Full wwPDB EM Validation Report

Jun 18, 2026 – 03:03 pm BST

PDB ID	:	7OIG / pdb_00007oig
EMDB ID	:	EMD-12929
Title	:	CspA-27 cotranslational folding intermediate 3
Authors	:	Agirrezabala, X.; Samatova, E.; Macher, M.; Liutkute, M.; Gil-Carton, D.; Novacek, J.; Valle, M.; Rodnina, M.V.
Deposited on	:	2021-05-11
Resolution	:	3.20 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 (i) 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 (1)) were used in the production of this report:

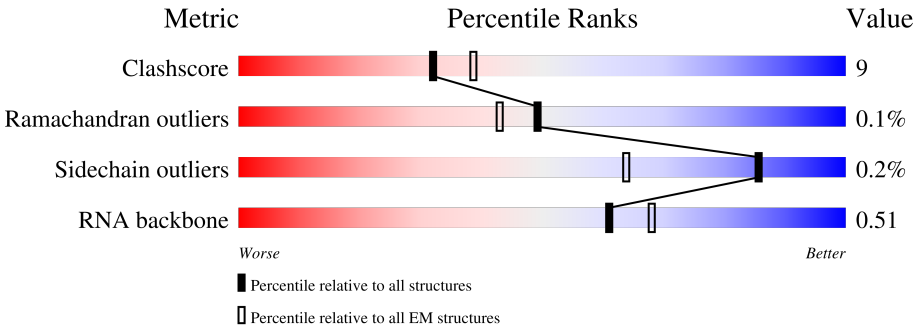
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal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

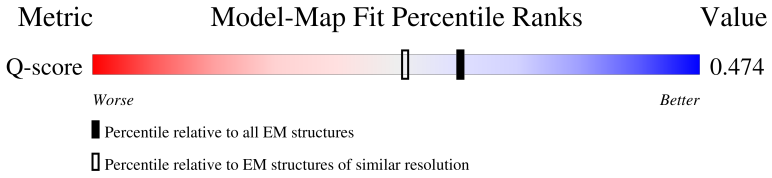
1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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 <=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	61% 31% 7%
2	2	1534	59% 34% 6%
3	3	120	72% 21% 7%

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Mol	Chain	Length	Quality of chain
4	4	6	67% 17% 17%
5	C	271	79% 21%
6	D	209	86% 12%
7	E	201	83% 16%
8	F	177	68% 32%
9	G	175	81% 19%
10	H	149	52% 61% 38%
11	I	142	85% 15%
12	J	123	85% 15%
13	K	144	84% 16%
14	L	136	83% 17%
15	M	119	81% 19%
16	N	116	79% 20%
17	O	114	87% 13%
18	P	117	79% 20%
19	Q	103	85% 13%
20	R	110	82% 18%
21	S	94	77% 23%
22	T	103	77% 23%
23	U	94	79% 21%
24	V	80	72% 28%
25	W	77	86% 14%
26	X	62	71% 29%
27	Y	58	79% 21%
28	Z	66	64% 36%

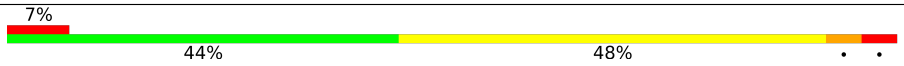
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Mol	Chain	Length	Quality of chain
29	a	56	64% 36%
30	b	52	88% 12%
31	c	46	72% 28%
32	d	64	81% 19%
33	e	38	87% 13%
34	f	225	72% 28%
35	g	208	75% 25%
36	h	205	79% 21%
37	i	156	69% 31%
38	j	104	63% 37%
39	k	151	70% 30%
40	l	129	74% 26%
41	m	127	72% 28%
42	n	99	63% 37%
43	o	117	72% 28%
44	p	123	75% 24%
45	q	116	73% 27%
46	r	100	75% 25%
47	s	88	80% 20%
48	t	82	76% 24%
49	u	80	71% 29%
50	v	66	88% 12%
51	w	83	72% 28%
52	x	86	81% 19%
53	y	70	6% 81% 17%

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Mol	Chain	Length	Quality of chain
54	z	88	
55	B	27	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145136 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
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

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

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

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

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

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	6	126	56	20	44	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

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

- Molecule 22 is a protein called 50S ribosomal protein L24.

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

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	80	Total	C	N	O	S	0	0
			601	370	121	109	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

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

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

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

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called 30S ribosomal protein S2.

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

- Molecule 35 is a protein called 30S ribosomal protein S3.

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

- Molecule 36 is a protein called 30S ribosomal protein S4.

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

- Molecule 37 is a protein called 30S ribosomal protein S5.

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

- Molecule 38 is a protein called 30S ribosomal protein S6.

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

- Molecule 39 is a protein called 30S ribosomal protein S7.

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

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

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

- Molecule 42 is a protein called 30S ribosomal protein S10.

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

- Molecule 43 is a protein called 30S ribosomal protein S11.

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

- Molecule 44 is a protein called 30S ribosomal protein S12.

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

- Molecule 45 is a protein called 30S ribosomal protein S13.

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

- Molecule 46 is a protein called 30S ribosomal protein S14.

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

- Molecule 47 is a protein called 30S ribosomal protein S15.

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

- Molecule 48 is a protein called 30S ribosomal protein S16.

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

- Molecule 49 is a protein called 30S ribosomal protein S17.

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

- Molecule 50 is a protein called 30S ribosomal protein S18.

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

- Molecule 51 is a protein called 30S ribosomal protein S19.

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

- Molecule 52 is a protein called 30S ribosomal protein S20.

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

- Molecule 53 is a protein called 30S ribosomal protein S21.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	88	Total	C	N	O	P	0	0
			1891	841	341	621	88		

- Molecule 55 is a protein called CspA transcriptional activator.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B	27	Total	C	N	O	S	0	0
			205	132	32	39	2		

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

Mol	Chain	Residues	Atoms	AltConf
56	1	270	Total Mg 270 270	0
56	2	113	Total Mg 113 113	0
56	3	8	Total Mg 8 8	0
56	4	1	Total Mg 1 1	0
56	C	1	Total Mg 1 1	0
56	D	2	Total Mg 2 2	0
56	M	1	Total Mg 1 1	0
56	a	1	Total Mg 1 1	0
56	h	1	Total Mg 1 1	0
56	q	1	Total Mg 1 1	0
56	z	1	Total Mg 1 1	0

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

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

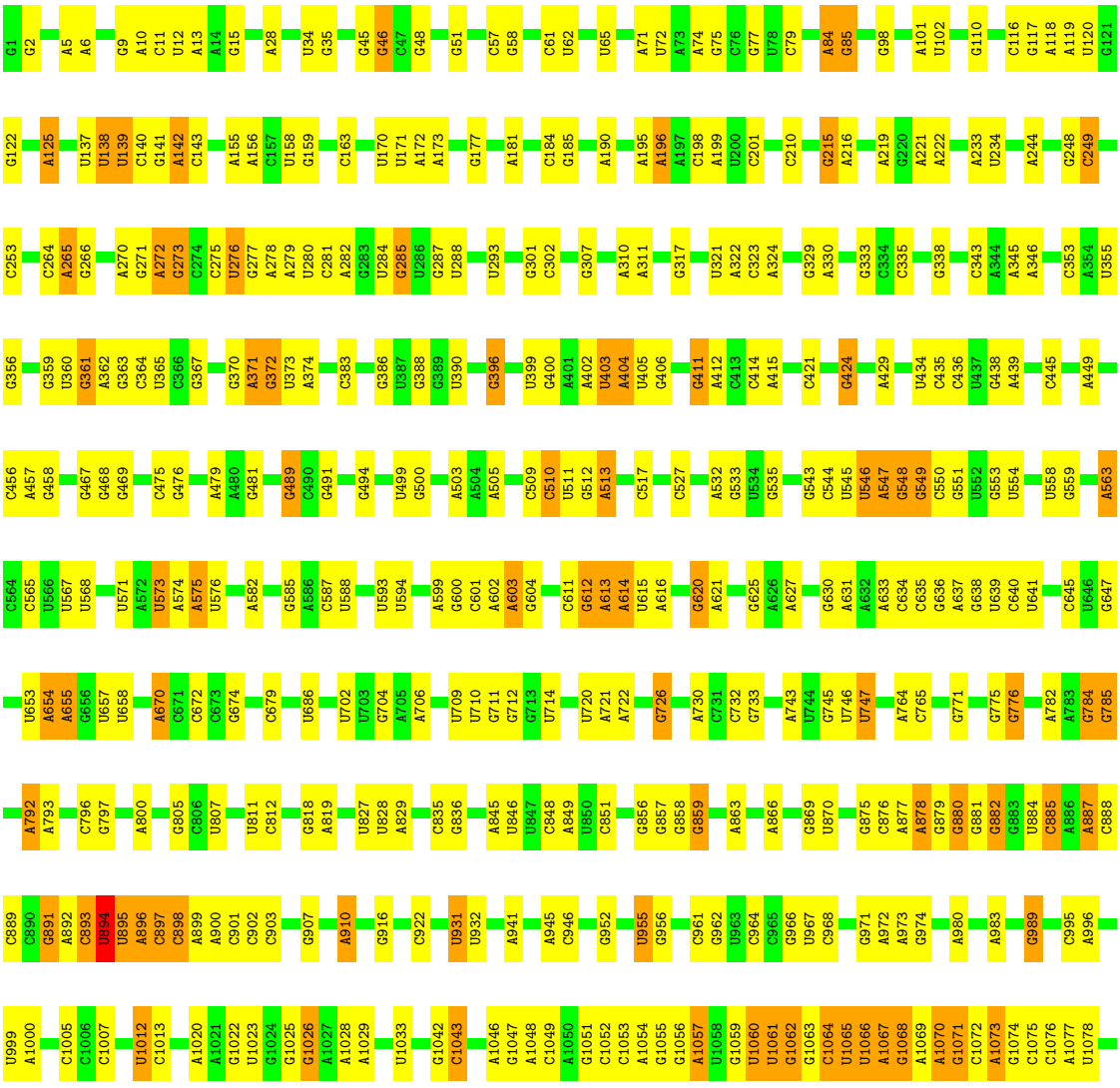
3 Residue-property plots (i)

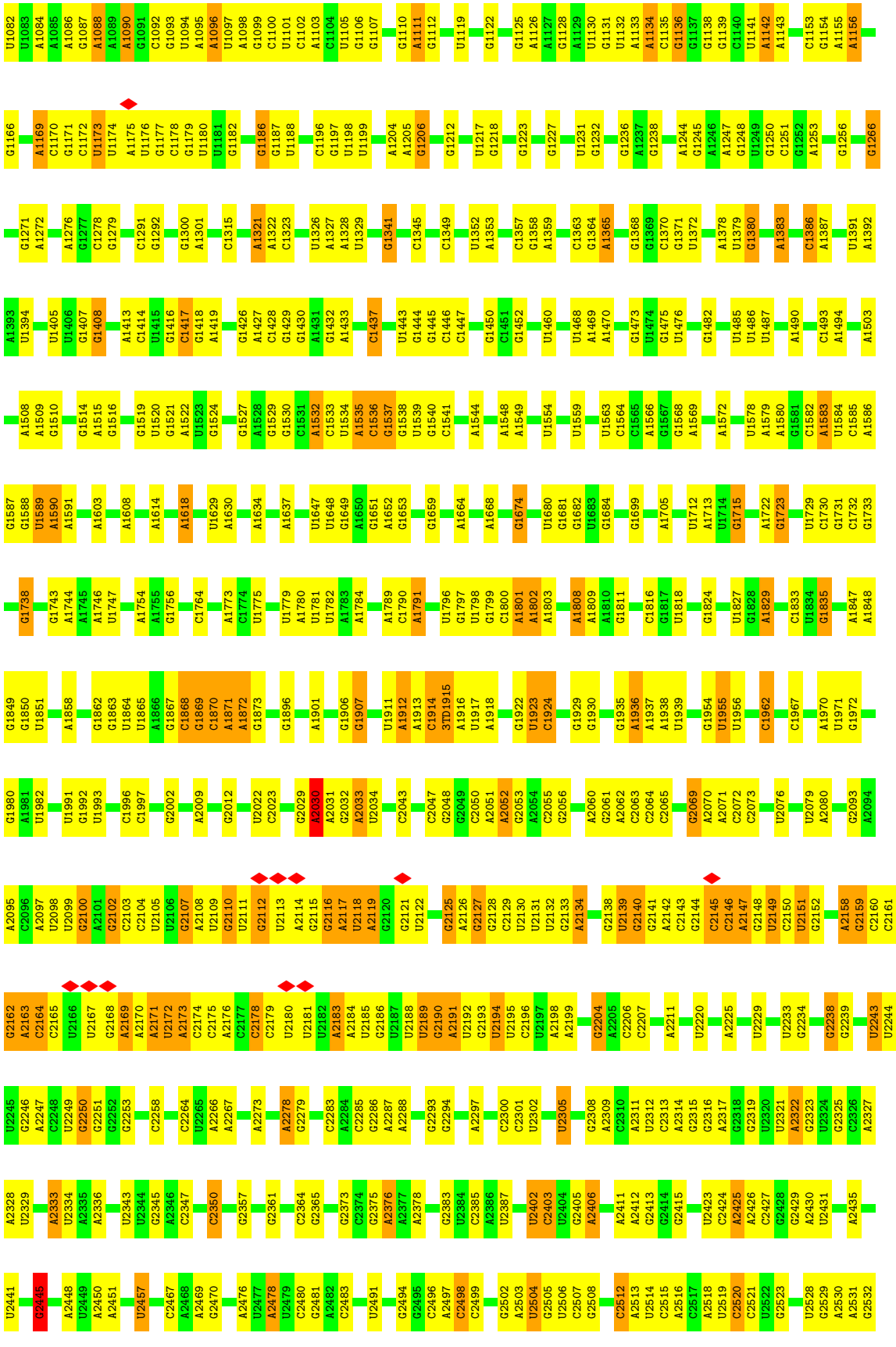
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 23S rRNA

Chain 1:





