5-C4-N3	4.13	118.83	115.31
2	2	527	G7M	C1'-N9-C4	4.12	138.73	126.50
2	2	1518	MA6	N9-C8-N7	-4.10	108.31	113.91
1	1	1915	3TD	C4-N3-C2	-4.01	120.26	124.61
1	1	1618	6MZ	C2-N3-C4	4.00	121.19	111.75
54	z	20	5MU	C5M-C5-C6	-3.98	117.53	122.85
1	1	747	5MU	C5M-C5-C4	3.95	123.11	118.77
2	2	527	G7M	C2-N3-C4	3.94	119.32	112.30
1	1	1618	6MZ	C4-C5-C6	3.94	119.86	116.81
54	z	76	5MU	O4-C4-C5	-3.93	120.34	124.90
54	z	55	5MU	C5M-C5-C4	3.91	123.07	118.77
54	z	8	5MU	C5M-C5-C4	3.87	123.02	118.77
54	z	69	5MU	C5-C4-N3	3.86	118.61	115.31
54	z	64	5MU	C5-C6-N1	-3.84	119.38	123.34
54	z	55	5MU	C5M-C5-C6	-3.84	117.72	122.85
54	z	64	5MU	O4-C4-C5	-3.84	120.45	124.90
54	z	76	5MU	C5-C6-N1	-3.82	119.41	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2552	OMU	N3-C2-N1	3.78	119.91	114.89
2	2	1518	MA6	C4-C5-C6	3.77	120.09	115.88
1	1	2030	6MZ	N9-C8-N7	-3.76	108.77	113.91
1	1	2069	G7M	C2-N3-C4	3.74	118.96	112.30
54	z	71	5MU	C5-C6-N1	-3.73	119.50	123.34
43	p	89	0TD	OD2-CG-CB	3.68	121.09	113.15
2	2	527	G7M	C5-C6-N1	3.67	119.46	111.79
54	z	71	5MU	O4-C4-C5	-3.66	120.65	124.90
54	z	40	5MU	O4-C4-C5	-3.65	120.67	124.90
2	2	1519	MA6	C2-N3-C4	3.65	120.38	111.75
1	1	2030	6MZ	C2-N3-C4	3.64	120.36	111.75
54	z	64	5MU	C2'-C1'-N1	-3.62	102.96	113.22
1	1	1618	6MZ	C5-C6-N1	3.60	122.03	118.20
54	z	39	5MU	O4-C4-C5	-3.58	120.75	124.90
54	z	42	5MU	C5M-C5-C6	-3.58	118.07	122.85
54	z	63	5MU	O4-C4-C5	-3.58	120.75	124.90
54	z	8	5MU	C5M-C5-C6	-3.56	118.10	122.85
1	1	2251	OMG	C2-N3-C4	3.56	118.63	112.30
2	2	1519	MA6	C4-C5-C6	3.50	119.80	115.88
2	2	527	G7M	O6-C6-C5	-3.49	120.18	128.06
2	2	1498	UR3	C4-N3-C2	-3.49	121.28	124.56
1	1	2069	G7M	C5-C6-N1	3.49	119.08	111.79
1	1	745	1MG	C2-N3-C4	3.41	119.64	111.98
1	1	1618	6MZ	N9-C8-N7	-3.41	109.26	113.91
1	1	745	1MG	N9-C4-N3	3.38	132.72	125.94
54	z	69	5MU	O4-C4-C5	-3.37	120.99	124.90
1	1	2580	PSU	O2-C2-N1	-3.35	119.10	122.79
2	2	966	2MG	N9-C4-N3	3.35	132.67	125.94
2	2	1518	MA6	N3-C4-N9	3.35	132.60	127.08
54	z	40	5MU	C5-C6-N1	-3.34	119.90	123.34
54	z	57	5MU	C5M-C5-C6	-3.34	118.39	122.85
2	2	1518	MA6	C2-N1-C6	3.32	119.58	111.75
2	2	1519	MA6	N3-C4-N9	3.30	132.52	127.08
1	1	2069	G7M	O6-C6-C5	-3.27	120.68	128.06
1	1	2069	G7M	C5-C4-N3	-3.27	121.89	128.15
2	2	527	G7M	N9-C4-N3	3.26	132.49	125.94
54	z	39	5MU	C5-C6-N1	-3.24	120.00	123.34
2	2	1518	MA6	C2-N3-C4	3.24	119.40	111.75
1	1	1835	2MG	N9-C4-N3	3.23	132.43	125.94
1	1	2503	2MA	C5-N7-C8	3.23	108.10	103.51
2	2	1519	MA6	C2-N1-C6	3.20	119.32	111.75
1	1	2251	OMG	C2-N1-C6	-3.19	119.27	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	64	5MU	C1'-N1-C2	3.19	123.34	117.57
1	1	1618	6MZ	C9-N6-C6	-3.18	120.13	122.87
1	1	2069	G7M	C1'-N9-C8	-3.16	116.06	126.74
1	1	2503	2MA	N3-C2-N1	-3.16	119.91	125.72
1	1	747	5MU	O2-C2-N1	-3.15	118.60	122.79
1	1	746	PSU	O2-C2-N1	-3.09	119.39	122.79
54	z	64	5MU	C1'-N1-C6	-3.08	116.00	121.12
2	2	527	G7M	C2-N1-C6	-3.08	119.49	125.10
54	z	39	5MU	C1'-N1-C2	3.03	123.06	117.57
1	1	2251	OMG	N9-C8-N7	-3.02	107.71	113.39
1	1	2030	6MZ	C5-N7-C8	2.95	107.69	103.51
1	1	745	1MG	N9-C8-N7	-2.94	107.85	113.39
1	1	1962	5MC	C5-C6-N1	-2.94	120.31	123.34
2	2	1407	5MC	C5-C6-N1	-2.93	120.33	123.34
1	1	2552	OMU	C5-C4-N3	2.92	119.21	114.84
1	1	1917	PSU	O2-C2-N1	-2.91	119.59	122.79
2	2	1207	2MG	C1'-N9-C4	-2.88	117.95	126.50
1	1	955	PSU	C6-C5-C4	2.87	120.21	118.20
1	1	2503	2MA	N3-C4-N9	2.85	130.95	126.99
54	z	8	5MU	O2-C2-N1	-2.84	119.01	122.79
2	2	1207	2MG	N9-C8-N7	-2.84	108.05	113.39
54	z	40	5MU	O4'-C1'-N1	2.82	114.82	108.36
54	z	69	5MU	C5-C6-N1	-2.82	120.43	123.34
54	z	55	5MU	O4-C4-N3	-2.80	114.75	120.12
2	2	1519	MA6	C5-N7-C8	2.79	107.47	103.51
54	z	20	5MU	O4-C4-N3	-2.78	114.78	120.12
1	1	2503	2MA	CM2-C2-N1	2.78	121.49	117.15
1	1	1911	PSU	O2-C2-N1	-2.78	119.73	122.79
54	z	40	5MU	C1'-N1-C2	2.77	122.59	117.57
54	z	40	5MU	C5M-C5-C4	2.77	121.81	118.77
1	1	2605	PSU	C6-C5-C4	2.77	120.13	118.20
54	z	42	5MU	C5M-C5-C4	2.76	121.80	118.77
1	1	2069	G7M	C1'-N9-C4	2.75	134.68	126.50
1	1	2445	2MG	CM2-N2-C2	-2.75	117.79	123.86
54	z	20	5MU	O2-C2-N1	-2.74	119.15	122.79
54	z	57	5MU	C5M-C5-C4	2.72	121.77	118.77
1	1	2504	PSU	O2-C2-N1	-2.72	119.79	122.79
1	1	2069	G7M	C2-N1-C6	-2.71	120.15	125.10
1	1	1939	5MU	O2-C2-N1	-2.71	119.18	122.79
1	1	1618	6MZ	C5-N7-C8	2.71	107.36	103.51
2	2	1516	2MG	N9-C8-N7	-2.70	108.30	113.39
1	1	2030	6MZ	C6-C5-N7	-2.70	129.47	132.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2445	2MG	N9-C4-N3	2.70	131.35	125.94
54	z	40	5MU	C2'-C1'-N1	-2.66	105.67	113.22
1	1	2457	PSU	O2-C2-N1	-2.66	119.86	122.79
1	1	2445	2MG	N9-C8-N7	-2.65	108.40	113.39
54	z	40	5MU	C1'-N1-C6	-2.63	116.75	121.12
2	2	966	2MG	N9-C8-N7	-2.60	108.49	113.39
1	1	2030	6MZ	C5-C6-N1	2.59	120.96	118.20
54	z	55	5MU	O2-C2-N1	-2.59	119.35	122.79
2	2	966	2MG	C5-C6-N1	2.58	119.75	113.19
2	2	1518	MA6	C5-N7-C8	2.58	107.17	103.51
54	z	42	5MU	O2-C2-N1	-2.58	119.36	122.79
2	2	967	5MC	C5-C6-N1	-2.58	120.69	123.34
1	1	2251	OMG	N9-C4-N3	2.57	131.09	125.94
1	1	1835	2MG	CM2-N2-C2	-2.55	118.23	123.86
2	2	516	PSU	O2-C2-N1	-2.55	119.99	122.79
1	1	1835	2MG	C5-C6-N1	2.54	119.65	113.19
2	2	1207	2MG	C5-C6-N1	2.53	119.62	113.19
2	2	1207	2MG	C1'-N9-C8	2.53	133.89	126.70
2	2	1207	2MG	CM2-N2-C2	-2.52	118.29	123.86
1	1	2552	OMU	O4-C4-C5	-2.52	120.73	125.16
1	1	2605	PSU	O2-C2-N1	-2.52	120.02	122.79
54	z	42	5MU	C6-C5-C4	2.51	120.13	118.03
54	z	39	5MU	O4'-C1'-N1	2.51	114.11	108.36
2	2	1516	2MG	N9-C4-N3	2.50	130.96	125.94
2	2	967	5MC	CM5-C5-C6	-2.50	119.51	122.85
54	z	64	5MU	O4'-C1'-N1	2.49	114.05	108.36
2	2	1516	2MG	C1'-N9-C4	-2.48	119.12	126.50
2	2	1207	2MG	N9-C4-N3	2.48	130.91	125.94
54	z	39	5MU	C1'-N1-C6	-2.46	117.03	121.12
1	1	2069	G7M	N2-C2-N1	2.45	121.92	116.71
2	2	1519	MA6	C4-N9-C8	2.44	108.37	105.73
54	z	40	5MU	C5M-C5-C6	-2.44	119.60	122.85
2	2	1516	2MG	C5-C6-N1	2.43	119.37	113.19
2	2	1518	MA6	C4-N9-C8	2.42	108.36	105.73
1	1	2251	OMG	C5-C6-N1	2.42	119.33	113.19
2	2	966	2MG	O6-C6-C5	-2.41	120.20	126.60
1	1	1835	2MG	N9-C8-N7	-2.41	108.85	113.39
1	1	2445	2MG	C5-C6-N1	2.41	119.30	113.19
54	z	57	5MU	O2-C2-N1	-2.40	119.59	122.79
1	1	2445	2MG	O6-C6-C5	-2.40	120.23	126.60
1	1	2030	6MZ	C9-N6-C6	-2.40	120.80	122.87
1	1	2504	PSU	C6-C5-C4	2.40	119.88	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1516	2MG	CM2-N2-C2	-2.40	118.56	123.86
1	1	1939	5MU	O4-C4-N3	-2.40	115.52	120.12
1	1	1917	PSU	C6-C5-C4	2.38	119.86	118.20
54	z	57	5MU	O4-C4-N3	-2.37	115.57	120.12
1	1	745	1MG	C5-C6-N1	2.37	119.48	114.91
2	2	1516	2MG	O6-C6-C5	-2.37	120.33	126.60
1	1	955	PSU	O2-C2-N1	-2.35	120.20	122.79
54	z	8	5MU	C1'-N1-C2	2.35	121.82	117.57
54	z	8	5MU	O4-C4-N3	-2.35	115.62	120.12
2	2	1207	2MG	O6-C6-C5	-2.35	120.38	126.60
54	z	63	5MU	C3'-C2'-C1'	2.33	105.85	101.43
1	1	2069	G7M	N9-C8-N7	-2.32	106.46	112.21
1	1	747	5MU	O4-C4-N3	-2.30	115.71	120.12
1	1	2580	PSU	O4'-C1'-C2'	2.29	108.37	105.14
1	1	1835	2MG	O6-C6-C5	-2.29	120.53	126.60
43	p	89	0TD	OD1-CG-CB	-2.28	117.66	122.44
54	z	69	5MU	C1'-N1-C2	2.27	121.67	117.57
54	z	63	5MU	C5M-C5-C4	2.26	121.25	118.77
54	z	76	5MU	O2-C2-N1	-2.25	119.79	122.79
54	z	64	5MU	O2-C2-N3	-2.25	117.31	121.50
1	1	2457	PSU	O4'-C1'-C2'	2.24	108.30	105.14
1	1	2445	2MG	C1'-N9-C4	-2.24	119.86	126.50
2	2	1516	2MG	C1'-N9-C8	2.23	133.05	126.70
54	z	39	5MU	O2-C2-N3	-2.22	117.36	121.50
1	1	2251	OMG	O6-C6-C5	-2.21	120.73	126.60
54	z	71	5MU	O2-C2-N1	-2.21	119.85	122.79
54	z	63	5MU	O2-C2-N1	-2.19	119.87	122.79
1	1	2457	PSU	C6-N1-C2	-2.19	120.44	122.68
1	1	746	PSU	C6-N1-C2	-2.19	120.45	122.68
1	1	1962	5MC	C5-C4-N4	-2.18	118.22	121.48
54	z	71	5MU	C5M-C5-C4	2.18	121.17	118.77
1	1	1917	PSU	C6-N1-C2	-2.18	120.46	122.68
54	z	57	5MU	C6-C5-C4	2.17	119.84	118.03
1	1	2580	PSU	C6-N1-C2	-2.15	120.49	122.68
1	1	955	PSU	C6-N1-C2	-2.14	120.49	122.68
1	1	1962	5MC	CM5-C5-C6	-2.14	120.00	122.85
1	1	1911	PSU	C6-N1-C2	-2.12	120.51	122.68
2	2	1498	UR3	C1'-N1-C2	2.12	120.57	116.99
54	z	42	5MU	O4-C4-N3	-2.12	116.06	120.12
1	1	2605	PSU	C6-N1-C2	-2.09	120.55	122.68
2	2	516	PSU	O4'-C1'-C2'	2.08	108.08	105.14
54	z	40	5MU	O2-C2-N1	-2.07	120.03	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	69	5MU	O2-C2-N3	-2.07	117.64	121.50
1	1	2552	OMU	O2-C2-N1	-2.07	120.03	122.79
1	1	747	5MU	C6-C5-C4	2.05	119.75	118.03
1	1	1911	PSU	C6-C5-C4	2.04	119.62	118.20
54	z	20	5MU	C1'-N1-C2	2.03	121.25	117.57
54	z	71	5MU	C2'-C1'-N1	-2.02	107.50	113.22
1	1	2580	PSU	C6-C5-C4	2.01	119.61	118.20
1	1	2251	OMG	C8-N7-C5	2.00	107.86	104.24
54	z	76	5MU	C5M-C5-C4	2.00	120.97	118.77