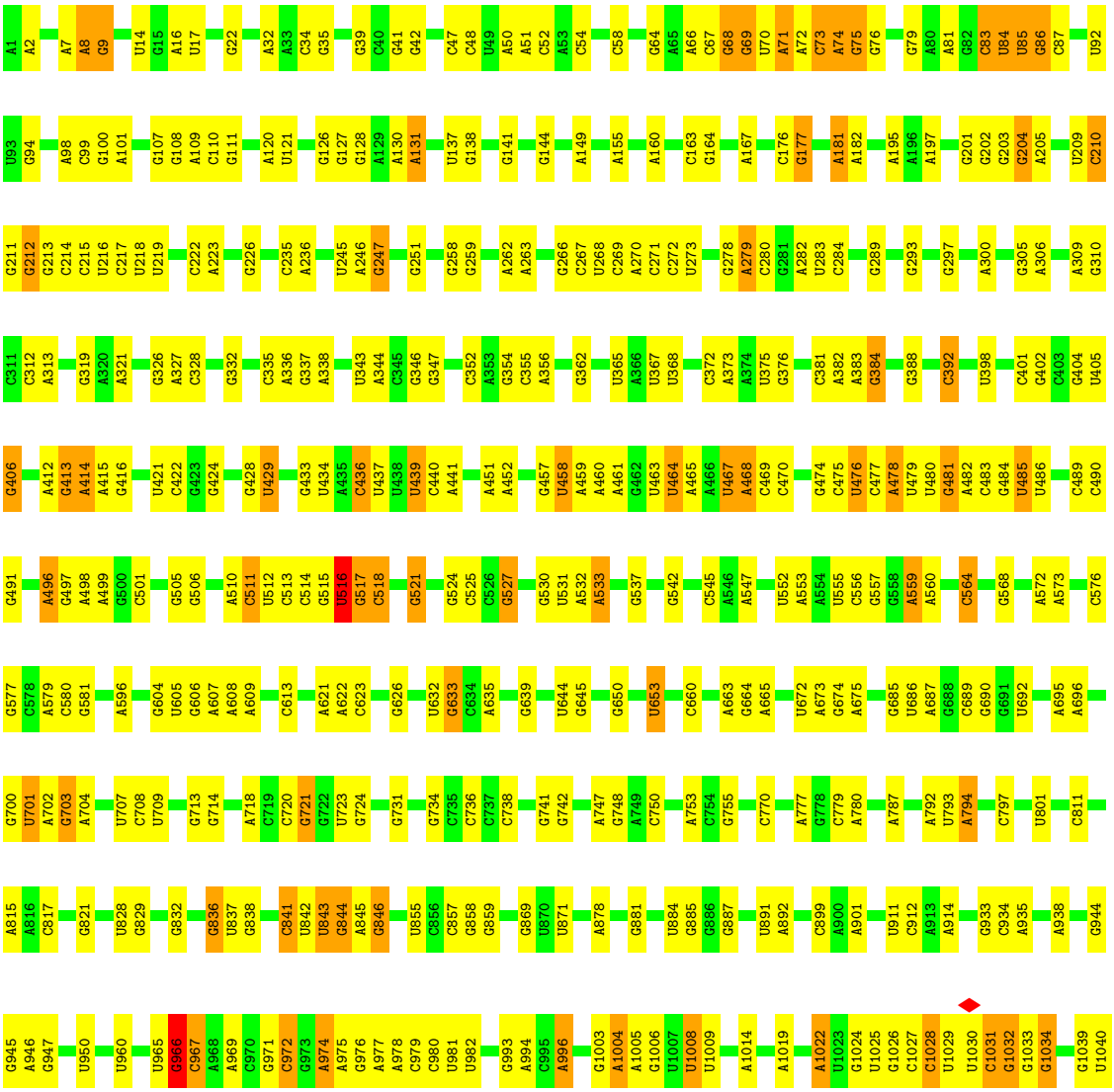


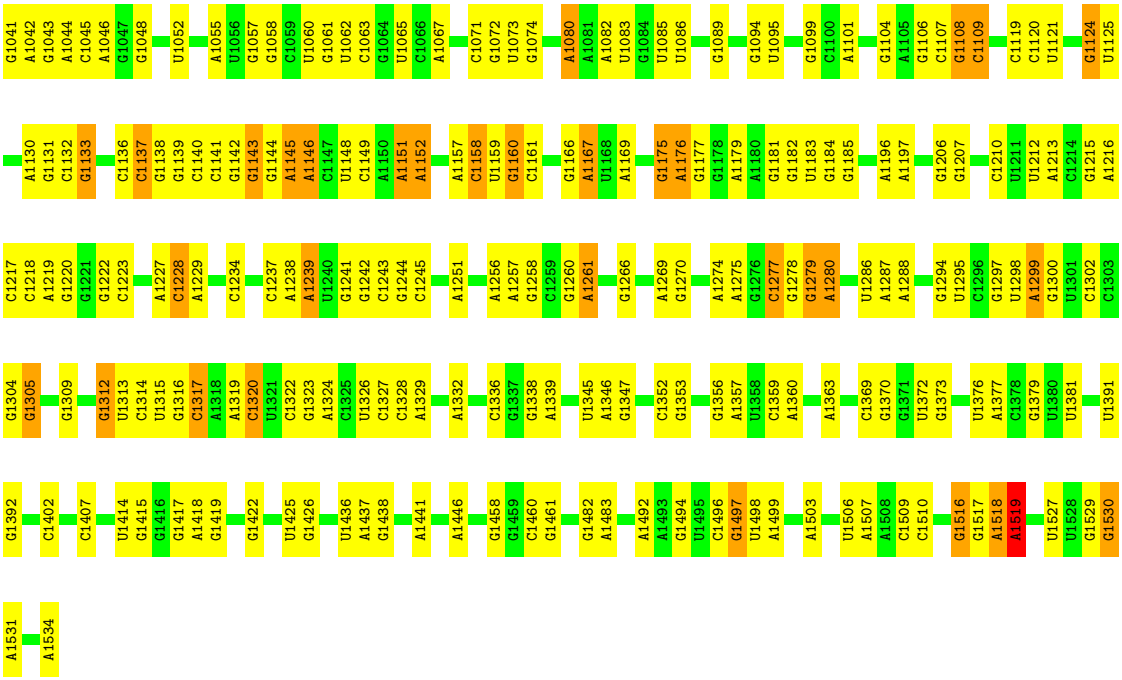


- Molecule 2: 16S rRNA

Chain 2:



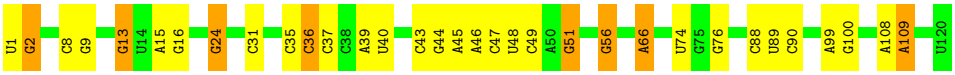




• Molecule 3: 5S rRNA

Chain 3:





• Molecule 4: mRNA

Chain 4:

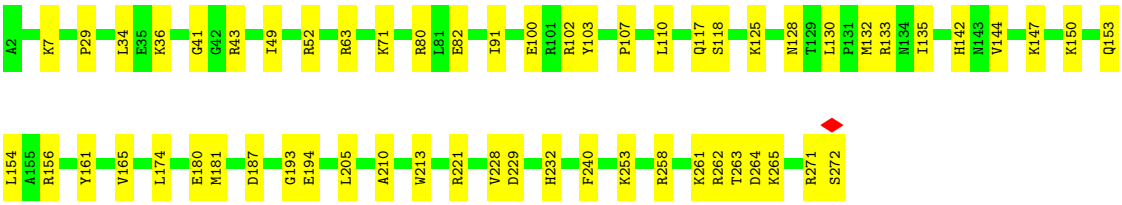




• Molecule 5: 50S ribosomal protein L2

Chain C:





• Molecule 6: 50S ribosomal protein L3

Chain D:

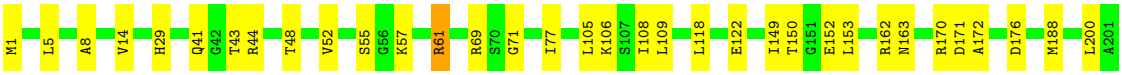




• Molecule 7: 50S ribosomal protein L4

Chain E:

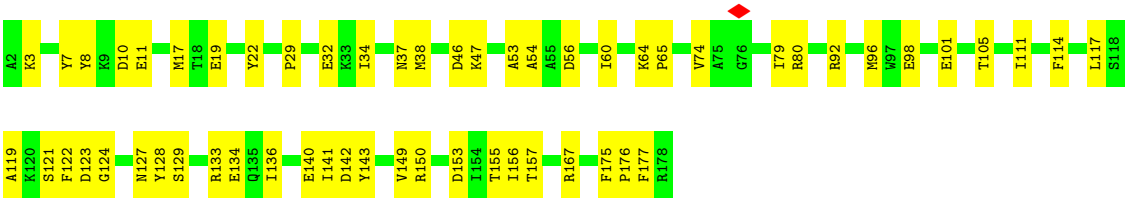




• Molecule 8: 50S ribosomal protein L5

Chain F:





• Molecule 9: 50S ribosomal protein L6

Chain G:

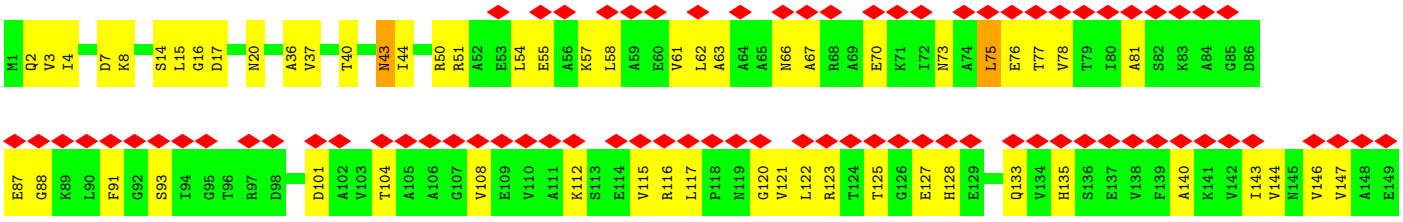




• Molecule 10: 50S ribosomal protein L9

Chain H:

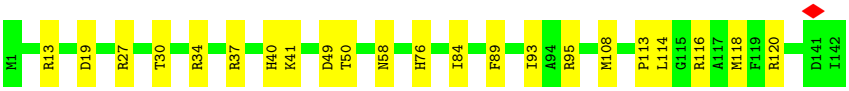




• Molecule 11: 50S ribosomal protein L13

Chain I:

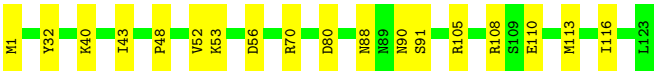




• Molecule 12: 50S ribosomal protein L14

Chain J:

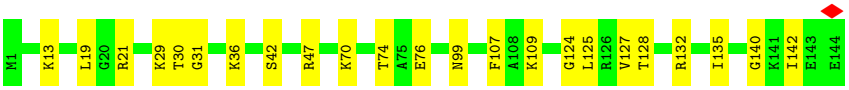




• Molecule 13: 50S ribosomal protein L15

Chain K:

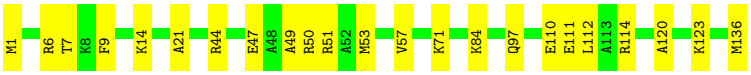




• Molecule 14: 50S ribosomal protein L16

Chain L:

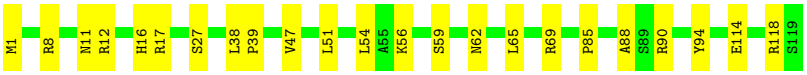




• Molecule 15: 50S ribosomal protein L17

Chain M:

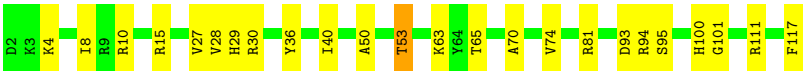




• Molecule 16: 50S ribosomal protein L18

Chain N:





• Molecule 17: 50S ribosomal protein L19

Chain O:





• Molecule 18: 50S ribosomal protein L20

Chain P:





• Molecule 19: 50S ribosomal protein L21

Chain Q:





• Molecule 20: 50S ribosomal protein L22

Chain R:





• Molecule 21: 50S ribosomal protein L23

Chain S:

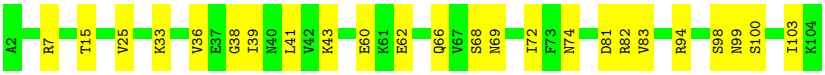




• Molecule 22: 50S ribosomal protein L24

Chain T:

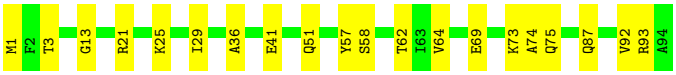




• Molecule 23: 50S ribosomal protein L25

Chain U:

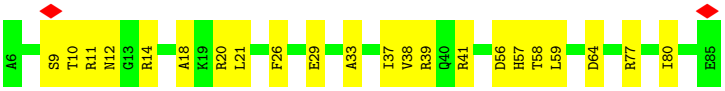




• Molecule 24: 50S ribosomal protein L27

Chain V:





• Molecule 25: 50S ribosomal protein L28

Chain W:





• Molecule 26: 50S ribosomal protein L29

Chain X:

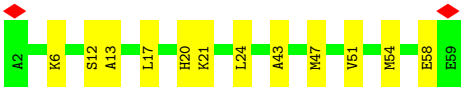




• Molecule 27: 50S ribosomal protein L30

Chain Y:

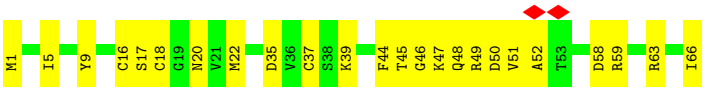




• Molecule 28: 50S ribosomal protein L31

Chain Z:

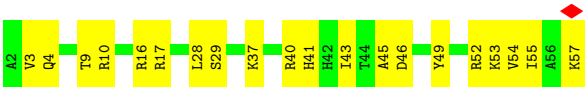




• Molecule 29: 50S ribosomal protein L32

Chain a:

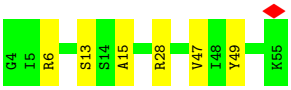




• Molecule 30: 50S ribosomal protein L33

Chain b:

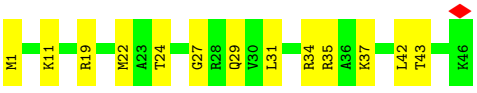




• Molecule 31: 50S ribosomal protein L34

Chain c:

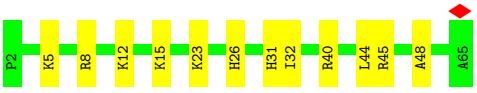




• Molecule 32: 50S ribosomal protein L35

Chain d:

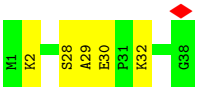




• Molecule 33: 50S ribosomal protein L36

Chain e:

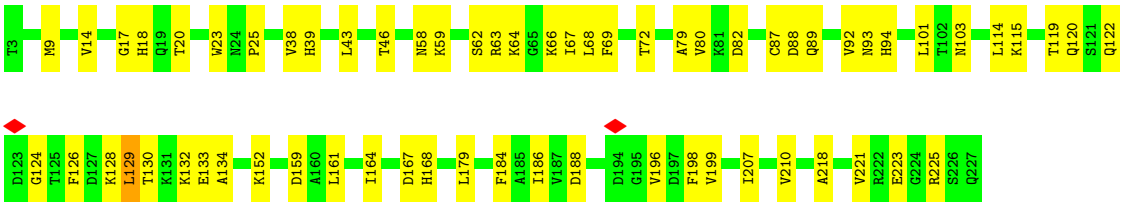




• Molecule 34: 30S ribosomal protein S2

Chain f:

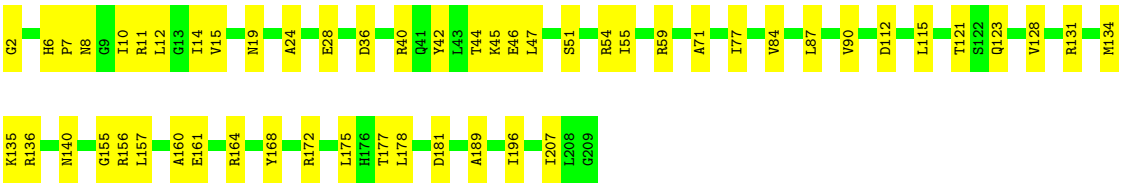




• Molecule 35: 30S ribosomal protein S3

Chain g:

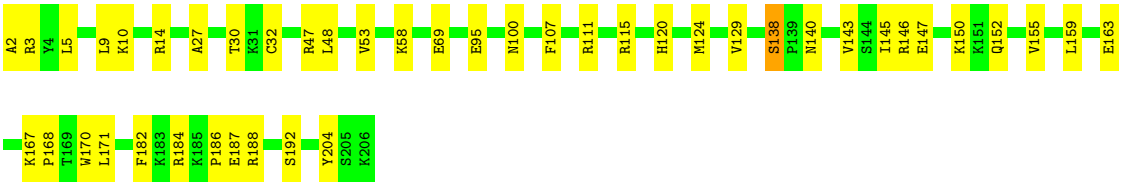




• Molecule 36: 30S ribosomal protein S4

Chain h:

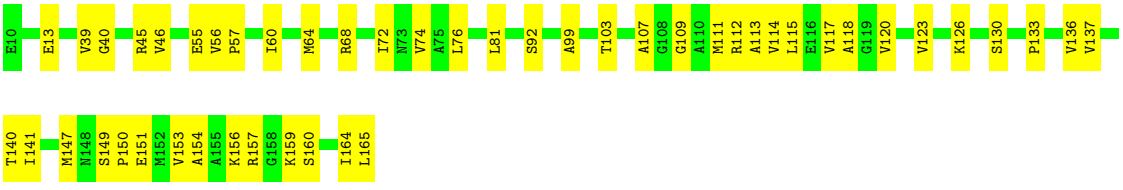




• Molecule 37: 30S ribosomal protein S5

Chain i:

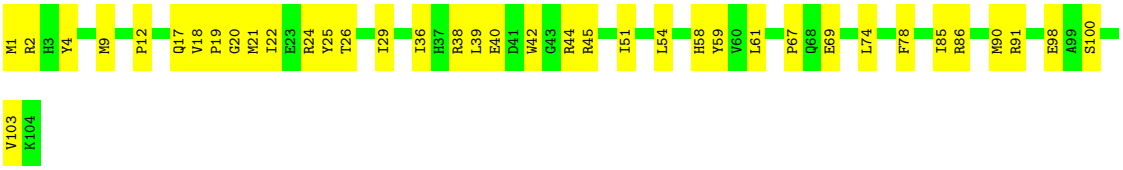




• Molecule 38: 30S ribosomal protein S6

Chain j:

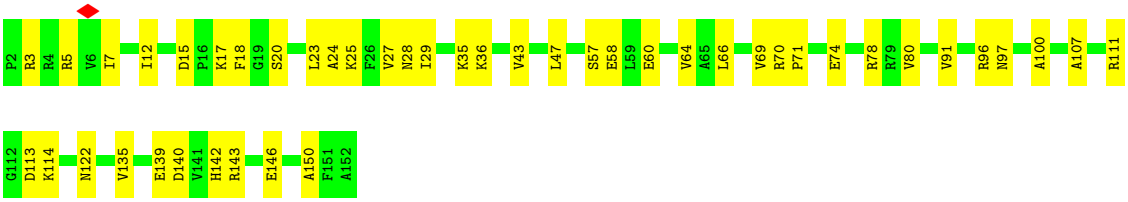




• Molecule 39: 30S ribosomal protein S7

Chain k:





• Molecule 40: 30S ribosomal protein S8

Chain l:

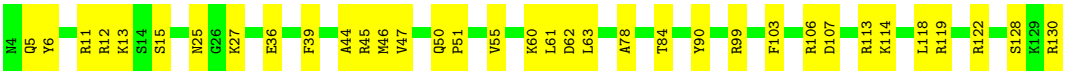




• Molecule 41: 30S ribosomal protein S9

Chain m:

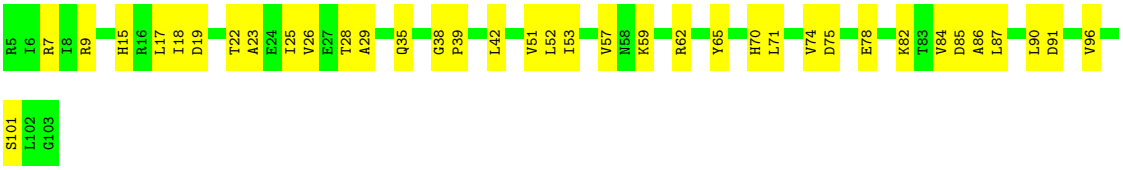




• Molecule 42: 30S ribosomal protein S10

Chain n:





• Molecule 43: 30S ribosomal protein S11

Chain o:

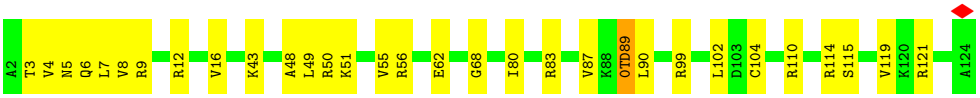




• Molecule 44: 30S ribosomal protein S12

Chain p:





• Molecule 45: 30S ribosomal protein S13

Chain q:

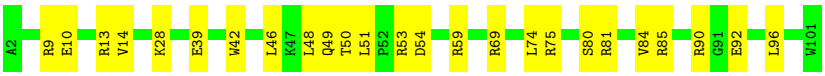




• Molecule 46: 30S ribosomal protein S14

Chain r:

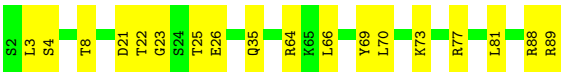




• Molecule 47: 30S ribosomal protein S15

Chain s:

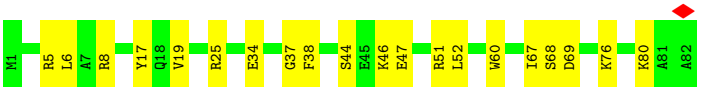




• Molecule 48: 30S ribosomal protein S16

Chain t:

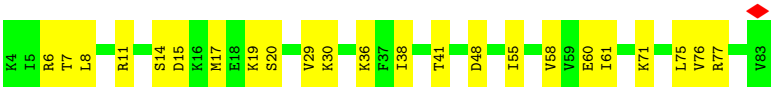




• Molecule 49: 30S ribosomal protein S17

Chain u:

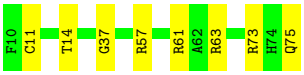




• Molecule 50: 30S ribosomal protein S18

Chain v:

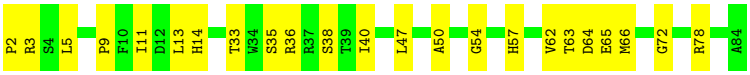




• Molecule 51: 30S ribosomal protein S19

Chain w:

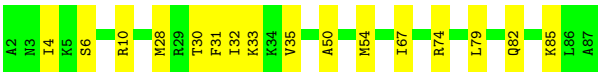




• Molecule 52: 30S ribosomal protein S20

Chain x:

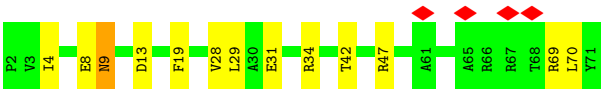




• Molecule 53: 30S ribosomal protein S21

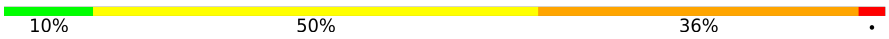
Chain y:

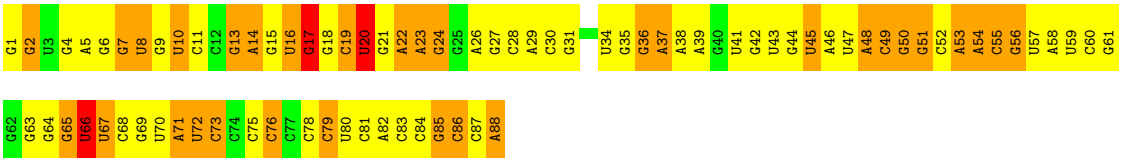




• Molecule 54: tRNA-Ser

Chain z:

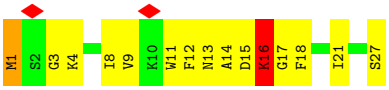




• Molecule 55: CspA transcriptional activator

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15459	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 ($e^-/Å^2$)	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	0.132	Depositor
Minimum map value	-0.058	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: MG, 5MC, 2MA, 2MG, OMG, PSU, 6MZ, OMC, UR3, 0TD, 5MU, ZN, 3TD, FME, G7M, 1MG, MA6, 4OC, OMU

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	0.52	0/69286	0.50	7/108087 (0.0%)
2	2	0.47	0/36590	0.47	0/57074
3	3	0.47	0/2872	0.45	0/4478
4	4	0.31	0/139	0.38	0/214
5	C	0.72	0/2121	0.60	0/2852
6	D	0.70	0/1586	0.60	0/2134
7	E	0.64	0/1571	0.66	0/2113
8	F	0.53	0/1434	0.64	0/1926
9	G	0.48	0/1333	0.60	0/1805
10	H	0.39	0/1122	0.76	0/1515
11	I	0.69	0/1152	0.58	0/1551
12	J	0.67	0/955	0.59	0/1279
13	K	0.68	0/1062	0.63	0/1413
14	L	0.66	0/1093	0.59	0/1460
15	M	0.70	0/964	0.66	0/1289
16	N	0.58	0/902	0.68	0/1209
17	O	0.66	0/929	0.55	0/1242
18	P	0.75	0/960	0.69	0/1278
19	Q	0.62	0/829	0.62	0/1107
20	R	0.72	0/864	0.63	0/1156
21	S	0.63	0/752	0.59	0/1005
22	T	0.52	0/796	0.55	0/1062
23	U	0.58	0/766	0.61	0/1025
24	V	0.66	0/608	0.58	0/804
25	W	0.65	0/635	0.62	0/848
26	X	0.58	0/502	0.71	0/667
27	Y	0.66	0/452	0.58	0/605
28	Z	0.41	0/531	0.65	0/709
29	a	0.66	0/450	0.59	0/599
30	b	0.54	0/433	0.55	0/576
31	c	0.73	0/380	0.65	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	d	0.73	0/513	0.70	0/676
33	e	0.68	0/303	0.61	0/397
34	f	0.48	0/1791	0.71	0/2413
35	g	0.56	0/1663	0.64	0/2241
36	h	0.56	0/1665	0.66	2/2227 (0.1%)
37	i	0.67	0/1165	0.73	2/1568 (0.1%)
38	j	0.53	0/867	0.65	0/1171
39	k	0.51	0/1195	0.68	0/1602
40	l	0.62	0/989	0.62	0/1326
41	m	0.55	0/1034	0.67	0/1375
42	n	0.51	0/800	0.71	0/1082
43	o	0.54	0/893	0.62	0/1205
44	p	0.60	0/960	0.61	0/1286
45	q	0.53	0/909	0.68	0/1215
46	r	0.57	0/817	0.64	0/1088
47	s	0.60	0/722	0.62	0/964
48	t	0.60	0/659	0.63	0/884
49	u	0.55	0/657	0.51	0/881
50	v	0.57	0/553	0.69	0/743
51	w	0.49	0/680	0.56	0/915
52	x	0.59	0/675	0.74	0/895
53	y	0.44	0/597	0.66	0/792
54	z	0.47	2/2062 (0.1%)	0.57	5/3208 (0.2%)
55	B	0.40	0/200	0.63	0/267
All	All	0.53	2/156438 (0.0%)	0.54	16/234001 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	20	U	C5-C6	6.74	1.47	1.34
54	z	20	U	C2-N3	5.61	1.49	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	z	67	U	O5'-P-OP1	-7.68	84.97	108.00
54	z	19	C	OP1-P-O3'	-7.21	86.36	108.00
54	z	8	U	O5'-P-OP1	-6.89	87.33	108.00
54	z	19	C	OP2-P-O3'	-6.69	87.92	108.00
1	1	2512	C	C5'-C4'-C3'	6.66	125.99	116.00
1	1	2602	A	C2'-C3'-O3'	6.47	119.20	109.50
36	h	138	SER	CA-C-N	6.27	126.63	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	h	138	SER	C-N-CA	6.27	126.63	119.92
1	1	894	U	C4'-C3'-O3'	5.69	117.94	109.40
37	i	149	SER	CA-C-N	5.52	125.88	119.47
37	i	149	SER	C-N-CA	5.52	125.88	119.47
54	z	67	U	C2'-C3'-O3'	-5.37	105.65	113.70
1	1	2149	U	N1-C1'-C2'	5.34	120.01	112.00
1	1	620	G	P-O3'-C3'	-5.21	112.39	120.20
1	1	403	U	C4'-C3'-O3'	-5.10	105.35	113.00
1	1	1328	A	N9-C1'-C2'	5.10	119.65	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62336	0	31365	669	0
2	2	32929	0	16583	384	0
3	3	2569	0	1301	23	0
4	4	126	0	65	1	0
5	C	2082	0	2154	45	0
6	D	1565	0	1616	24	0
7	E	1552	0	1619	28	0
8	F	1410	0	1444	39	0
9	G	1313	0	1358	26	0
10	H	1111	0	1148	60	0
11	I	1129	0	1162	17	0
12	J	946	0	1023	16	0
13	K	1053	0	1129	19	0
14	L	1074	0	1156	16	0
15	M	951	0	994	18	0
16	N	892	0	923	20	0
17	O	917	0	962	11	0
18	P	947	0	1019	19	0
19	Q	816	0	839	14	0
20	R	857	0	922	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	S	746	0	811	18	0
22	T	788	0	843	21	0
23	U	753	0	780	12	0
24	V	601	0	615	22	0
25	W	625	0	652	9	0
26	X	501	0	531	15	0
27	Y	448	0	488	7	0
28	Z	522	0	520	25	0
29	a	444	0	458	16	0
30	b	426	0	464	4	0
31	c	377	0	418	11	0
32	d	504	0	572	10	0
33	e	302	0	340	4	0
34	f	1760	0	1787	52	0
35	g	1636	0	1710	49	0
36	h	1643	0	1707	38	0
37	i	1152	0	1196	41	0
38	j	848	0	846	33	0
39	k	1181	0	1238	33	0
40	l	979	0	1031	28	0
41	m	1022	0	1070	27	0
42	n	790	0	831	31	0
43	o	877	0	887	21	0
44	p	957	0	1017	26	0
45	q	900	0	965	30	0
46	r	805	0	844	22	0
47	s	714	0	734	13	0
48	t	649	0	666	15	0
49	u	648	0	691	18	0
50	v	544	0	560	7	0
51	w	663	0	688	22	0
52	x	669	0	719	12	0
53	y	589	0	629	11	0
54	z	1891	0	955	102	0
55	B	205	0	195	13	0
56	1	270	0	0	0	0
56	2	113	0	0	0	0
56	3	8	0	0	0	0
56	4	1	0	0	0	0
56	C	1	0	0	0	0
56	D	2	0	0	0	0
56	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	a	1	0	0	0	0
56	h	1	0	0	0	0
56	q	1	0	0	0	0
56	z	1	0	0	0	0
57	Z	1	0	0	0	0
57	e	1	0	0	0	0
All	All	145136	0	97240	1999	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 9.