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	C2'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
54	z	8	5MU	O4'-C4'-C5'-O5'
54	z	39	5MU	O4'-C1'-N1-C2
54	z	39	5MU	O4'-C1'-N1-C6
54	z	40	5MU	O4'-C1'-N1-C2
54	z	40	5MU	O4'-C1'-N1-C6
54	z	64	5MU	O4'-C1'-N1-C2
54	z	64	5MU	O4'-C1'-N1-C6
54	z	69	5MU	C2'-C1'-N1-C2
54	z	69	5MU	C3'-C4'-C5'-O5'
54	z	69	5MU	C2'-C1'-N1-C6
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
54	z	8	5MU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	2503	2MA	O4'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
54	z	69	5MU	O4'-C4'-C5'-O5'
54	z	71	5MU	C3'-C4'-C5'-O5'
54	z	71	5MU	O4'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'
54	z	64	5MU	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
1	1	2503	2MA	C3'-C4'-C5'-O5'
43	p	89	0TD	CG-CB-SB-CSB
2	2	527	G7M	C4'-C5'-O5'-P
43	p	89	0TD	SB-CB-CG-OD1
54	z	64	5MU	O4'-C4'-C5'-O5'
54	z	71	5MU	C4'-C5'-O5'-P
1	1	2069	G7M	O4'-C4'-C5'-O5'
54	z	39	5MU	O4'-C4'-C5'-O5'
54	z	20	5MU	C2'-C1'-N1-C6
2	2	1402	4OC	C3'-C4'-C5'-O5'
54	z	69	5MU	O4'-C1'-N1-C6
1	1	746	PSU	O4'-C1'-C5-C6
54	z	20	5MU	C2'-C1'-N1-C2