All (1999) 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)
6:D:151:THR:HG23	6:D:152:PRO:HD3	1.35	1.02
35:g:15:VAL:HG11	35:g:207:ILE:HD13	1.45	0.97
10:H:66:ASN:OD1	10:H:67:ALA:N	2.01	0.93
54:z:9:G:O2'	54:z:10:U:OP1	1.88	0.91
54:z:17:OMG:HM22	54:z:69:G:H22	1.36	0.90
1:1:2640:G:OP1	11:I:95:ARG:NH2	2.05	0.90
34:f:119:THR:O	34:f:124:GLY:N	2.05	0.89
2:2:1031:C:O3'	2:2:1032:G:N2	2.07	0.88
54:z:6:G:H2'	54:z:7:G:C8	2.09	0.88
2:2:501:C:OP1	44:p:114:ARG:NH2	2.07	0.87
2:2:203:G:O2'	2:2:465:A:N1	2.07	0.87
41:m:36:GLU:OE1	41:m:45:ARG:NH1	2.08	0.86
2:2:626:G:O3'	48:t:51:ARG:NH1	2.09	0.86
5:C:271:ARG:O	5:C:272:SER:OG	1.94	0.85
1:1:877:A:O2'	1:1:900:A:N6	2.09	0.85
1:1:276:U:O2'	1:1:277:G:N7	2.06	0.85
1:1:2483:C:N3	14:L:123:LYS:NZ	2.23	0.85
20:R:2:GLU:N	20:R:2:GLU:OE1	2.10	0.84
1:1:2305:U:O2'	8:F:133:ARG:NH1	2.11	0.84
36:h:124:MET:HE3	36:h:146:ARG:HE	1.40	0.84
51:w:33:THR:HG22	51:w:35:SER:H	1.42	0.84
1:1:2880:C:O3'	15:M:90:ARG:NH2	2.11	0.84
1:1:1754:A:N1	1:1:2716:C:O2'	2.09	0.84
9:G:24:ILE:HD11	9:G:43:VAL:HG11	1.60	0.84
21:S:6:ARG:NH1	21:S:37:ASP:OD1	2.10	0.84
2:2:107:G:N7	52:x:10:ARG:NH2	2.26	0.83
35:g:40:ARG:NH1	35:g:55:ILE:O	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:219:A:N3	1:1:234:U:O2'	2.11	0.83
54:z:51:G:O6	54:z:55:C:N4	2.12	0.83
1:1:2119:A:N6	1:1:2167:U:O2	2.12	0.82
1:1:125:A:OP2	31:c:19:ARG:NH2	2.13	0.82
1:1:565:C:N4	1:1:576:U:O4	2.12	0.81
38:j:51:ILE:HD12	38:j:85:ILE:HG21	1.62	0.81
44:p:87:VAL:HG11	44:p:90:LEU:HD12	1.61	0.81
2:2:1516:2MG:N2	2:2:1519:MA6:OP2	2.12	0.81
1:1:1668:A:O2'	1:1:1674:G:N7	2.14	0.81
1:1:1801:A:OP2	5:C:150:LYS:NZ	2.11	0.81
1:1:2188:U:O4	1:1:2189:U:O4	1.99	0.81
1:1:65:U:O2'	1:1:456:C:N3	2.13	0.81
3:3:51:G:OP1	16:N:63:LYS:NZ	2.13	0.81
35:g:131:ARG:NH2	35:g:168:TYR:OH	2.13	0.81
45:q:16:VAL:O	45:q:20:THR:HG23	1.80	0.80
45:q:9:ILE:HG23	45:q:18:ALA:HB1	1.62	0.80
2:2:1028:C:O2	2:2:1033:G:N1	2.14	0.80
2:2:1266:G:N2	2:2:1269:A:OP2	2.13	0.80
26:X:9:LYS:O	26:X:60:LYS:NZ	2.15	0.79
3:3:43:C:O2	8:F:92:ARG:NH2	2.14	0.79
50:v:73:ARG:O	50:v:75:GLN:NE2	2.15	0.79
7:E:149:ILE:HD11	7:E:188:MET:HG2	1.64	0.78
1:1:2109:U:O2	1:1:2180:U:N3	2.16	0.78
2:2:1055:A:N3	35:g:156:ARG:NH1	2.31	0.78
1:1:1056:G:O2'	1:1:1103:A:N6	2.16	0.78
2:2:996:A:N1	2:2:1045:C:O2'	2.16	0.78
23:U:58:SER:O	23:U:73:LYS:NZ	2.16	0.78
1:1:956:G:O6	14:L:14:LYS:NZ	2.15	0.78
2:2:1005:A:H3'	2:2:1006:G:C8	2.17	0.78
1:1:896:A:H1'	1:1:897:C:C5	2.18	0.78
1:1:2144:G:H21	1:1:2148:G:H1	1.32	0.78
50:v:37:GLY:O	50:v:63:ARG:NH2	2.16	0.78
1:1:2278:A:OP2	24:V:12:ASN:ND2	2.17	0.78
1:1:1169:A:N6	1:1:1180:U:O4	2.16	0.78
35:g:28:GLU:OE1	35:g:28:GLU:N	2.14	0.78
1:1:1223:G:OP1	19:Q:68:ARG:NH2	2.17	0.78
53:y:4:ILE:HD12	53:y:19:PHE:HD1	1.47	0.78
8:F:117:LEU:N	8:F:177:PHE:O	2.17	0.77
1:1:2571:U:O2'	6:D:151:THR:HG21	1.84	0.77
41:m:84:THR:HG21	41:m:103:PHE:HB3	1.67	0.77
38:j:22:ILE:HG21	38:j:39:LEU:HD21	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2199:A:OP1	25:W:37:ARG:NH1	2.18	0.77
2:2:1309:G:OP2	45:q:98:ARG:NE	2.17	0.77
1:1:475:C:O2	1:1:479:A:N6	2.19	0.76
1:1:1068:G:O2'	1:1:1070:A:N6	2.18	0.76
1:1:2683:C:O2	12:J:70:ARG:NH2	2.17	0.76
1:1:301:G:OP2	22:T:82:ARG:NH1	2.17	0.76
2:2:1241:G:OP1	39:k:35:LYS:NZ	2.19	0.76
2:2:938:A:N3	2:2:1376:U:O2'	2.19	0.76
54:z:67:U:O2	54:z:67:U:H2'	1.84	0.76
1:1:1416:G:O6	1:1:1583:A:N6	2.19	0.76
10:H:55:GLU:OE1	10:H:55:GLU:N	2.18	0.76
1:1:585:G:N7	18:P:6:ARG:NH1	2.34	0.75
2:2:356:A:N3	2:2:368:U:O2'	2.19	0.75
2:2:1060:U:OP1	46:r:85:ARG:NH1	2.19	0.75
1:1:563:A:N3	18:P:37:GLN:NE2	2.35	0.75
38:j:51:ILE:O	38:j:54:LEU:HD23	1.86	0.75
39:k:66:LEU:HD21	39:k:97:ASN:OD1	1.85	0.75
42:n:29:ALA:HB2	42:n:87:LEU:HD11	1.69	0.75
2:2:1261:A:N6	2:2:1274:A:O2'	2.19	0.75
1:1:1068:G:HO2'	1:1:1070:A:N6	1.85	0.74
1:1:1912:A:OP2	1:1:1918:A:N6	2.12	0.74
1:1:2258:C:O2'	1:1:2427:C:OP2	2.04	0.74
2:2:405:U:O4	36:h:2:ALA:N	2.20	0.74
12:J:113:MET:SD	12:J:116:ILE:HD11	2.26	0.74
16:N:4:LYS:NZ	16:N:8:ILE:HD11	2.02	0.74
1:1:2102:G:H4'	1:1:2102:G:OP1	1.85	0.74
2:2:401:C:O2'	2:2:621:A:N3	2.19	0.74
2:2:1131:G:O6	2:2:1143:G:N2	2.19	0.74
8:F:8:TYR:OH	8:F:29:PRO:O	2.04	0.74
11:I:19:ASP:OD1	11:I:58:ASN:ND2	2.18	0.74
1:1:621:A:OP2	13:K:99:ASN:ND2	2.21	0.74
14:L:14:LYS:O	14:L:71:LYS:NZ	2.19	0.74
15:M:59:SER:OG	15:M:62:ASN:OD1	2.05	0.73
2:2:16:A:H2	2:2:1080:A:H1'	1.53	0.73
38:j:98:GLU:OE1	38:j:98:GLU:N	2.20	0.73
38:j:69:GLU:OE1	38:j:69:GLU:N	2.20	0.73
54:z:51:G:OP1	54:z:52:C:N4	2.20	0.73
1:1:458:G:O2'	1:1:469:G:O6	2.06	0.73
10:H:133:GLN:NE2	10:H:135:HIS:O	2.21	0.73
16:N:4:LYS:HZ3	16:N:8:ILE:HD11	1.54	0.73
1:1:372:G:O2'	1:1:400:G:O6	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:933:G:O6	39:k:3:ARG:NH2	2.21	0.73
7:E:61:ARG:HD2	55:B:16:LYS:HE2	1.71	0.73
2:2:738:C:OP1	38:j:4:TYR:OH	2.06	0.73
20:R:55:ILE:HG23	20:R:66:ILE:HD12	1.71	0.73
28:Z:35:ASP:OD2	45:q:57:ARG:NE	2.22	0.73
1:1:2114:A:H62	1:1:2169:A:H61	1.37	0.72
2:2:1179:A:OP2	41:m:99:ARG:NH2	2.22	0.72
1:1:1266:G:OP2	29:a:17:ARG:NE	2.22	0.72
9:G:170:ARG:NH2	33:e:29:ALA:O	2.21	0.72
2:2:1280:A:OP2	42:n:9:ARG:NH2	2.22	0.72
2:2:1222:G:OP2	2:2:1322:C:N4	2.22	0.72
1:1:1094:U:O2'	1:1:1096:A:N7	2.21	0.72
1:1:2102:G:C8	1:1:2102:G:H5"	2.25	0.72
39:k:12:ILE:HD11	39:k:28:ASN:ND2	2.05	0.71
41:m:106:ARG:NH1	41:m:107:ASP:O	2.23	0.71
1:1:2076:U:OP2	1:1:2238:G:N2	2.23	0.71
29:a:45:ALA:O	29:a:57:LYS:NZ	2.23	0.71
14:L:47:GLU:OE2	14:L:51:ARG:NE	2.22	0.71
1:1:1365:A:OP1	25:W:3:ARG:NH2	2.24	0.71
40:l:5:ASP:OD2	40:l:77:ARG:NH1	2.23	0.71
1:1:280:U:O4	1:1:361:G:N2	2.24	0.71
2:2:552:U:O2'	44:p:83:ARG:O	2.08	0.71
1:1:1028:A:OP2	1:1:1126:A:N6	2.24	0.71
1:1:1715:G:O2'	1:1:1743:G:O6	2.08	0.70
1:1:2279:G:N7	24:V:14:ARG:NH2	2.37	0.70
37:i:151:GLU:OE1	37:i:151:GLU:N	2.24	0.70
9:G:23:VAL:HG22	9:G:36:THR:OG1	1.91	0.70
48:t:6:LEU:HD23	48:t:17:TYR:CG	2.25	0.70
34:f:122:GLN:OE1	34:f:122:GLN:N	2.24	0.70
5:C:262:ARG:O	5:C:265:LYS:NZ	2.24	0.70
1:1:863:A:O3'	3:3:100:G:N2	2.25	0.70
37:i:107:ALA:O	37:i:112:ARG:NH2	2.24	0.70
10:H:121:VAL:HG22	10:H:123:ARG:HG3	1.73	0.70
24:V:33:ALA:N	24:V:64:ASP:OD1	2.25	0.70
54:z:67:U:O2	54:z:67:U:C2'	2.40	0.69
1:1:1798:U:OP2	5:C:271:ARG:NH2	2.26	0.69
34:f:129:LEU:HD11	34:f:134:ALA:N	2.07	0.69
49:u:48:ASP:CG	49:u:75:LEU:HD21	2.16	0.69
38:j:38:ARG:NH1	38:j:98:GLU:O	2.26	0.69
10:H:14:SER:N	10:H:17:ASP:OD2	2.24	0.69
53:y:31:GLU:OE2	53:y:34:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2293:G:OP1	16:N:94:ARG:NH1	2.25	0.69
1:1:2808:G:O2'	1:1:2890:G:O6	2.10	0.69
1:1:796:C:OP1	7:E:57:LYS:NZ	2.24	0.69
39:k:113:ASP:OD2	39:k:122:ASN:ND2	2.25	0.69
54:z:6:G:H2'	54:z:7:G:H8	1.54	0.69
48:t:51:ARG:C	48:t:52:LEU:HD12	2.17	0.69
1:1:776:G:N7	1:1:793:A:O2'	2.26	0.69
1:1:1869:G:N2	1:1:1871:A:O2'	2.26	0.69
2:2:501:C:OP2	44:p:121:ARG:NH1	2.25	0.69
18:P:105:ALA:HB1	19:Q:40:MET:HE1	1.73	0.69
40:l:11:LEU:HD22	40:l:75:ILE:HD11	1.75	0.69
54:z:55:C:O2'	54:z:56:G:OP2	2.10	0.69
40:l:93:PRO:O	40:l:117:ARG:NH2	2.26	0.69
1:1:2445:2MG:OP1	7:E:69:ARG:NH1	2.25	0.69
2:2:1152:A:OP1	42:n:70:HIS:ND1	2.25	0.69
6:D:116:LYS:HD2	15:M:1:MET:HE1	1.75	0.69
2:2:406:G:H5'	36:h:5:LEU:HD22	1.73	0.68
36:h:184:ARG:NH1	36:h:187:GLU:OE1	2.26	0.68
45:q:50:GLU:OE1	45:q:50:GLU:N	2.24	0.68
2:2:464:U:N3	2:2:467:U:OP2	2.24	0.68
6:D:136:ASN:OD1	6:D:139:SER:OG	2.10	0.68
1:1:672:C:OP2	13:K:42:SER:OG	2.11	0.68
8:F:74:VAL:HG22	8:F:79:ILE:HD11	1.76	0.68
39:k:15:ASP:OD1	39:k:20:SER:N	2.26	0.68
1:1:2125:G:N1	1:1:2171:A:OP2	2.24	0.68
2:2:685:G:N2	2:2:704:A:OP2	2.27	0.68
28:Z:44:PHE:CD2	28:Z:45:THR:HG23	2.28	0.68
41:m:27:LYS:NZ	41:m:62:ASP:OD2	2.22	0.68
1:1:1789:A:OP2	5:C:221:ARG:NH1	2.27	0.68
2:2:1005:A:H3'	2:2:1006:G:H8	1.58	0.68
10:H:115:VAL:HG12	10:H:117:LEU:HD11	1.76	0.68
1:1:2188:U:C4	1:1:2189:U:O4	2.47	0.68
5:C:43:ARG:NH2	5:C:49:ILE:HD11	2.09	0.68
16:N:111:ARG:NH2	16:N:117:PHE:OXT	2.27	0.68
37:i:13:GLU:HG2	37:i:39:VAL:HG22	1.76	0.68
1:1:2051:A:O2'	1:1:2614:A:N6	2.26	0.68
2:2:980:C:O2'	46:r:13:ARG:NH1	2.27	0.68
2:2:1338:G:N3	54:z:42:G:O2'	2.27	0.67
1:1:1244:A:O2'	7:E:29:HIS:NE2	2.27	0.67
2:2:521:G:OP2	44:p:51:LYS:NZ	2.25	0.67
43:o:28:ASN:O	43:o:57:LYS:NZ	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:545:U:O2'	1:1:546:U:O3'	2.11	0.67
54:z:17:OMG:HM23	54:z:17:OMG:O3'	1.94	0.67