There are no ring outliers.

28 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1915	3TD	2	0
54	z	76	5MU	1	0
54	z	64	5MU	1	0
1	1	2503	2MA	1	0
1	1	1939	5MU	1	0
2	2	1407	5MC	1	0
1	1	2552	OMU	1	0
43	p	89	0TD	1	0
1	1	2504	PSU	1	0
1	1	2498	OMC	1	0
54	z	39	5MU	2	0
54	z	69	5MU	6	0
2	2	1498	UR3	1	0
2	2	1516	2MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	z	71	5MU	4	0
54	z	55	5MU	1	0
1	1	955	PSU	1	0
2	2	1519	MA6	2	0
54	z	20	5MU	4	0
1	1	2445	2MG	1	0
54	z	40	5MU	1	0
1	1	2580	PSU	1	0
2	2	516	PSU	2	0
54	z	57	5MU	1	0
1	1	2030	6MZ	2	0
1	1	1618	6MZ	1	0
1	1	1962	5MC	2	0
2	2	1518	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 396 ligands modelled in this entry, 396 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

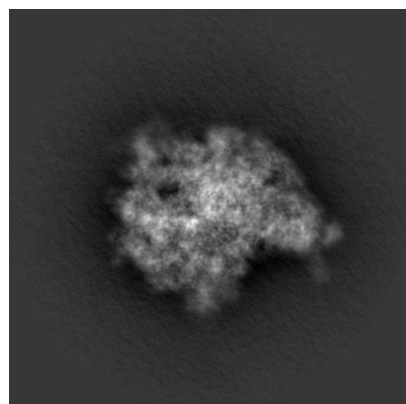
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13055. These allow visual inspection of the internal detail of the map and identification of artifacts.

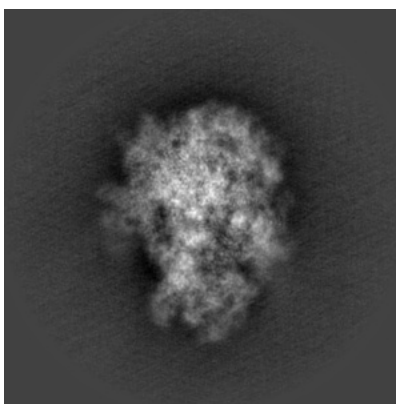
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

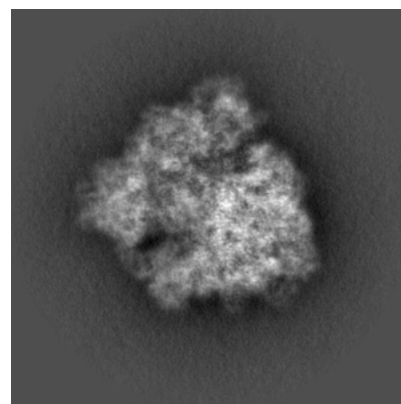
6.1.1 Primary map



X

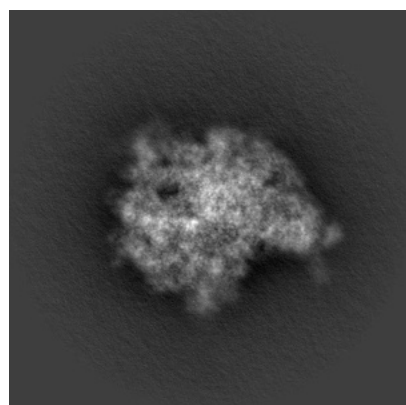


Y

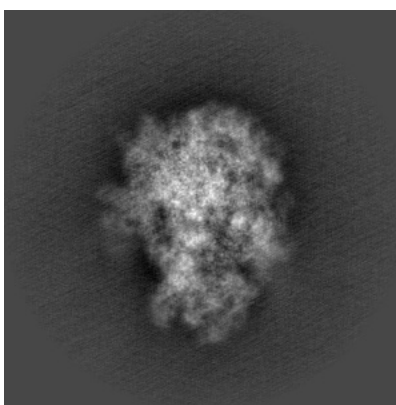


Z

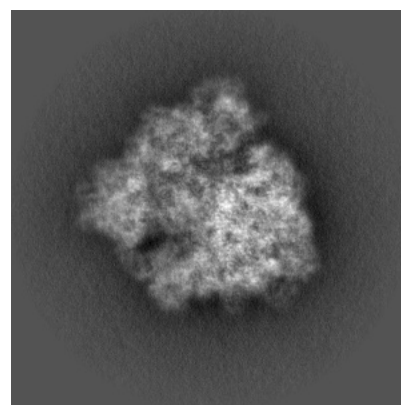
6.1.2 Raw map



X



Y

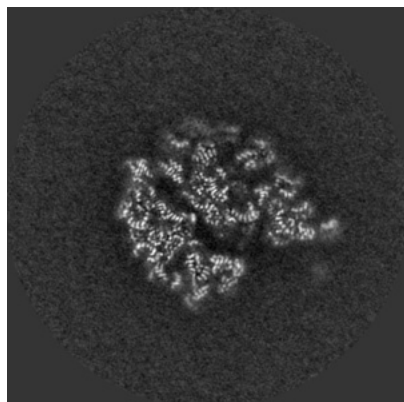


Z

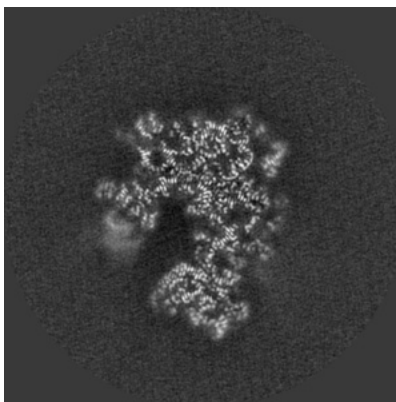
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