2:2:83:C:O2'	2:2:86:G:O6	2.07	0.67
2:2:1376:U:OP2	39:k:25:LYS:NZ	2.21	0.67
10:H:7:ASP:OD1	10:H:8:LYS:N	2.28	0.67
38:j:100:SER:OG	38:j:103:VAL:HG23	1.94	0.67
2:2:346:G:OP1	17:O:39:ARG:NH2	2.27	0.67
2:2:1160:G:OP1	34:f:132:LYS:NZ	2.23	0.67
19:Q:51:VAL:HB	19:Q:52:PRO:HD3	1.77	0.67
37:i:136:VAL:O	37:i:140:THR:HG23	1.95	0.67
1:1:1064:C:H41	1:1:1070:A:P	2.17	0.67
19:Q:38:VAL:HG13	19:Q:54:VAL:HB	1.77	0.67
38:j:18:VAL:HG21	38:j:58:HIS:CD2	2.30	0.67
38:j:26:THR:HG23	38:j:36:ILE:HG13	1.77	0.67
10:H:54:LEU:O	10:H:57:LYS:HG3	1.94	0.67
35:g:134:MET:HE2	35:g:168:TYR:HD2	1.60	0.67
1:1:2128:G:N3	1:1:2173:A:O2'	2.27	0.67
2:2:545:C:OP1	36:h:58:LYS:NZ	2.28	0.67
1:1:1070:A:N7	1:1:1096:A:O2'	2.24	0.67
2:2:35:G:N3	44:p:115:SER:OG	2.27	0.67
2:2:653:U:O4'	40:l:56:LYS:NZ	2.27	0.66
1:1:1069:A:O2'	1:1:1074:G:N1	2.27	0.66
1:1:2684:U:O4'	12:J:70:ARG:NH1	2.28	0.66
17:O:90:GLY:O	17:O:113:ARG:NH1	2.29	0.66
2:2:1518:MA6:N6	2:2:1519:MA6:H93	2.09	0.66
8:F:32:GLU:OE2	8:F:157:THR:HG22	1.95	0.66
54:z:17:OMG:HM21	54:z:18:G:N7	2.09	0.66
1:1:489:G:N2	1:1:1321:A:OP1	2.25	0.66
1:1:2125:G:H2'	1:1:2173:A:H61	1.59	0.66
16:N:53:THR:HG21	16:N:70:ALA:HB1	1.75	0.66
21:S:11:LEU:O	26:X:29:ARG:NH1	2.29	0.66
43:o:16:VAL:HG12	43:o:77:TYR:HB3	1.77	0.66
1:1:2134:A:H4'	1:1:2159:G:H21	1.59	0.66
2:2:855:U:OP2	2:2:871:U:N3	2.26	0.66
37:i:74:VAL:HG12	37:i:76:LEU:HD12	1.78	0.66
2:2:1315:U:O2'	2:2:1360:A:N3	2.21	0.66
39:k:140:ASP:OD1	39:k:143:ARG:NH1	2.29	0.66
1:1:253:C:OP2	32:d:5:LYS:NZ	2.17	0.66
1:1:573:U:O2'	1:1:575:A:OP1	2.11	0.66
1:1:611:C:C2'	1:1:612:G:H5'	2.26	0.66
47:s:26:GLU:HG3	47:s:81:LEU:HD22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:107:PHE:CD1	36:h:159:LEU:HD21	2.30	0.66
41:m:60:LYS:HB3	41:m:61:LEU:HD12	1.78	0.66
1:1:2114:A:H62	1:1:2169:A:N6	1.94	0.65
2:2:1317:C:OP2	46:r:28:LYS:NZ	2.22	0.65
24:V:37:ILE:HG22	24:V:38:VAL:HG23	1.77	0.65
35:g:47:LEU:HD12	35:g:47:LEU:N	2.11	0.65
1:1:1153:C:OP1	18:P:92:ARG:NH2	2.28	0.65
1:1:2147:A:N7	1:1:2148:G:N2	2.44	0.65
2:2:1006:G:H8	2:2:1006:G:O5'	1.80	0.65
34:f:58:ASN:ND2	34:f:223:GLU:OE1	2.28	0.65
1:1:2249:U:N3	1:1:2253:G:OP2	2.28	0.65
28:Z:63:ARG:NH1	51:w:5:LEU:HD21	2.11	0.65
54:z:17:OMG:HM22	54:z:69:G:N2	2.09	0.65
2:2:673:A:H2'	2:2:674:G:C8	2.31	0.65
35:g:36:ASP:OD1	35:g:59:ARG:NH2	2.29	0.65
2:2:16:A:C2	2:2:1080:A:H1'	2.31	0.65
2:2:452:A:H62	2:2:480:U:H3	1.44	0.65
10:H:54:LEU:HD12	10:H:57:LYS:HE2	1.77	0.65
38:j:17:GLN:OE1	38:j:17:GLN:N	2.29	0.65
1:1:2848:G:O2'	1:1:2867:G:N2	2.29	0.65
10:H:58:LEU:O	10:H:62:LEU:HD23	1.97	0.65
36:h:27:ALA:O	36:h:30:THR:OG1	2.14	0.65
5:C:228:VAL:HG13	5:C:229:ASP:OD1	1.96	0.65
17:O:33:VAL:HG22	17:O:38:LYS:HG2	1.79	0.65
52:x:4:ILE:HG22	52:x:6:SER:H	1.62	0.65
1:1:370:G:O2'	1:1:424:G:OP1	2.15	0.64
2:2:673:A:O3'	38:j:86:ARG:NH2	2.30	0.64
2:2:131:A:O2'	2:2:262:A:N3	2.25	0.64
10:H:66:ASN:HB2	10:H:135:HIS:HB2	1.78	0.64
14:L:136:MET:HE1	23:U:74:ALA:O	1.96	0.64
21:S:69:ARG:NH2	21:S:72:GLN:O	2.30	0.64
1:1:2749:A:OP1	9:G:2:SER:OG	2.15	0.64
9:G:103:ILE:HD12	9:G:117:LEU:HD21	1.78	0.64
6:D:3:GLY:C	6:D:4:LEU:HD12	2.23	0.64
5:C:100:GLU:OE2	5:C:102:ARG:NE	2.31	0.64
38:j:22:ILE:CG2	38:j:39:LEU:HD21	2.27	0.64
44:p:48:ALA:C	44:p:49:LEU:HD12	2.22	0.64
53:y:8:GLU:N	53:y:8:GLU:OE1	2.30	0.64
1:1:1818:U:O2'	5:C:153:GLN:O	2.11	0.64
2:2:110:C:O2'	48:t:25:ARG:O	2.14	0.64
2:2:481:G:O2'	2:2:483:C:N4	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:1:MET:HE3	23:U:62:THR:OG1	1.97	0.64
1:1:249:C:O2	32:d:12:LYS:NZ	2.31	0.63
54:z:1:G:N7	54:z:85:G:N2	2.46	0.63
2:2:362:G:N2	2:2:365:U:OP2	2.28	0.63
5:C:142:HIS:ND1	5:C:193:GLY:O	2.29	0.63
17:O:14:LYS:HE2	17:O:77:HIS:HA	1.80	0.63
2:2:738:C:OP1	38:j:2:ARG:NH2	2.29	0.63
2:2:770:C:O2'	2:2:899:C:N3	2.30	0.63
24:V:11:ARG:O	24:V:14:ARG:NH1	2.31	0.63
1:1:2159:G:H2'	1:1:2160:C:C6	2.34	0.63
1:1:2194:U:H2'	1:1:2195:U:C6	2.34	0.63
2:2:974:A:OP1	46:r:69:ARG:NH1	2.31	0.63
2:2:1320:C:N3	51:w:36:ARG:NH1	2.46	0.63
7:E:41:GLN:HG2	7:E:43:THR:HG23	1.81	0.63
8:F:60:ILE:HA	8:F:140:GLU:HG3	1.79	0.63
37:i:99:ALA:HB1	37:i:103:THR:HG21	1.80	0.63
1:1:1172:C:O2'	1:1:1173:U:O4'	2.13	0.63
10:H:75:LEU:H	10:H:75:LEU:HD23	1.63	0.63
42:n:42:LEU:HB2	42:n:71:LEU:HB3	1.81	0.63
44:p:68:GLY:O	44:p:99:ARG:NH1	2.30	0.63
1:1:210:C:OP1	31:c:29:GLN:NE2	2.31	0.63
3:3:13:G:N2	3:3:16:G:N3	2.46	0.63
4:4:2:G:O2'	4:4:3:C:O4'	2.13	0.63
20:R:69:LEU:HD22	20:R:107:VAL:HG22	1.81	0.62
1:1:1475:G:O2'	1:1:1514:G:O6	2.16	0.62
8:F:121:SER:OG	8:F:129:SER:O	2.16	0.62
24:V:18:ALA:O	24:V:20:ARG:NH1	2.31	0.62
45:q:4:ILE:CG1	45:q:9:ILE:HD12	2.29	0.62
54:z:54:A:O2'	54:z:55:C:O5'	2.18	0.62
1:1:278:A:H61	1:1:361:G:H2'	1.63	0.62
2:2:1298:U:OP2	39:k:114:LYS:NZ	2.23	0.62
28:Z:51:VAL:HG23	28:Z:52:ALA:H	1.65	0.62
40:l:30:SER:O	40:l:34:VAL:HG23	1.99	0.62
54:z:16:U:O2'	54:z:73:C:OP1	2.17	0.62
20:R:34:ASP:OD2	29:a:37:LYS:NZ	2.30	0.62
1:1:894:U:OP2	1:1:894:U:H6	1.83	0.62
36:h:47:ARG:NE	36:h:47:ARG:HA	2.15	0.62
45:q:106:ALA:HB3	45:q:110:LYS:HD3	1.81	0.62
1:1:964:C:O2'	1:1:2273:A:N3	2.31	0.62
2:2:1167:A:O2'	2:2:1169:A:N7	2.33	0.62
28:Z:63:ARG:HH11	51:w:5:LEU:HD21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1137:C:O2	2:2:1138:G:N2	2.34	0.61
14:L:49:ALA:HB1	14:L:120:ALA:HB1	1.82	0.61
28:Z:58:ASP:OD1	28:Z:59:ARG:N	2.33	0.61
51:w:64:ASP:OD1	51:w:65:GLU:N	2.33	0.61
1:1:468:G:OP2	31:c:37:LYS:NZ	2.30	0.61
1:1:2175:C:H2'	1:1:2176:A:C8	2.34	0.61
13:K:132:ARG:HG3	13:K:142:ILE:HD12	1.82	0.61
18:P:74:ILE:HD11	18:P:78:LYS:HB3	1.82	0.61
1:1:2311:A:O2'	1:1:2312:U:O4'	2.17	0.61
13:K:70:LYS:O	13:K:74:THR:HG23	2.00	0.61
35:g:24:ALA:HB1	35:g:28:GLU:HG2	1.81	0.61
2:2:966:2MG:HM22	54:z:35:G:H5'	1.82	0.61
1:1:9:G:O2'	1:1:2800:A:N6	2.33	0.61
5:C:125:LYS:HG2	5:C:128:ASN:OD1	2.01	0.61
16:N:50:ALA:O	16:N:81:ARG:NH2	2.33	0.61
38:j:40:GLU:CD	38:j:103:VAL:HG21	2.26	0.61
1:1:2469:A:N6	1:1:2481:G:O2'	2.32	0.61
1:1:2655:G:O2'	1:1:2664:G:O6	2.15	0.61
2:2:1312:G:OP2	28:Z:63:ARG:NH2	2.31	0.61
6:D:181:ASP:OD2	6:D:184:ARG:NH2	2.33	0.61
1:1:714:U:OP2	47:s:88:ARG:NH1	2.30	0.61
37:i:165:LEU:HD12	40:l:114:ARG:HD2	1.83	0.61
42:n:19:ASP:HA	42:n:22:THR:HG22	1.82	0.61
2:2:564:C:OP1	44:p:12:ARG:NH1	2.34	0.60
15:M:54:LEU:HD11	15:M:62:ASN:HD22	1.66	0.60
37:i:154:ALA:HA	37:i:164:ILE:HD11	1.82	0.60
39:k:69:VAL:HG12	39:k:135:VAL:HG12	1.83	0.60
49:u:15:ASP:OD1	49:u:55:ILE:HD11	2.00	0.60
1:1:321:U:O3'	7:E:162:ARG:NH1	2.34	0.60
1:1:1042:G:O2'	1:1:1043:C:H5"	2.01	0.60
1:1:2530:A:N7	9:G:172:LYS:NZ	2.49	0.60
21:S:6:ARG:O	21:S:10:VAL:HG23	2.01	0.60
22:T:41:LEU:HB3	22:T:60:GLU:OE2	2.02	0.60
1:1:620:G:H4'	1:1:621:A:O5'	2.01	0.60
34:f:59:LYS:O	34:f:62:SER:OG	2.16	0.60
35:g:121:THR:HG23	35:g:189:ALA:HB2	1.81	0.60
1:1:2130:U:O3'	1:1:2158:A:N6	2.34	0.60
1:1:517:C:OP2	29:a:10:ARG:NH2	2.35	0.60
1:1:1364:G:OP2	25:W:2:SER:N	2.35	0.60
34:f:114:LEU:C	34:f:114:LEU:HD23	2.27	0.60
35:g:10:ILE:HG23	35:g:11:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:x:82:GLN:O	52:x:85:LYS:HG3	2.02	0.60
54:z:51:G:N1	54:z:55:C:N3	2.45	0.60
29:a:43:ILE:HG22	29:a:49:TYR:HB2	1.84	0.60
5:C:107:PRO:HD2	5:C:110:LEU:HD22	1.83	0.60
1:1:1870:C:O2'	1:1:1871:A:O4'	2.18	0.59
7:E:118:LEU:HD11	7:E:188:MET:SD	2.41	0.59
38:j:90:MET:HE1	50:v:61:ARG:CZ	2.32	0.59
1:1:1363:C:O2'	1:1:1809:A:N3	2.34	0.59
1:1:2178:C:H2'	1:1:2179:C:C5	2.37	0.59
1:1:2316:G:H2'	1:1:2317:A:H8	1.67	0.59
10:H:15:LEU:HD23	10:H:16:GLY:N	2.17	0.59
11:I:37:ARG:HD2	11:I:118:MET:HE1	1.85	0.59
41:m:25:ASN:OD1	41:m:27:LYS:NZ	2.34	0.59
10:H:15:LEU:HD23	10:H:15:LEU:C	2.28	0.59
42:n:22:THR:O	42:n:26:VAL:HG23	2.02	0.59
2:2:1527:U:OP2	53:y:42:THR:HG22	2.02	0.59
8:F:46:ASP:OD1	8:F:47:LYS:N	2.35	0.59
38:j:1:MET:HE3	38:j:67:PRO:HD3	1.84	0.59
49:u:7:THR:C	49:u:8:LEU:HD12	2.27	0.59
10:H:78:VAL:HB	10:H:144:VAL:HG22	1.85	0.59
34:f:20:THR:HG22	34:f:39:HIS:NE2	2.17	0.59
36:h:107:PHE:HD1	36:h:159:LEU:HD21	1.67	0.59
1:1:1245:G:OP1	13:K:13:LYS:NZ	2.35	0.59
1:1:1534:U:H4'	1:1:1535:A:H2	1.68	0.59
10:H:63:ALA:O	10:H:66:ASN:OD1	2.20	0.59
27:Y:47:MET:O	27:Y:51:VAL:HG22	2.02	0.59
37:i:55:GLU:HG3	37:i:57:PRO:HD2	1.84	0.59
10:H:115:VAL:HG12	10:H:117:LEU:CD1	2.33	0.59
39:k:60:GLU:O	39:k:64:VAL:HG23	2.03	0.59
8:F:3:LYS:NZ	8:F:101:GLU:OE2	2.30	0.59
16:N:28:VAL:HG12	16:N:93:ASP:O	2.02	0.59
1:1:611:C:H2'	1:1:612:G:H5'	1.83	0.58
1:1:784:G:O2'	1:1:785:G:O5'	2.20	0.58
1:1:2350:C:OP2	32:d:45:ARG:NH2	2.36	0.58
2:2:9:G:OP2	37:i:126:LYS:NZ	2.25	0.58
40:l:106:THR:OG1	40:l:109:GLY:O	2.17	0.58
54:z:44:G:O2'	54:z:45:U:OP1	2.20	0.58
34:f:207:ILE:H	34:f:207:ILE:HD12	1.68	0.58
41:m:12:ARG:HG3	41:m:13:LYS:H	1.68	0.58
1:1:279:A:N6	1:1:361:G:H1'	2.19	0.58
1:1:706:A:OP1	5:C:7:LYS:NZ	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1084:A:N3	1:1:1105:U:O2'	2.35	0.58
1:1:1378:A:O2'	1:1:1380:G:N7	2.37	0.58
34:f:67:ILE:N	34:f:89:GLN:OE1	2.36	0.58
23:U:36:ALA:O	23:U:93:ARG:NH2	2.36	0.58
42:n:25:ILE:HD11	42:n:90:LEU:HD22	1.85	0.58
1:1:79:C:O2'	1:1:346:A:N3	2.33	0.58
1:1:371:A:N6	1:1:402:A:OP2	2.28	0.58
1:1:2117:A:O2'	1:1:2119:A:OP1	2.20	0.58
1:1:2141:G:H22	1:1:2151:U:C2'	2.16	0.58
2:2:944:G:N1	2:2:1338:G:OP2	2.35	0.58
46:r:80:SER:O	46:r:84:VAL:HG23	2.02	0.58
1:1:402:A:H2'	1:1:403:U:H5'	1.86	0.58
1:1:2885:G:O6	29:a:29:SER:OG	2.21	0.58
2:2:521:G:N7	44:p:50:ARG:NH2	2.51	0.58
10:H:4:ILE:HD12	10:H:17:ASP:C	2.29	0.58
31:c:34:ARG:NE	31:c:42:LEU:O	2.36	0.58
54:z:5:A:H2'	54:z:6:G:O4'	2.04	0.58
54:z:14:A:N6	54:z:22:A:O2'	2.34	0.58
1:1:870:U:OP1	14:L:6:ARG:NH1	2.36	0.58
1:1:1722:A:O2'	1:1:1723:G:H5'	2.04	0.58
54:z:50:G:N2	54:z:56:G:C2	2.72	0.58
1:1:500:G:N1	1:1:503:A:OP2	2.36	0.58
1:1:2134:A:C4'	1:1:2159:G:H21	2.17	0.58
2:2:841:C:H2'	2:2:843:U:H5'	1.86	0.58
2:2:842:U:H2'	2:2:844:G:H21	1.69	0.58
54:z:48:A:N6	54:z:49:C:C4	2.72	0.58
1:1:404:A:N6	1:1:421:C:O2'	2.37	0.57
1:1:1527:G:N1	1:1:1544:A:OP2	2.33	0.57
24:V:21:LEU:HD21	24:V:41:ARG:HH21	1.69	0.57
30:b:13:SER:HA	30:b:49:TYR:CD1	2.39	0.57
1:1:2375:G:N2	1:1:2378:A:OP2	2.34	0.57
44:p:5:ASN:OD1	49:u:36:LYS:NZ	2.36	0.57
2:2:1006:G:C8	2:2:1006:G:O5'	2.57	0.57
2:2:1124:G:O2'	2:2:1145:A:N6	2.36	0.57
16:N:70:ALA:O	16:N:74:VAL:HG23	2.04	0.57
1:1:1954:G:O2'	1:1:1956:U:O4	2.16	0.57
1:1:2051:A:N6	1:1:2614:A:O2'	2.37	0.57
37:i:133:PRO:HA	37:i:136:VAL:HG12	1.86	0.57
39:k:27:VAL:HG12	39:k:43:VAL:HG21	1.86	0.57
42:n:39:PRO:HA	42:n:74:VAL:HG22	1.86	0.57
1:1:630:G:N2	1:1:633:A:OP2	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2835:A:N6	1:1:2879:A:O5'	2.36	0.57
2:2:1086:U:H3	2:2:1099:G:H22	1.51	0.57
8:F:74:VAL:CG2	8:F:79:ILE:HD11	2.34	0.57
36:h:188:ARG:NH1	36:h:192:SER:O	2.28	0.57
45:q:100:GLN:OE1	45:q:100:GLN:N	2.37	0.57
1:1:190:A:N3	1:1:679:C:O2'	2.35	0.57
2:2:14:U:N3	2:2:17:U:OP2	2.33	0.57
2:2:413:G:N2	2:2:428:G:O3'	2.38	0.57
5:C:80:ARG:NH1	5:C:82:GLU:OE2	2.35	0.57
10:H:116:ARG:HG3	10:H:116:ARG:HH11	1.69	0.57
34:f:207:ILE:HA	34:f:210:VAL:HG22	1.86	0.57
54:z:54:A:O2'	54:z:55:C:O4'	2.22	0.57
1:1:1062:G:H2'	1:1:1063:G:C8	2.39	0.57
37:i:109:GLY:O	37:i:112:ARG:HG2	2.04	0.57
1:1:743:A:O2'	1:1:1659:G:OP1	2.23	0.57
2:2:413:G:H22	2:2:429:U:P	2.27	0.57
45:q:11:ASP:OD1	45:q:12:HIS:N	2.38	0.57
1:1:1901:A:OP2	5:C:253:LYS:NZ	2.36	0.57
2:2:1234:C:OP1	41:m:119:ARG:NH2	2.38	0.57
36:h:187:GLU:OE1	36:h:187:GLU:N	2.37	0.57
1:1:511:U:H2'	1:1:512:G:H5'	1.86	0.57
1:1:1248:G:OP1	7:E:44:ARG:NH2	2.37	0.56
1:1:1266:G:OP1	29:a:16:ARG:NE	2.26	0.56
3:3:74:U:O2	23:U:29:ILE:HD13	2.05	0.56
24:V:20:ARG:O	24:V:39:ARG:NH1	2.38	0.56
29:a:52:ARG:NH2	29:a:54:VAL:HG12	2.20	0.56
43:o:47:ALA:HB1	43:o:62:ALA:HB1	1.87	0.56
44:p:48:ALA:O	44:p:49:LEU:HD12	2.05	0.56
1:1:1652:A:OP1	15:M:8:ARG:NH2	2.36	0.56
1:1:1980:G:O2'	1:1:1982:U:OP2	2.21	0.56
1:1:2149:U:H2'	1:1:2150:C:O4'	2.06	0.56
2:2:972:C:OP2	42:n:59:LYS:NZ	2.32	0.56
7:E:77:ILE:HG22	7:E:77:ILE:O	2.04	0.56
14:L:7:THR:OG1	14:L:9:PHE:O	2.20	0.56
55:B:9:VAL:HA	55:B:12:PHE:CD1	2.40	0.56
1:1:1055:G:N1	1:1:1105:U:C4	2.73	0.56
1:1:2250:G:O2'	1:1:2496:C:OP1	2.22	0.56
1:1:2831:G:N2	1:1:2884:U:OP2	2.38	0.56
5:C:165:VAL:HG21	5:C:181:MET:HE1	1.86	0.56
14:L:110:GLU:O	14:L:114:ARG:HG2	2.05	0.56
22:T:36:VAL:HG11	22:T:39:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:t:44:SER:N	48:t:47:GLU:OE2	2.30	0.56
1:1:818:G:N1	1:1:1188:U:OP2	2.28	0.56
21:S:72:GLN:OE1	21:S:72:GLN:N	2.38	0.56
1:1:887:A:H4'	1:1:889:C:H41	1.71	0.56
2:2:1422:G:H4'	12:J:48:PRO:HB3	1.87	0.56
22:T:94:ARG:HB3	22:T:103:ILE:HD12	1.88	0.56
37:i:157:ARG:NH1	40:l:43:GLU:OE2	2.39	0.56
54:z:56:G:C2	54:z:57:U:C5	2.94	0.56
1:1:1055:G:N1	1:1:1105:U:N3	2.54	0.56
1:1:244:A:OP2	32:d:8:ARG:NH2	2.29	0.56
1:1:278:A:N1	1:1:361:G:O2'	2.25	0.56
1:1:445:C:OP1	18:P:2:ALA:N	2.38	0.56
22:T:74:ASN:ND2	22:T:81:ASP:OD2	2.36	0.56
1:1:2405:G:O2'	1:1:2411:A:N6	2.38	0.56
2:2:1314:C:N4	51:w:2:PRO:O	2.38	0.56
46:r:49:GLN:NE2	51:w:11:ILE:O	2.31	0.56
2:2:1176:A:H2'	2:2:1177:G:C8	2.41	0.55
1:1:639:U:H2'	1:1:640:C:H6	1.70	0.55
2:2:811:C:O2'	2:2:901:A:N1	2.40	0.55
2:2:1239:A:H62	2:2:1299:A:N6	2.02	0.55
31:c:42:LEU:HD23	31:c:43:THR:HG23	1.88	0.55
34:f:20:THR:HG22	34:f:39:HIS:CD2	2.40	0.55
35:g:14:ILE:HG22	35:g:15:VAL:HG23	1.88	0.55
35:g:51:SER:HB3	35:g:115:LEU:HD22	1.89	0.55
2:2:701:U:O2	2:2:703:G:N1	2.39	0.55
44:p:87:VAL:HG11	44:p:90:LEU:CD1	2.34	0.55
54:z:26:A:C4	54:z:27:G:C8	2.94	0.55
1:1:2343:U:HO2'	1:1:2373:G:HO2'	1.53	0.55
2:2:1305:G:H21	2:2:1332:A:H2	1.53	0.55
11:I:76:HIS:O	11:I:84:ILE:HD12	2.06	0.55
19:Q:52:PRO:O	19:Q:53:PHE:CG	2.59	0.55
1:1:476:G:N1	1:1:479:A:OP2	2.39	0.55
1:1:1062:G:N1	1:1:1063:G:C6	2.74	0.55
5:C:29:PRO:HG2	5:C:34:LEU:HD11	1.87	0.55
5:C:41:GLY:O	5:C:43:ARG:NH1	2.40	0.55
9:G:105:LEU:HD13	9:G:107:LEU:HD11	1.88	0.55
16:N:15:ARG:NH2	16:N:95:SER:OG	2.37	0.55
29:a:40:ARG:HG3	29:a:41:HIS:ND1	2.22	0.55
1:1:85:G:OP2	22:T:7:ARG:HB2	2.07	0.55
12:J:88:ASN:ND2	12:J:90:ASN:OD1	2.39	0.55
23:U:75:GLN:HB2	23:U:92:VAL:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:55:THR:HG23	40:l:56:LYS:H	1.72	0.55
54:z:13:G:O2'	54:z:23:A:N6	2.26	0.55
35:g:15:VAL:CG1	35:g:207:ILE:HD13	2.30	0.55
1:1:1914:C:H2'	1:1:1915:3TD:O4	2.06	0.55
10:H:101:ASP:O	10:H:104:THR:HG22	2.06	0.55
14:L:47:GLU:OE2	14:L:50:ARG:NH1	2.40	0.55
26:X:7:ARG:NH1	26:X:59:GLU:OE1	2.40	0.55
26:X:49:ASP:OD1	26:X:52:ARG:NH2	2.39	0.55
28:Z:66:ILE:HG22	46:r:39:GLU:OE1	2.06	0.55
44:p:99:ARG:NE	44:p:104:CYS:SG	2.79	0.55
12:J:48:PRO:O	12:J:53:LYS:NZ	2.39	0.55
15:M:56:LYS:NZ	15:M:94:TYR:OH	2.36	0.55
20:R:55:ILE:CG2	20:R:66:ILE:HD12	2.37	0.55
22:T:38:GLY:N	22:T:62:GLU:OE2	2.39	0.55
35:g:123:GLN:HB3	35:g:128:VAL:HG21	1.88	0.55
1:1:1055:G:O6	1:1:1105:U:O4	2.24	0.55
2:2:1183:U:O2'	2:2:1185:G:OP2	2.24	0.55
28:Z:46:GLY:O	28:Z:49:ARG:HG3	2.06	0.55
1:1:324:A:OP2	1:1:1205:A:N6	2.39	0.54
1:1:2052:A:C8	6:D:146:ILE:HD11	2.43	0.54
1:1:2902:C:N4	1:1:2903:U:O4	2.39	0.54
2:2:516:PSU:N1	2:2:533:A:N7	2.53	0.54
6:D:152:PRO:O	6:D:154:LYS:N	2.40	0.54
36:h:146:ARG:O	36:h:150:LYS:HG3	2.08	0.54
1:1:1062:G:C6	1:1:1063:G:C6	2.96	0.54
1:1:2112:G:P	1:1:2119:A:H2'	2.48	0.54
2:2:933:G:N7	39:k:3:ARG:NE	2.55	0.54
9:G:102:VAL:HG22	9:G:116:GLN:OE1	2.07	0.54
10:H:57:LYS:HD2	10:H:58:LEU:N	2.23	0.54
54:z:44:G:O2'	54:z:45:U:P	2.66	0.54
1:1:2683:C:OP1	17:O:51:ARG:NH2	2.34	0.54
1:1:1064:C:O2'	1:1:1065:U:O5'	2.24	0.54
1:1:2148:G:H2'	1:1:2149:U:C6	2.43	0.54
2:2:1251:A:N3	2:2:1369:C:O2'	2.38	0.54
19:Q:52:PRO:HD2	19:Q:53:PHE:H	1.72	0.54
51:w:3:ARG:NH1	51:w:9:PRO:O	2.40	0.54
54:z:17:OMG:HM22	54:z:69:G:H1	1.72	0.54
1:1:721:A:H2'	1:1:722:A:C8	2.43	0.54
1:1:1173:U:O2	1:1:1174:U:N3	2.31	0.54
1:1:1754:A:O3'	17:O:103:ARG:NH2	2.39	0.54
1:1:2100:G:C6	1:1:2190:G:C6	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:43:ILE:HD12	12:J:56:ASP:HB2	1.88	0.54
22:T:36:VAL:CG1	22:T:39:ILE:HD12	2.37	0.54
5:C:117:GLN:O	5:C:128:ASN:ND2	2.36	0.54
35:g:155:GLY:O	35:g:196:ILE:HG12	2.07	0.54
44:p:4:VAL:O	44:p:8:VAL:HG23	2.07	0.54
1:1:631:A:N3	1:1:2415:G:O2'	2.38	0.54
1:1:811:U:O4	13:K:21:ARG:NH1	2.41	0.54
1:1:1173:U:H4'	1:1:1174:U:H5'	1.90	0.54
1:1:2171:A:O2'	1:1:2173:A:OP1	2.26	0.54
40:l:35:ALA:O	40:l:39:VAL:HG23	2.08	0.54
46:r:46:LEU:O	46:r:50:THR:HG23	2.08	0.54
1:1:2308:G:O6	1:1:2311:A:N7	2.41	0.54
2:2:1359:C:OP2	46:r:75:ARG:NE	2.41	0.54
24:V:59:LEU:CD1	24:V:80:ILE:HD12	2.38	0.54
30:b:15:ALA:HB2	30:b:47:VAL:HG11	1.90	0.54
2:2:881:G:OP2	44:p:9:ARG:NH1	2.41	0.54
10:H:54:LEU:HD12	10:H:57:LYS:CE	2.38	0.54
28:Z:16:CYS:SG	28:Z:17:SER:N	2.81	0.54
37:i:111:MET:HA	37:i:114:VAL:HG12	1.88	0.54
1:1:639:U:H2'	1:1:640:C:C6	2.42	0.53