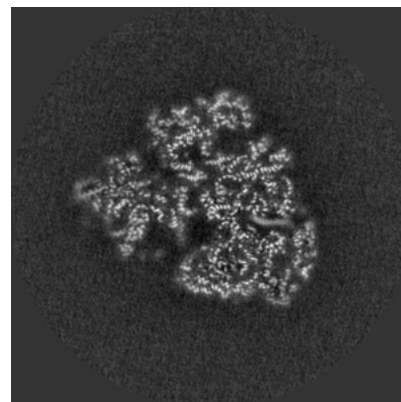
6.2.1 Primary map



X Index: 200

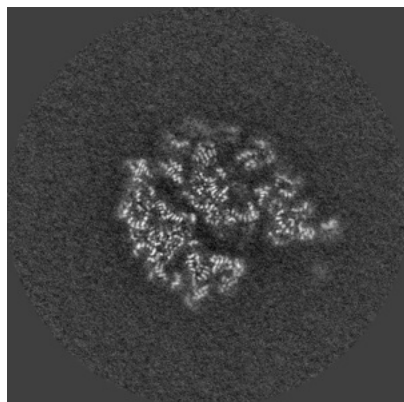


Y Index: 200

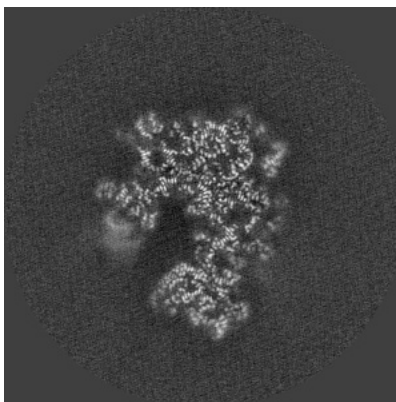


Z Index: 200

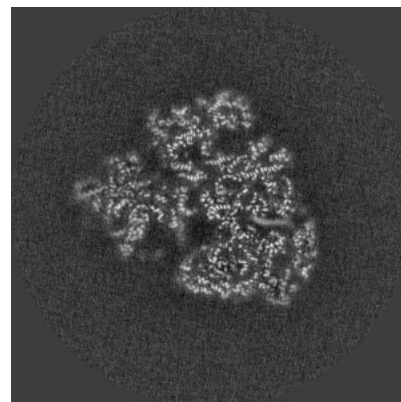
6.2.2 Raw map



X Index: 200



Y Index: 200

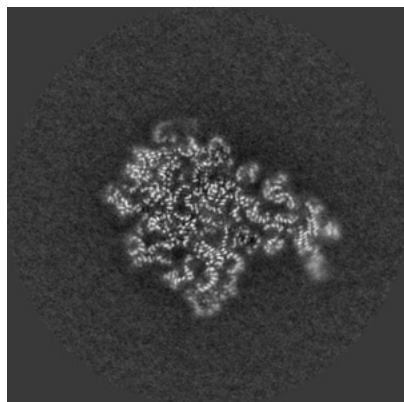


Z Index: 200

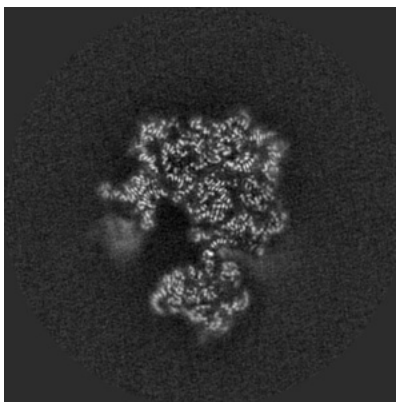
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

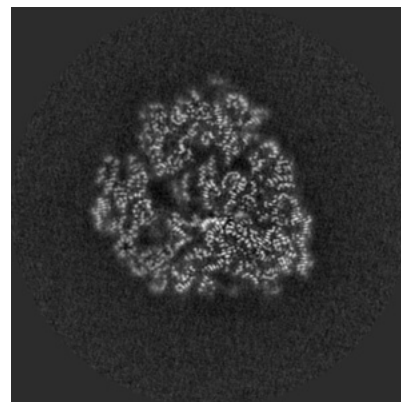
6.3.1 Primary map



X Index: 216

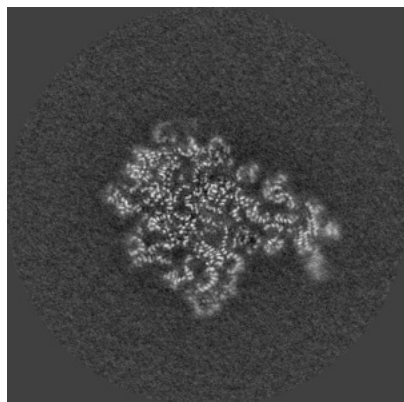


Y Index: 206

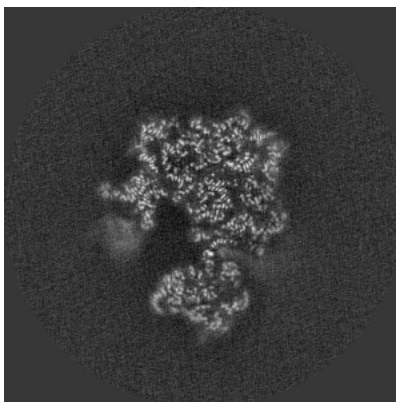


Z Index: 188

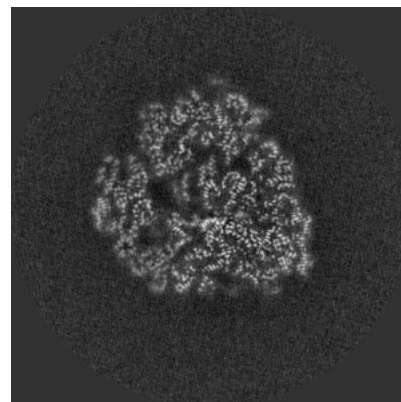
6.3.2 Raw map



X Index: 216



Y Index: 206

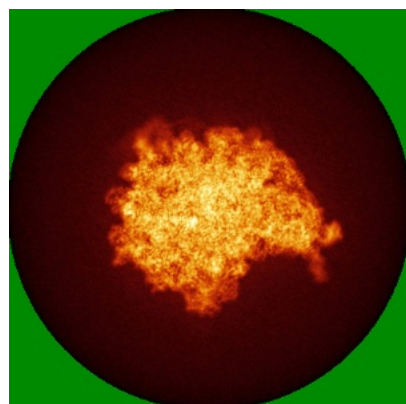


Z Index: 188

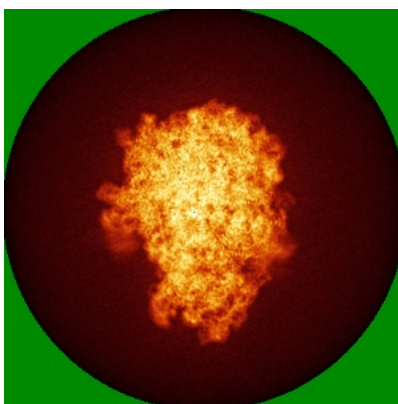
The images above show the largest variance slices of the map in three orthogonal directions.