1:1:2250:G:OP1	14:L:84:LYS:NZ	2.29	0.53
2:2:496:A:H2'	2:2:496:A:N3	2.22	0.53
31:c:35:ARG:HG3	31:c:42:LEU:HD11	1.90	0.53
44:p:56:ARG:NE	44:p:62:GLU:OE1	2.39	0.53
1:1:881:G:H2'	1:1:882:G:O4'	2.08	0.53
1:1:2402:U:O2'	1:1:2403:C:H5"	2.08	0.53
1:1:2822:G:OP1	6:D:164:GLN:NE2	2.41	0.53
49:u:48:ASP:OD2	49:u:75:LEU:HD21	2.08	0.53
54:z:1:G:O2'	54:z:2:G:P	2.66	0.53
1:1:1915:3TD:H2'	1:1:1916:A:O4'	2.09	0.53
2:2:216:U:H2'	2:2:217:C:C6	2.43	0.53
2:2:1119:C:OP2	41:m:11:ARG:NH1	2.41	0.53
1:1:989:G:OP2	27:Y:12:SER:OG	2.24	0.53
31:c:24:THR:HG23	31:c:27:GLY:H	1.74	0.53
1:1:797:G:OP1	7:E:55:SER:OG	2.23	0.53
1:1:1075:C:H2'	1:1:1076:C:C6	2.43	0.53
2:2:1222:G:H5"	51:w:78:ARG:HD2	1.89	0.53
9:G:86:LYS:HG2	9:G:132:VAL:HG22	1.91	0.53
16:N:53:THR:HB	16:N:65:THR:HB	1.90	0.53
40:l:48:ASP:OD1	40:l:49:PHE:N	2.42	0.53
1:1:599:A:O2'	1:1:600:G:H5'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:258:ARG:NH2	5:C:263:THR:OG1	2.42	0.53
24:V:26:PHE:N	24:V:29:GLU:OE1	2.37	0.53
1:1:402:A:H2'	1:1:403:U:C5'	2.38	0.53
1:1:1125:G:O6	1:1:1126:A:N6	2.40	0.53
1:1:2148:G:H2'	1:1:2149:U:H6	1.73	0.53
1:1:2149:U:HO2'	1:1:2172:U:H3	1.56	0.53
43:o:19:GLY:C	43:o:82:LEU:HD12	2.34	0.53
44:p:16:VAL:O	44:p:16:VAL:HG13	2.07	0.53
1:1:587:C:OP2	13:K:21:ARG:NH2	2.38	0.53
1:1:1473:G:C6	1:1:1519:G:C6	2.96	0.53
10:H:4:ILE:HD12	10:H:17:ASP:O	2.08	0.53
34:f:129:LEU:HG	34:f:134:ALA:HB2	1.90	0.53
1:1:1450:G:N2	1:1:1452:G:O6	2.41	0.53
1:1:1870:C:HO2'	1:1:1871:A:C1'	2.21	0.53
1:1:2193:G:C6	1:1:2194:U:C4	2.96	0.53
3:3:36:C:N4	3:3:49:C:O2	2.42	0.53
18:P:82:GLY:HA3	18:P:113:ALA:HB1	1.91	0.53
20:R:25:ARG:NH1	20:R:74:ILE:O	2.41	0.53
42:n:90:LEU:HD23	42:n:90:LEU:C	2.34	0.53
1:1:1590:A:H2'	1:1:1591:A:C8	2.44	0.53
5:C:71:LYS:O	5:C:118:SER:OG	2.27	0.53
8:F:64:LYS:HE3	28:Z:5:ILE:HD12	1.91	0.53
23:U:1:MET:HE2	23:U:3:THR:OG1	2.09	0.53
28:Z:51:VAL:HG23	28:Z:52:ALA:N	2.24	0.53
49:u:76:VAL:HG23	49:u:77:ARG:HG2	1.90	0.53
1:1:2162:G:O2'	1:1:2163:A:N7	2.39	0.52
46:r:42:TRP:O	46:r:46:LEU:HD23	2.09	0.52
9:G:2:SER:OG	9:G:3:ARG:N	2.43	0.52
38:j:51:ILE:CD1	38:j:85:ILE:HG21	2.38	0.52
49:u:17:MET:HE3	49:u:20:SER:HB3	1.92	0.52
2:2:542:G:OP1	36:h:10:LYS:NZ	2.42	0.52
41:m:39:PHE:O	41:m:45:ARG:NH2	2.42	0.52
53:y:9:ASN:N	53:y:9:ASN:OD1	2.43	0.52
1:1:2009:A:OP1	20:R:41:LYS:NZ	2.35	0.52
1:1:2478:A:OP2	33:e:2:LYS:NZ	2.25	0.52
2:2:1316:G:N1	2:2:1319:A:OP2	2.40	0.52
34:f:115:LYS:NZ	34:f:152:LYS:O	2.42	0.52
37:i:57:PRO:HA	37:i:60:ILE:HG12	1.91	0.52
54:z:54:A:O2'	54:z:55:C:C5'	2.58	0.52
1:1:1731:G:C2	1:1:1733:G:C4	2.97	0.52
6:D:151:THR:CG2	6:D:152:PRO:HD3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:434:U:O2	1:1:436:C:N4	2.42	0.52
1:1:955:PSU:HN3	1:1:962:G:H1	1.58	0.52
1:1:1437:C:HO2'	1:1:1516:G:HO2'	1.58	0.52
2:2:972:C:O2'	42:n:57:VAL:HG23	2.10	0.52
41:m:62:ASP:C	41:m:63:LEU:HD12	2.34	0.52
1:1:811:U:H2'	13:K:21:ARG:HA	1.90	0.52
1:1:894:U:O2'	1:1:895:U:H2'	2.09	0.52
2:2:516:PSU:H4'	2:2:517:G:OP1	2.09	0.52
10:H:50:ARG:HD3	10:H:50:ARG:N	2.24	0.52
38:j:100:SER:OG	38:j:103:VAL:N	2.34	0.52
46:r:90:ARG:HB2	46:r:92:GLU:OE1	2.09	0.52
1:1:2313:C:H2'	1:1:2314:A:H8	1.74	0.52
2:2:950:U:O5'	45:q:101:ARG:NH2	2.43	0.52
2:2:1458:G:OP1	52:x:30:THR:OG1	2.25	0.52
15:M:118:ARG:NH1	29:a:54:VAL:O	2.43	0.52
42:n:85:ASP:OD1	42:n:86:ALA:N	2.43	0.52
1:1:2168:G:H8	1:1:2168:G:O5'	1.93	0.52
2:2:542:G:O3'	36:h:14:ARG:NH2	2.39	0.52
14:L:53:MET:O	14:L:57:VAL:HG22	2.10	0.52
1:1:793:A:N6	1:1:2073:C:OP1	2.42	0.51
1:1:1094:U:N3	1:1:1097:U:OP2	2.35	0.51
1:1:1540:G:C6	1:1:1541:C:C4	2.98	0.51
2:2:663:A:H61	2:2:742:G:H1	1.56	0.51
2:2:1220:G:P	46:r:53:ARG:HH12	2.33	0.51
26:X:7:ARG:O	26:X:60:LYS:NZ	2.31	0.51
45:q:4:ILE:HG12	45:q:9:ILE:HD12	1.91	0.51
2:2:213:G:C8	2:2:214:C:C5	2.98	0.51
2:2:246:A:C2	2:2:282:A:C5	2.97	0.51
2:2:859:G:OP2	2:2:869:G:N1	2.29	0.51
1:1:1664:A:H2	12:J:1:MET:HE1	1.76	0.51
20:R:13:SER:O	20:R:17:VAL:HG23	2.09	0.51
1:1:355:U:H2'	1:1:356:G:H8	1.76	0.51
1:1:582:A:OP1	18:P:14:HIS:ND1	2.39	0.51
1:1:966:G:C6	1:1:967:U:C4	2.98	0.51
2:2:1166:G:N1	2:2:1169:A:OP2	2.43	0.51
2:2:1309:G:OP2	45:q:98:ARG:NH2	2.44	0.51
34:f:87:CYS:O	34:f:88:ASP:OD1	2.28	0.51
35:g:161:GLU:N	35:g:161:GLU:OE1	2.37	0.51
39:k:12:ILE:HD11	39:k:28:ASN:HD21	1.75	0.51
48:t:6:LEU:HD23	48:t:17:TYR:CB	2.40	0.51
1:1:2098:U:H2'	1:1:2099:U:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1218:C:H2'	2:2:1219:A:C8	2.46	0.51
2:2:1347:G:O2'	2:2:1373:G:O6	2.25	0.51
3:3:40:U:N3	3:3:44:G:OP2	2.35	0.51
10:H:127:GLU:O	10:H:128:HIS:ND1	2.44	0.51
54:z:1:G:O2'	54:z:2:G:O5'	2.24	0.51
54:z:6:G:N2	54:z:80:U:O2	2.43	0.51
54:z:30:C:H2'	54:z:31:G:O4'	2.11	0.51
2:2:1073:U:O2	34:f:103:ASN:ND2	2.43	0.51
24:V:41:ARG:O	24:V:57:HIS:ND1	2.41	0.51
35:g:77:ILE:HG12	35:g:84:VAL:HG21	1.93	0.51
1:1:2053:G:O6	1:1:2614:A:H2	1.94	0.51
2:2:687:A:C2	2:2:704:A:C5	2.98	0.51
35:g:131:ARG:O	35:g:135:LYS:HG2	2.11	0.51
35:g:136:ARG:O	35:g:140:ASN:ND2	2.44	0.51
1:1:527:C:O2'	1:1:2779:U:O2'	2.23	0.51
1:1:2141:G:N1	1:1:2151:U:C2	2.73	0.51
54:z:60:C:HO2'	54:z:71:A:HO2'	1.49	0.51
1:1:1266:G:O2'	1:1:2012:G:O6	2.27	0.51
1:1:2104:C:C5	1:1:2105:U:C4	2.99	0.51
1:1:2140:G:C5	1:1:2152:G:N7	2.79	0.51
1:1:2636:C:H2'	1:1:2637:U:H6	1.76	0.51
2:2:672:U:H2'	2:2:673:A:C8	2.46	0.51
9:G:102:VAL:HG12	9:G:103:ILE:N	2.26	0.51
10:H:87:GLU:OE2	38:j:24:ARG:NH2	2.44	0.51
22:T:7:ARG:O	22:T:25:VAL:HB	2.11	0.51
22:T:72:ILE:HD12	22:T:83:VAL:HG21	1.91	0.51
35:g:51:SER:HB2	35:g:71:ALA:HB3	1.91	0.51
38:j:42:TRP:HB2	38:j:59:TYR:HB2	1.93	0.51
41:m:44:ALA:HA	41:m:47:VAL:HG22	1.93	0.51
1:1:1779:U:H5"	1:1:1780:A:H5"	1.92	0.51
39:k:135:VAL:O	39:k:139:GLU:HG2	2.10	0.51
41:m:39:PHE:O	41:m:45:ARG:NE	2.44	0.51
1:1:1722:A:H2'	1:1:1723:G:O4'	2.10	0.50
2:2:209:U:H3'	2:2:210:C:O2	2.11	0.50
34:f:72:THR:HG22	34:f:93:ASN:C	2.36	0.50
36:h:168:PRO:HG2	36:h:171:LEU:HD12	1.92	0.50
54:z:53:A:H5"	54:z:54:A:C5	2.47	0.50
2:2:2:A:N3	2:2:613:C:O2'	2.41	0.50
2:2:269:C:H2'	2:2:270:A:C8	2.47	0.50
2:2:878:A:OP1	40:l:80:ARG:NH1	2.44	0.50
43:o:60:PRO:HD3	43:o:91:PRO:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2116:G:H22	1:1:2161:C:H5”	1.76	0.50
1:1:2250:G:H5’	1:1:2250:G:N3	2.26	0.50
1:1:2508:G:H1	1:1:2580:PSU:HN3	1.59	0.50
2:2:392:C:OP1	48:t:8:ARG:NH2	2.45	0.50
2:2:459:A:H2’	2:2:460:A:H8	1.76	0.50
2:2:1425:U:H2’	2:2:1426:G:H8	1.76	0.50
8:F:34:ILE:HD12	8:F:96:MET:HG3	1.94	0.50
34:f:128:LYS:HD2	34:f:128:LYS:O	2.11	0.50
37:i:137:VAL:O	37:i:141:ILE:HG12	2.11	0.50
49:u:7:THR:HG21	49:u:60:GLU:OE2	2.11	0.50
18:P:74:ILE:HG21	18:P:110:VAL:HG13	1.93	0.50
54:z:66:5MU:C6	54:z:67:U:C4	3.00	0.50
55:B:15:ASP:O	55:B:16:LYS:C	2.54	0.50
1:1:1418:G:N1	1:1:1579:A:OP2	2.38	0.50
1:1:2512:C:O5’	1:1:2512:C:H6	1.94	0.50
10:H:2:GLN:OE1	10:H:20:ASN:HB2	2.12	0.50
21:S:10:VAL:HG13	21:S:38:ALA:CB	2.40	0.50
38:j:74:LEU:HG	38:j:78:PHE:CE2	2.46	0.50
45:q:16:VAL:HG23	45:q:17:ILE:HD12	1.92	0.50
54:z:44:G:HO2’	54:z:45:U:P	2.34	0.50
1:1:72:U:OP2	26:X:54:LYS:NZ	2.44	0.50
1:1:568:U:O5’	1:1:945:A:N6	2.45	0.50
1:1:1871:A:H1’	1:1:1872:A:C8	2.47	0.50
1:1:2142:A:H3’	1:1:2143:C:C6	2.46	0.50
2:2:109:A:C6	2:2:326:G:C6	3.00	0.50
2:2:1039:G:H2’	2:2:1040:U:C6	2.47	0.50
2:2:1071:C:H2’	2:2:1072:G:H8	1.77	0.50
8:F:134:GLU:OE2	8:F:136:ILE:HD12	2.11	0.50
34:f:23:TRP:CZ3	34:f:25:PRO:HA	2.46	0.50
37:i:150:PRO:HA	37:i:153:VAL:HG22	1.92	0.50
47:s:21:ASP:O	47:s:22:THR:HG22	2.12	0.50
54:z:48:A:C6	54:z:58:A:N1	2.80	0.50
5:C:130:LEU:HD23	5:C:130:LEU:N	2.27	0.50
7:E:8:ALA:HB3	7:E:122:GLU:OE2	2.11	0.50
19:Q:75:VAL:HG22	19:Q:86:GLN:OE1	2.12	0.50
1:1:574:A:N6	1:1:2034:U:OP1	2.36	0.50
1:1:1323:C:OP1	20:R:98:LYS:HE2	2.11	0.50
1:1:2266:A:H4’	1:1:2267:A:N3	2.26	0.50
2:2:966:2MG:HM22	54:z:35:G:C5’	2.41	0.50
48:t:76:LYS:O	48:t:80:LYS:HG2	2.12	0.50
51:w:63:THR:HG22	51:w:64:ASP:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:y:13:ASP:N	53:y:13:ASP:OD1	2.44	0.50
1:1:535:G:C6	1:1:559:G:C6	2.99	0.50
1:1:807:U:OP1	13:K:36:LYS:HE2	2.12	0.50
2:2:1220:G:N2	51:w:54:GLY:O	2.40	0.50
8:F:32:GLU:HG3	8:F:157:THR:O	2.12	0.50
18:P:76:TYR:OH	18:P:92:ARG:NE	2.45	0.50
34:f:129:LEU:HD11	34:f:133:GLU:C	2.36	0.50
36:h:9:LEU:HD13	36:h:32:CYS:SG	2.51	0.50
37:i:156:LYS:HG2	40:l:71:VAL:HG13	1.94	0.50
42:n:90:LEU:HD23	42:n:91:ASP:N	2.26	0.50