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

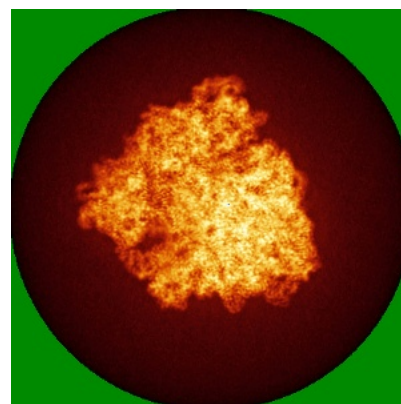
6.4.1 Primary map



X

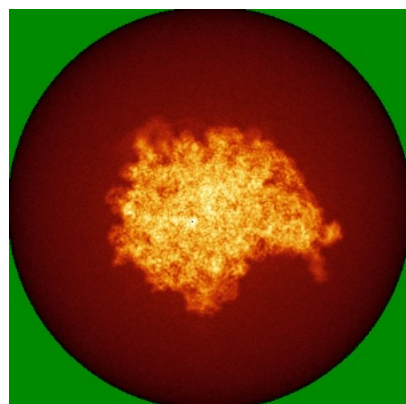


Y

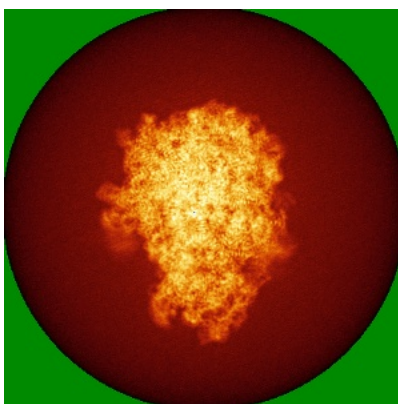


Z

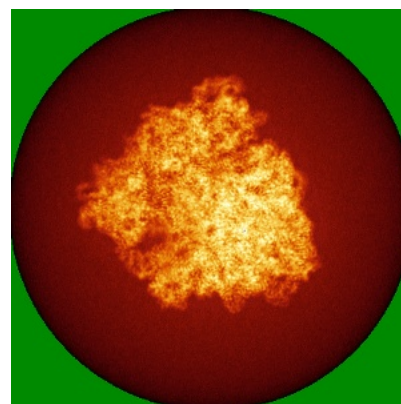
6.4.2 Raw map



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



X



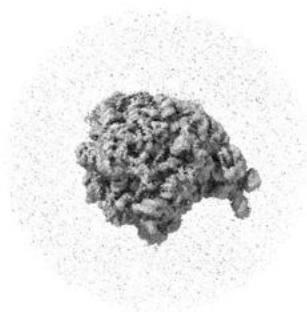
Y



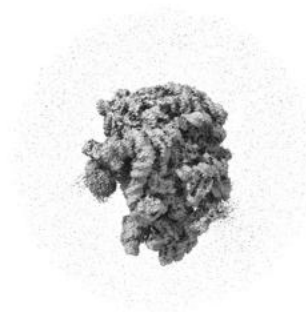
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

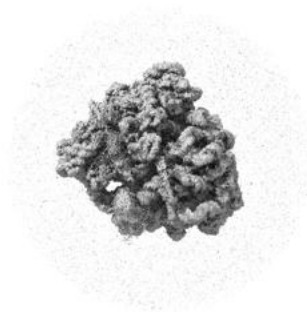
6.5.2 Raw map



X



Y



Z

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.

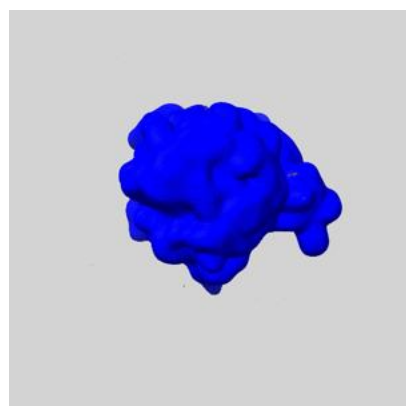
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

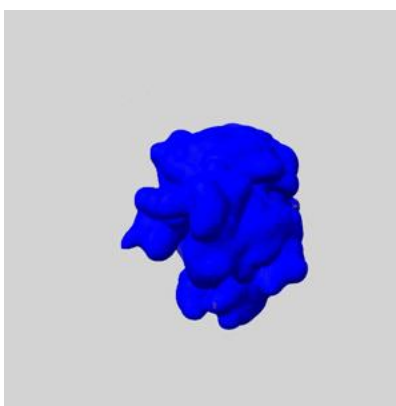
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

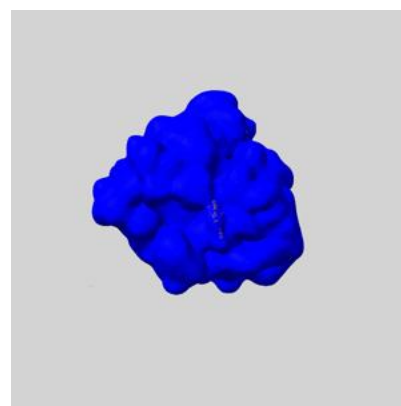
6.6.1 emd_13055_msk_1.map [i](#)



X



Y

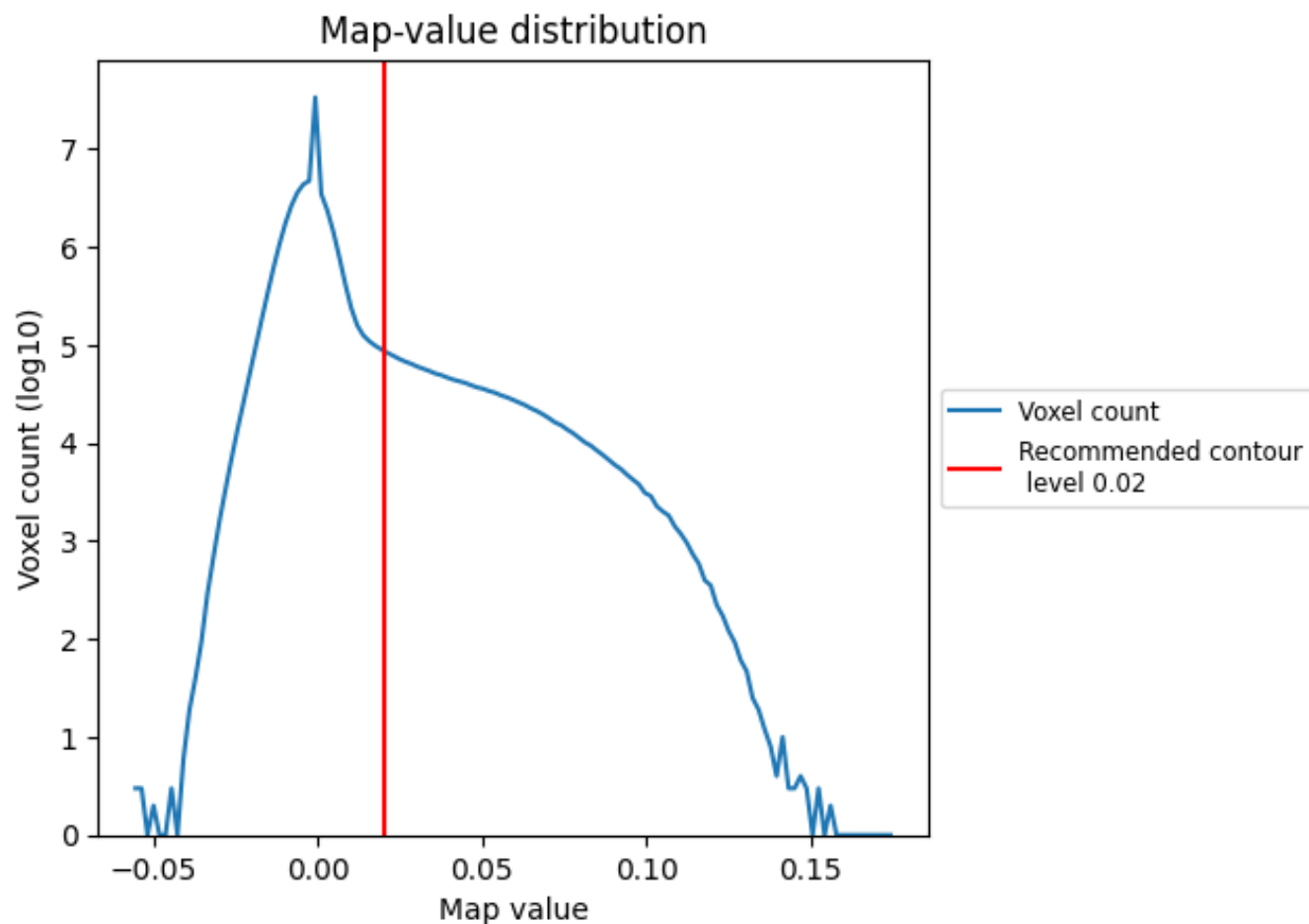


Z

7 Map analysis [i](#)

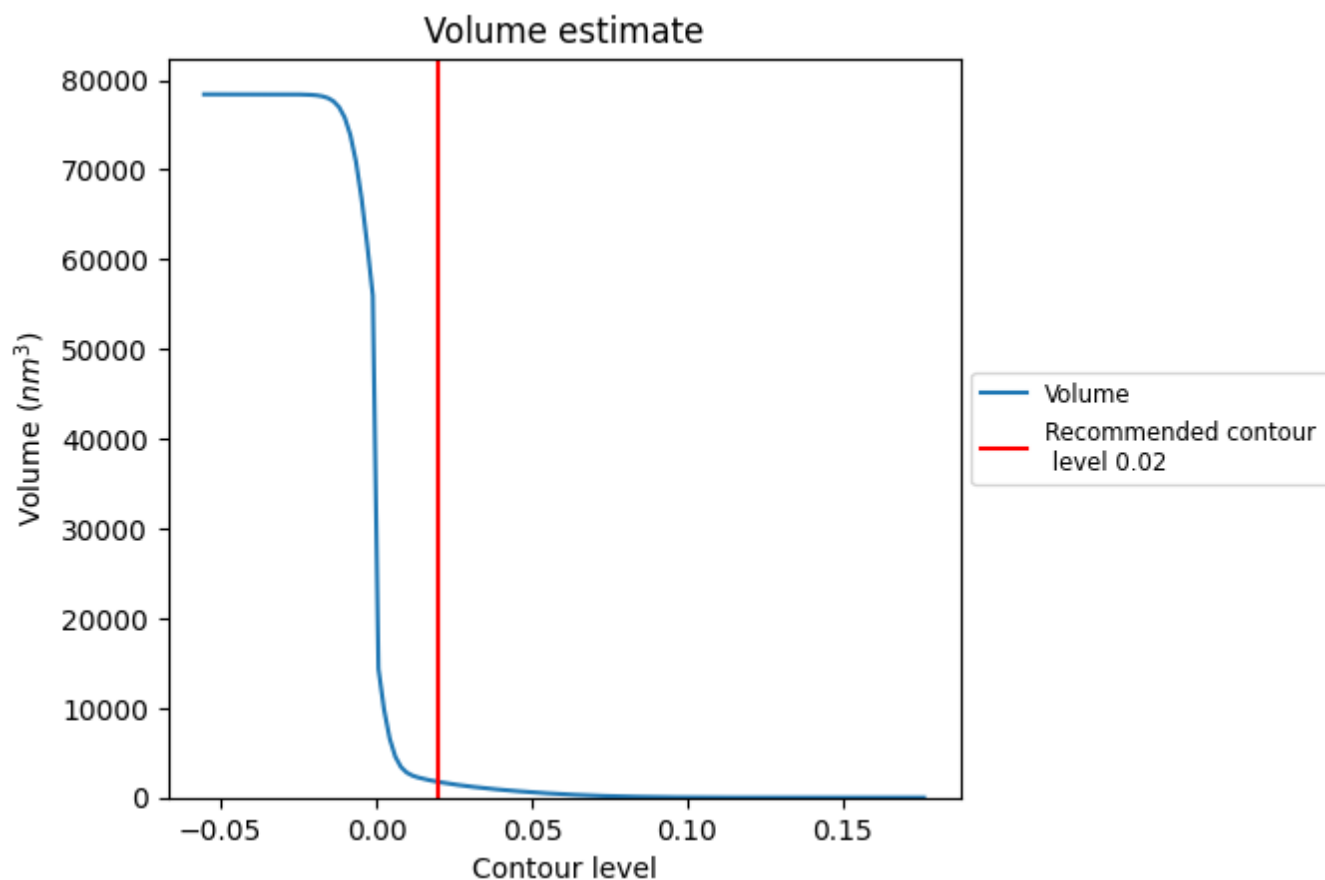
This section contains the results of statistical analysis of the map.

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.

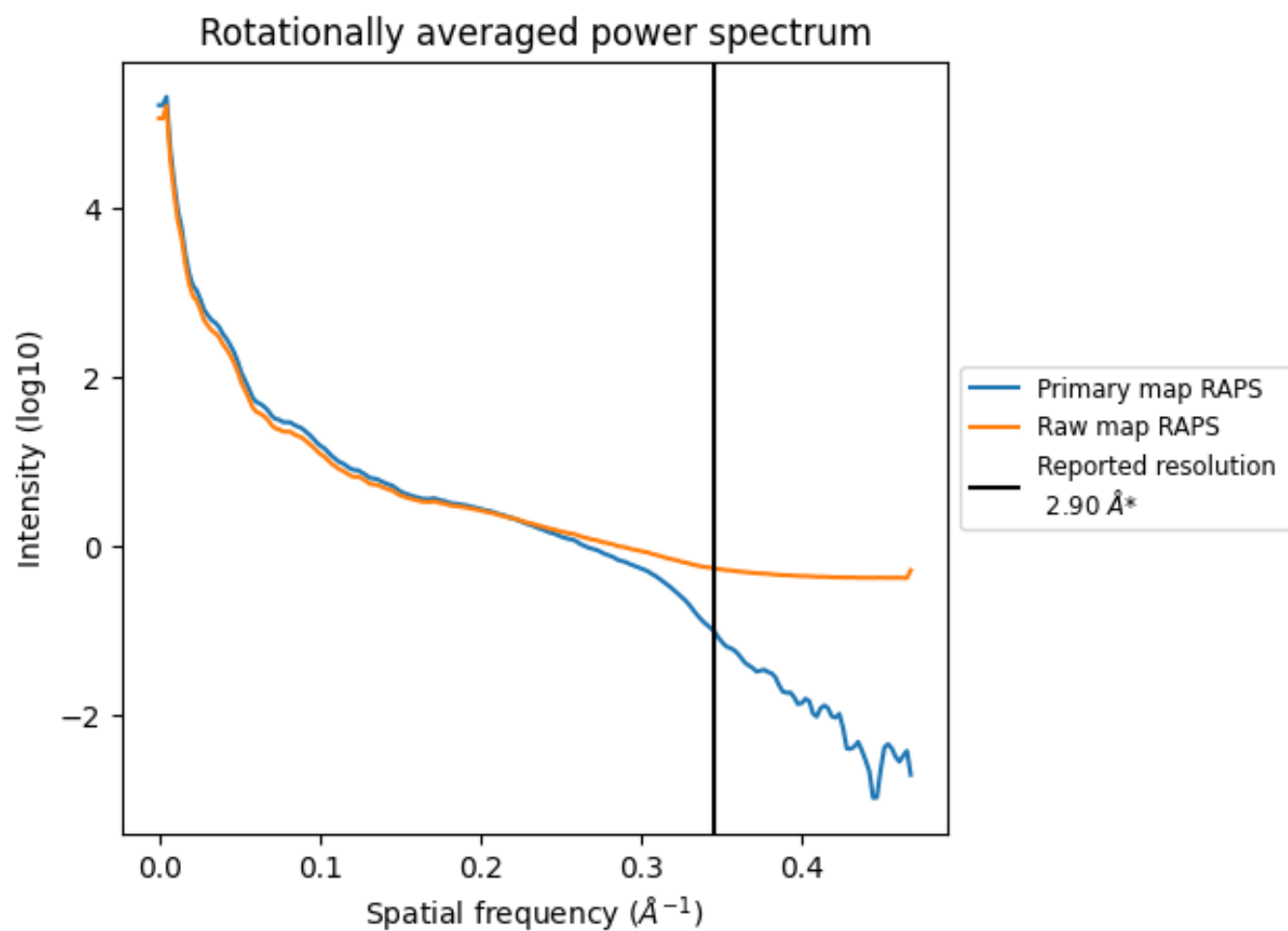
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1746 nm^3 ; this corresponds to an approximate mass of 1577 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 ⓘ

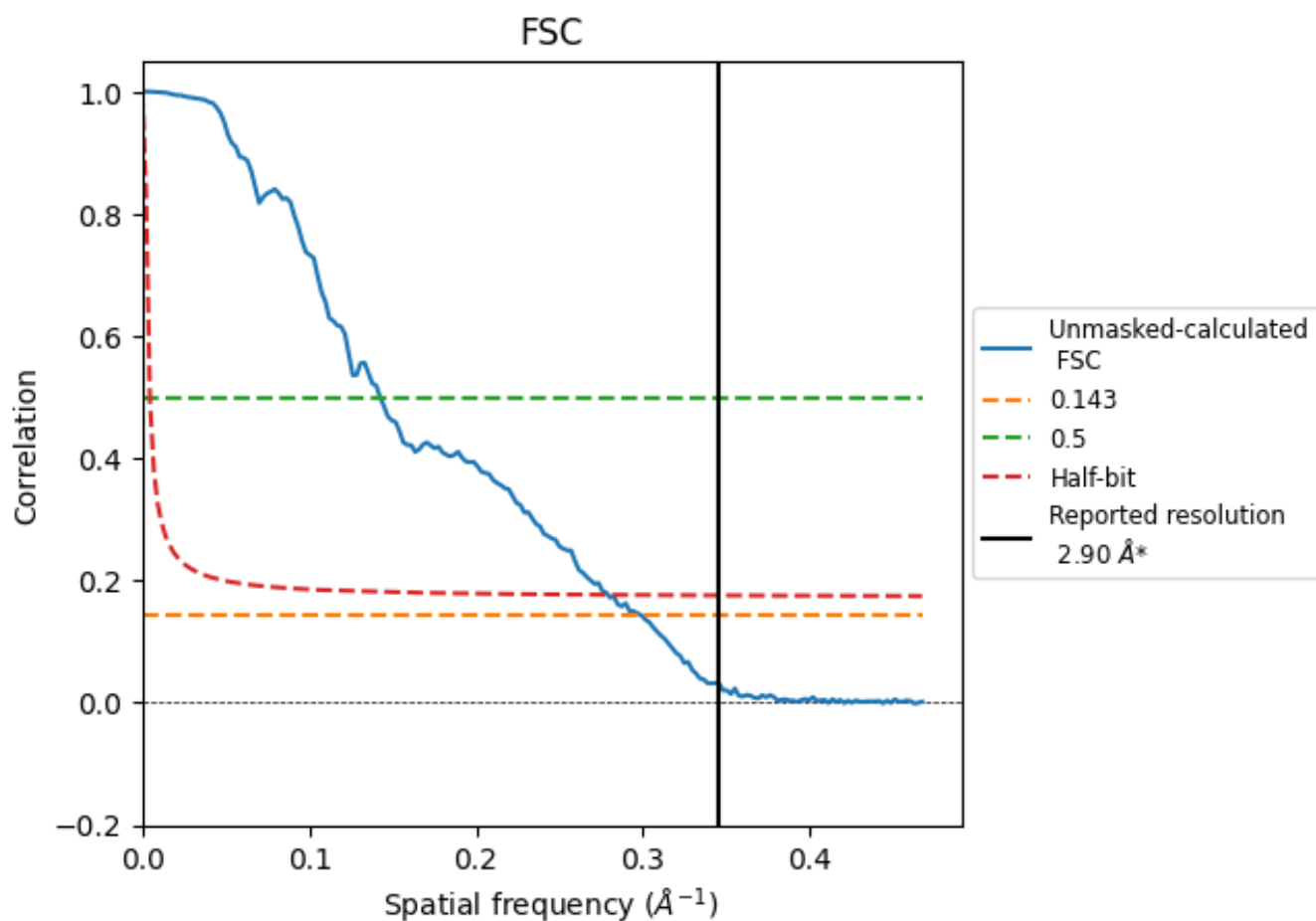


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

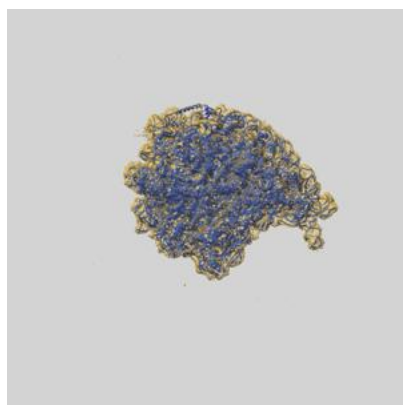
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	7.01	3.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.34 differs from the reported value 2.9 by more than 10 %

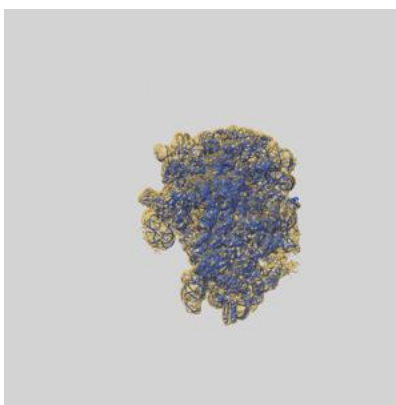
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13055 and PDB model 7OT5. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

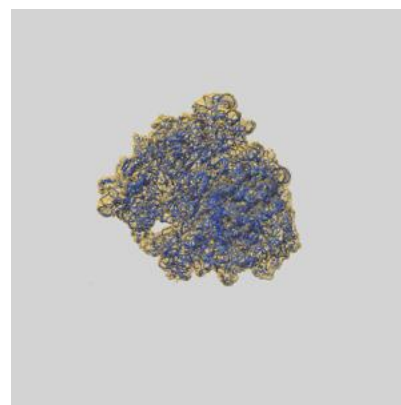
9.1 Map-model overlay [i](#)



X



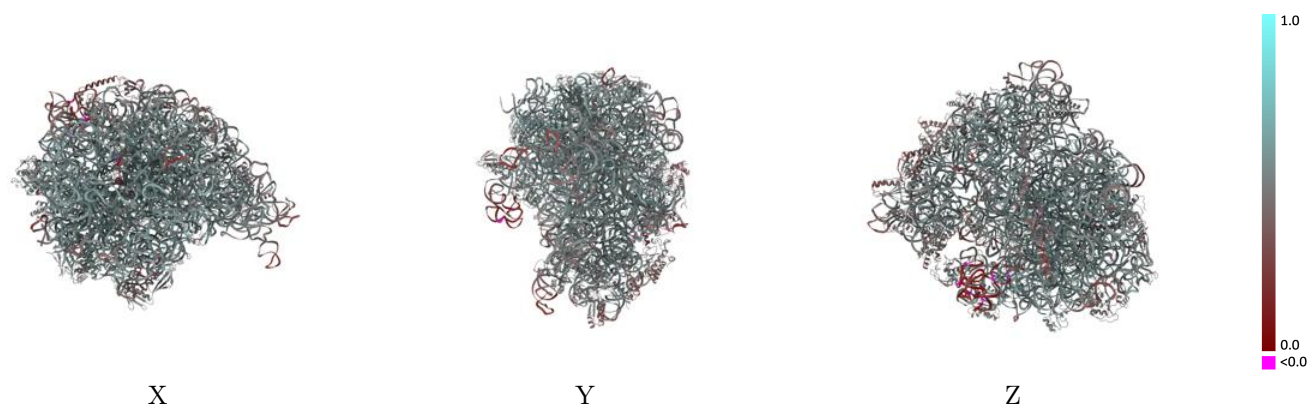
Y



Z

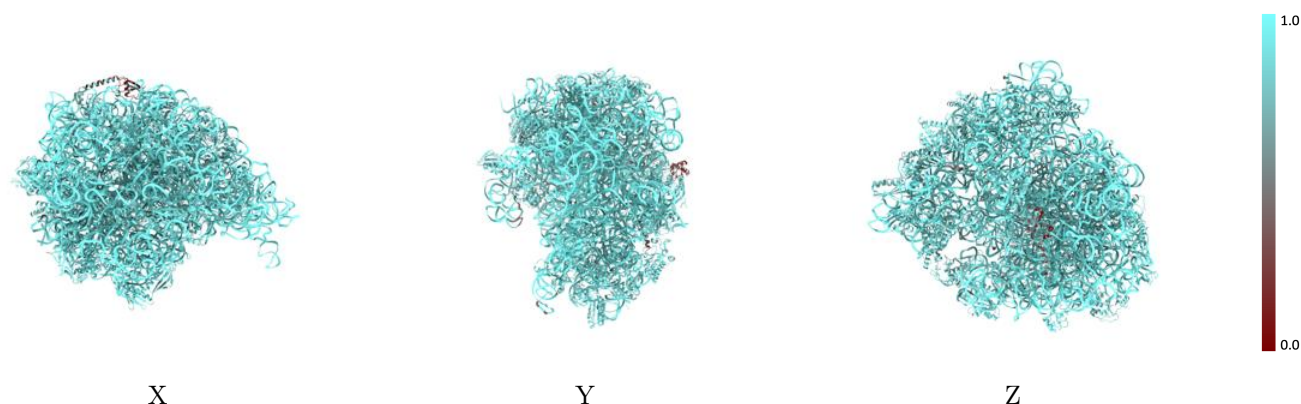
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



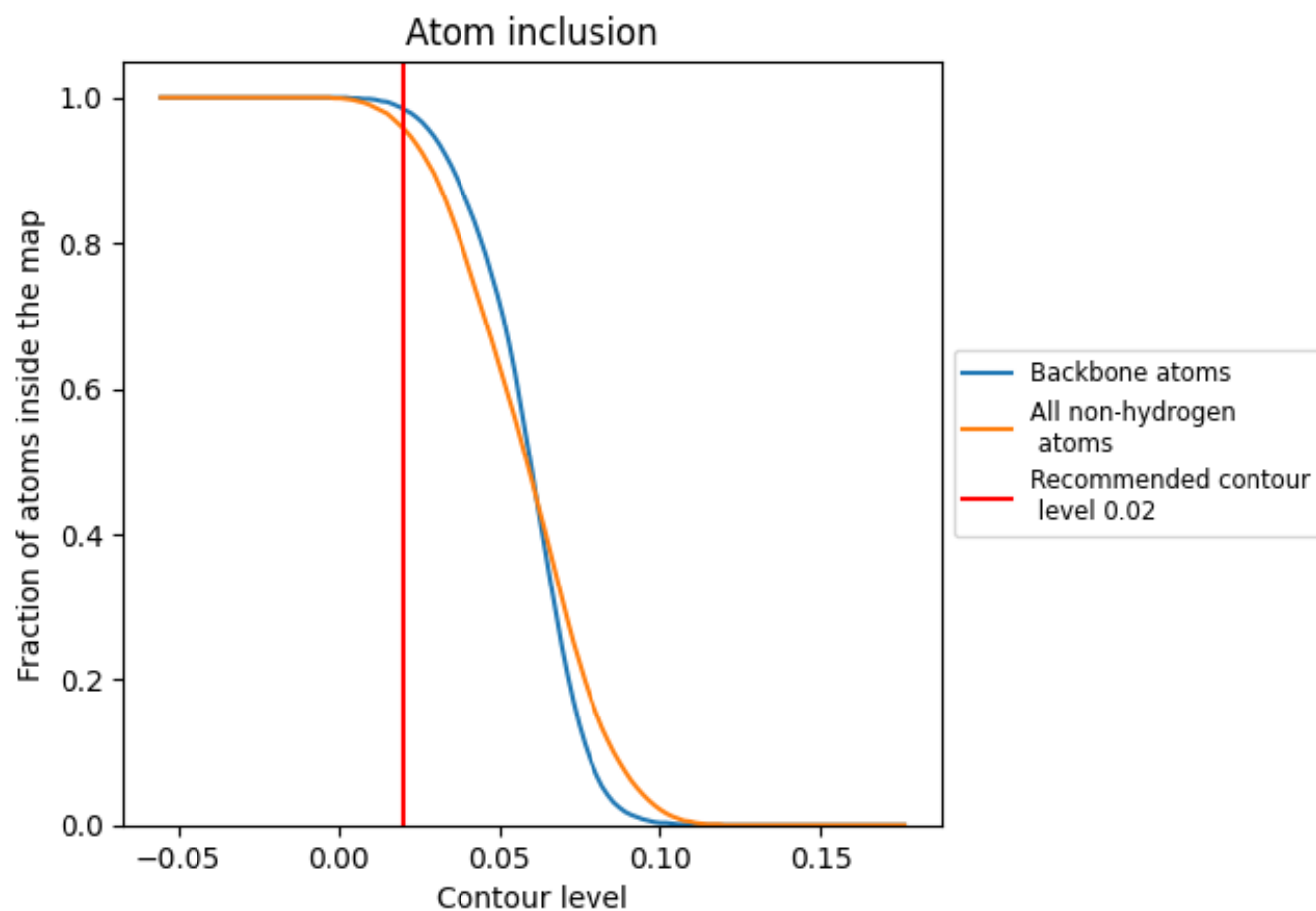
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.5150
1	 0.9880	 0.5290
2	 0.9940	 0.5210
3	 0.9970	 0.5180
4	 1.0000	 0.5110
B	 0.7870	 0.2210
C	 0.9090	 0.5600
D	 0.9260	 0.5480
E	 0.9180	 0.5130
F	 0.8940	 0.4580
G	 0.9210	 0.4640
H	 0.4720	 0.3550
I	 0.9140	 0.5370
J	 0.8720	 0.5360
K	 0.9160	 0.5330
L	 0.8930	 0.5340
M	 0.9430	 0.5470
N	 0.9320	 0.4880
O	 0.9030	 0.5330
P	 0.9350	 0.5340
Q	 0.9270	 0.5290
R	 0.8890	 0.5230
S	 0.8750	 0.5100
T	 0.9160	 0.5060
U	 0.9130	 0.5130
V	 0.8840	 0.5480
W	 0.9080	 0.5320
X	 0.8790	 0.4560
Y	 0.9010	 0.5240
Z	 0.8710	 0.4060
a	 0.8880	 0.5340
b	 0.8470	 0.5070
c	 0.8930	 0.5690
d	 0.9230	 0.5690
e	 0.9040	 0.5310



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Chain	Atom inclusion	Q-score
f	 0.8460	 0.4240
g	 0.8930	 0.4770
h	 0.9060	 0.4780
i	 0.9050	 0.5160
j	 0.9030	 0.4690
k	 0.8620	 0.4420
l	 0.9010	 0.5080
m	 0.9110	 0.4710
n	 0.8540	 0.4370
o	 0.9050	 0.4830
p	 0.8700	 0.5220
q	 0.9060	 0.4610
r	 0.9160	 0.4880
s	 0.9040	 0.4780
t	 0.9220	 0.4930
u	 0.8720	 0.4880
v	 0.9010	 0.4870
w	 0.9290	 0.4750
x	 0.9050	 0.4740
y	 0.7370	 0.4060
z	 0.9560	 0.4630