1:1:1062:G:C6	1:1:1063:G:O6	2.65	0.49
1:1:1066:U:H2'	1:1:1067:A:H2'	1.92	0.49
1:1:2116:G:O6	1:1:2171:A:C6	2.65	0.49
1:1:2174:C:H2'	1:1:2175:C:C6	2.47	0.49
7:E:152:GLU:CD	7:E:153:LEU:N	2.69	0.49
34:f:17:GLY:O	34:f:38:VAL:HG13	2.12	0.49
34:f:79:ALA:HA	34:f:82:ASP:OD2	2.12	0.49
1:1:11:C:H2'	1:1:12:U:H5'	1.94	0.49
1:1:636:G:N7	13:K:109:LYS:HE2	2.27	0.49
1:1:1935:G:N2	1:1:1962:5MC:O2'	2.38	0.49
1:1:2451:A:OP1	1:1:2497:A:N6	2.44	0.49
2:2:127:G:O2'	49:u:6:ARG:NH1	2.45	0.49
2:2:203:G:N2	2:2:215:C:C2	2.80	0.49
2:2:632:U:H5"	2:2:633:G:C8	2.47	0.49
1:1:301:G:C6	1:1:317:G:C6	3.00	0.49
1:1:1028:A:H2'	1:1:1029:A:C8	2.48	0.49
1:1:1469:A:H2'	1:1:1470:A:C8	2.46	0.49
1:1:2376:A:N3	16:N:111:ARG:NH1	2.60	0.49
1:1:2185:U:H2'	1:1:2186:G:C8	2.47	0.49
2:2:71:A:N1	2:2:99:C:O2'	2.42	0.49
2:2:73:C:C6	2:2:73:C:H5"	2.48	0.49
2:2:1008:U:N3	2:2:1022:A:C2	2.80	0.49
3:3:76:G:OP1	23:U:13:GLY:N	2.32	0.49
5:C:232:HIS:CG	5:C:240:PHE:HE1	2.30	0.49
7:E:48:THR:O	7:E:52:VAL:HG23	2.12	0.49
8:F:149:VAL:HG23	8:F:149:VAL:O	2.11	0.49
34:f:130:THR:HG23	34:f:133:GLU:HB3	1.93	0.49
36:h:69:GLU:OE2	36:h:204:TYR:OH	2.21	0.49
51:w:50:ALA:HB1	51:w:57:HIS:HB3	1.94	0.49
54:z:75:C:N4	54:z:76:C:H41	2.11	0.49
1:1:307:G:N1	1:1:310:A:OP2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:792:A:N3	1:1:2072:C:O2'	2.43	0.49
1:1:1781:U:H5	31:c:1:MET:HE1	1.77	0.49
1:1:2313:C:H2'	1:1:2314:A:C8	2.46	0.49
52:x:32:ILE:HG12	52:x:54:MET:HE2	1.94	0.49
1:1:195:A:H61	1:1:198:C:H3'	1.77	0.49
1:1:859:G:O2'	1:1:916:G:O6	2.28	0.49
1:1:1383:A:N3	1:1:1405:U:O2'	2.45	0.49
1:1:1682:G:OP2	1:1:1699:G:N2	2.44	0.49
1:1:2146:C:O2'	1:1:2147:A:O5'	2.21	0.49
2:2:1052:U:O2'	2:2:1055:A:OP2	2.11	0.49
3:3:24:G:N7	3:3:56:G:H2'	2.27	0.49
9:G:170:ARG:NH2	33:e:28:SER:O	2.42	0.49
10:H:91:PHE:O	10:H:123:ARG:NH1	2.45	0.49
47:s:25:THR:HG23	47:s:66:LEU:HD22	1.95	0.49
54:z:86:C:O2'	54:z:87:C:H5'	2.12	0.49
1:1:548:G:H3'	1:1:549:G:O4'	2.12	0.49
1:1:636:G:N1	13:K:76:GLU:OE1	2.37	0.49
1:1:653:U:H5	1:1:654:A:H62	1.60	0.49
22:T:43:LYS:HG2	22:T:60:GLU:OE1	2.12	0.49
26:X:18:LEU:O	26:X:18:LEU:HD23	2.12	0.49
35:g:7:PRO:HA	35:g:10:ILE:HG22	1.95	0.49
1:1:1276:A:O2'	15:M:16:HIS:NE2	2.45	0.49
1:1:1278:C:O2'	15:M:27:SER:OG	2.26	0.49
1:1:1432:G:H2'	1:1:1433:A:C8	2.48	0.49
1:1:1582:C:H42	1:1:1583:A:N6	2.11	0.49
1:1:1827:U:OP2	5:C:221:ARG:NE	2.45	0.49
1:1:2118:U:H5"	1:1:2148:G:O2'	2.12	0.49
2:2:1145:A:O2'	2:2:1146:A:O4'	2.31	0.49
2:2:1244:G:C6	2:2:1294:G:C6	3.01	0.49
8:F:19:GLU:O	8:F:19:GLU:HG2	2.13	0.49
34:f:130:THR:HG23	34:f:130:THR:O	2.12	0.49
36:h:146:ARG:CG	36:h:147:GLU:N	2.75	0.49
42:n:17:LEU:HD21	42:n:96:VAL:HG23	1.95	0.49
54:z:26:A:H2'	54:z:27:G:O4'	2.13	0.49
1:1:1065:U:O2'	1:1:1066:U:C6	2.65	0.49
1:1:1315:C:O2'	1:1:1392:A:N3	2.44	0.49
1:1:1357:C:H2'	1:1:1358:G:O4'	2.13	0.49
1:1:2128:G:H2'	1:1:2129:C:O4'	2.13	0.49
1:1:2849:U:N3	1:1:2867:G:O4'	2.45	0.49
10:H:40:THR:OG1	10:H:43:ASN:HB3	2.13	0.49
19:Q:52:PRO:CD	19:Q:53:PHE:H	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:43:LYS:CG	22:T:60:GLU:OE1	2.61	0.49
54:z:51:G:H5"	54:z:52:C:C5	2.48	0.49
1:1:84:A:N1	1:1:98:G:O2'	2.42	0.49
1:1:894:U:OP2	1:1:894:U:H2'	2.13	0.49
21:S:93:LEU:HD23	21:S:94:ASP:N	2.28	0.49
26:X:32:ALA:HB2	26:X:37:LEU:HD23	1.94	0.49
42:n:7:ARG:HB2	42:n:101:SER:HB2	1.94	0.49
1:1:284:U:C2	1:1:285:G:C8	3.01	0.48
1:1:324:A:N6	1:1:338:G:O2'	2.44	0.48
1:1:411:G:OP2	1:1:2406:A:O2'	2.28	0.48
1:1:1007:C:OP1	11:I:37:ARG:NH2	2.45	0.48
1:1:1712:U:OP2	1:1:1713:A:O2'	2.28	0.48
1:1:2520:C:C6	1:1:2567:G:H1'	2.48	0.48
5:C:133:ARG:NE	5:C:187:ASP:OD1	2.34	0.48
10:H:3:VAL:HG23	10:H:37:VAL:O	2.13	0.48
21:S:33:LYS:HG3	21:S:80:TRP:CE3	2.48	0.48
37:i:76:LEU:HD21	37:i:120:VAL:HG23	1.94	0.48
37:i:160:SER:O	37:i:164:ILE:HG13	2.13	0.48
38:j:18:VAL:HB	38:j:19:PRO:HD3	1.95	0.48
1:1:613:A:O4'	1:1:614:A:C8	2.66	0.48
1:1:635:C:H2'	1:1:636:G:O4'	2.14	0.48
1:1:1358:G:C8	1:1:1371:G:O6	2.65	0.48
1:1:2102:G:H2'	1:1:2102:G:N3	2.28	0.48
32:d:26:HIS:CE1	32:d:48:ALA:HB2	2.47	0.48
43:o:96:THR:HG23	43:o:97:ILE:N	2.27	0.48
48:t:34:GLU:OE1	48:t:60:TRP:NE1	2.43	0.48
2:2:842:U:C2'	2:2:844:G:H21	2.25	0.48
21:S:14:PRO:HD3	26:X:30:MET:SD	2.53	0.48
1:1:510:C:C2'	1:1:511:U:H5'	2.44	0.48
1:1:1156:A:C8	18:P:51:ARG:HG2	2.49	0.48
1:1:1590:A:H2'	1:1:1591:A:H8	1.76	0.48
1:1:2116:G:N1	1:1:2162:G:OP2	2.42	0.48
2:2:214:C:H2'	2:2:215:C:H6	1.78	0.48
15:M:114:GLU:OE1	15:M:118:ARG:NH1	2.46	0.48
16:N:100:HIS:CD2	16:N:101:GLY:N	2.82	0.48
40:l:55:THR:HG23	40:l:56:LYS:N	2.28	0.48
54:z:79:C:H2'	54:z:80:U:C6	2.48	0.48
1:1:287:G:H2'	1:1:288:U:C6	2.48	0.48
2:2:212:G:C2	2:2:213:G:C8	3.02	0.48
2:2:518:C:O2'	2:2:530:G:N2	2.35	0.48
2:2:579:A:H2'	2:2:580:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:720:C:OP2	2:2:721:G:O2'	2.31	0.48
9:G:104:ASN:ND2	9:G:114:ASP:OD1	2.42	0.48
35:g:42:TYR:CE2	35:g:90:VAL:HG21	2.48	0.48
36:h:95:GLU:HA	36:h:100:ASN:ND2	2.28	0.48
49:u:17:MET:HG3	49:u:20:SER:HB2	1.96	0.48
54:z:27:G:C4	54:z:28:C:C5	3.01	0.48
1:1:170:U:H2'	1:1:171:U:C6	2.49	0.48
1:1:2029:G:N1	1:1:2033:A:OP2	2.38	0.48
2:2:459:A:H2'	2:2:460:A:C8	2.48	0.48
39:k:17:LYS:HG3	39:k:18:PHE:CE1	2.48	0.48
41:m:118:LEU:HD12	41:m:118:LEU:N	2.29	0.48
48:t:69:ASP:OD1	48:t:69:ASP:N	2.47	0.48
54:z:20:U:H6	54:z:20:U:H5'	1.77	0.48
55:B:11:TRP:O	55:B:14:ALA:N	2.47	0.48
1:1:48:G:N2	1:1:177:G:OP2	2.47	0.48
1:1:601:C:H2'	1:1:602:A:O4'	2.14	0.48
1:1:613:A:H4'	1:1:614:A:OP1	2.13	0.48
1:1:1394:U:H4'	1:1:1603:A:H4'	1.96	0.48
1:1:1936:A:OP2	1:1:1962:5MC:N4	2.42	0.48
2:2:85:U:H1'	2:2:86:G:N7	2.29	0.48
2:2:950:U:C5	45:q:101:ARG:NH1	2.81	0.48
21:S:93:LEU:HD23	21:S:94:ASP:O	2.14	0.48
32:d:32:ILE:O	32:d:32:ILE:HG22	2.13	0.48
35:g:10:ILE:HG23	35:g:11:ARG:CD	2.43	0.48
35:g:87:LEU:HA	35:g:90:VAL:HG22	1.95	0.48
37:i:56:VAL:HB	37:i:57:PRO:HD3	1.96	0.48
41:m:130:ARG:NH1	54:z:34:U:OP2	2.45	0.48
1:1:285:G:C6	1:1:356:G:C6	3.01	0.48
1:1:1074:G:H2'	1:1:1075:C:C6	2.49	0.48
1:1:2116:G:C6	1:1:2164:C:C6	3.02	0.48
1:1:2118:U:C2	1:1:2147:A:N1	2.82	0.48
1:1:2595:G:N2	1:1:2598:A:OP2	2.36	0.48
2:2:1060:U:H2'	2:2:1061:G:H8	1.79	0.48
2:2:1391:U:H2'	2:2:1392:G:C8	2.48	0.48
2:2:1519:MA6:O5'	2:2:1519:MA6:H8	2.12	0.48
16:N:29:HIS:HB3	16:N:36:TYR:HB2	1.96	0.48
28:Z:18:CYS:SG	28:Z:20:ASN:HB2	2.54	0.48
43:o:86:VAL:HG11	43:o:93:ARG:HE	1.79	0.48
54:z:29:A:O2'	54:z:30:C:H5'	2.14	0.48
1:1:396:G:OP2	25:W:10:LYS:NZ	2.47	0.48
1:1:2591:C:H2'	1:1:2592:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:559:A:H4'	2:2:560:A:H3'	1.94	0.48
2:2:1518:MA6:O5'	2:2:1518:MA6:H8	2.14	0.48
9:G:86:LYS:C	9:G:87:LEU:HD12	2.39	0.48
39:k:47:LEU:HB3	39:k:58:GLU:HB3	1.95	0.48
46:r:10:GLU:O	46:r:14:VAL:HG23	2.14	0.48
54:z:17:OMG:O3'	54:z:17:OMG:CM2	2.60	0.48
54:z:48:A:C6	54:z:49:C:C4	3.01	0.48
1:1:362:A:C4	1:1:363:G:C8	3.02	0.48
1:1:1519:G:C6	1:1:1520:U:C4	3.02	0.48
1:1:2425:A:H5"	1:1:2427:C:O4'	2.14	0.48
2:2:126:G:OP1	2:2:605:U:O2'	2.26	0.48
2:2:685:G:N1	2:2:704:A:OP2	2.46	0.48
13:K:29:LYS:HG3	13:K:30:THR:HG23	1.96	0.48
45:q:4:ILE:HG13	45:q:9:ILE:HD12	1.95	0.48
1:1:1746:A:H2'	1:1:1747:U:C6	2.49	0.47
1:1:2305:U:HO2'	8:F:133:ARG:HH11	1.58	0.47
1:1:2515:C:H2'	1:1:2516:A:H8	1.79	0.47
2:2:477:C:H2'	2:2:478:A:C8	2.49	0.47
2:2:713:G:H2'	2:2:714:G:C8	2.49	0.47
2:2:780:A:C2	2:2:801:U:C5	3.02	0.47
2:2:946:A:H2'	2:2:947:G:C8	2.48	0.47
11:I:114:LEU:HG	11:I:118:MET:HE3	1.96	0.47
14:L:1:MET:HE3	14:L:44:ARG:HG3	1.96	0.47
49:u:19:LYS:HA	49:u:48:ASP:O	2.13	0.47
1:1:402:A:C2'	1:1:403:U:H5'	2.43	0.47
1:1:1370:C:H2'	1:1:1371:G:O4'	2.13	0.47
1:1:1444:G:C4	1:1:1445:G:C8	3.02	0.47
1:1:2109:U:H5"	1:1:2110:G:OP1	2.13	0.47
1:1:2457:PSU:HN3	1:1:2494:G:H1	1.60	0.47
1:1:2561:U:O3'	12:J:40:LYS:NZ	2.45	0.47
1:1:2602:A:H4'	1:1:2603:G:O5'	2.13	0.47
2:2:246:A:N1	2:2:278:G:O2'	2.45	0.47
2:2:514:C:H2'	2:2:515:G:H8	1.79	0.47
3:3:43:C:H5"	28:Z:1:MET:HG2	1.96	0.47
8:F:47:LYS:HE2	8:F:47:LYS:HA	1.96	0.47
1:1:271:G:C6	1:1:367:G:C6	3.02	0.47
1:1:657:U:H2'	1:1:658:U:C6	2.49	0.47
1:1:732:C:H2'	1:1:733:G:O4'	2.13	0.47
1:1:1020:A:N1	1:1:1141:U:O2'	2.34	0.47
1:1:1090:A:C2	1:1:1102:C:H1'	2.49	0.47
28:Z:48:GLN:OE1	28:Z:48:GLN:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:z:9:G:N2	54:z:13:G:H1	2.11	0.47
1:1:1105:U:H2'	1:1:1106:G:H8	1.79	0.47
1:1:1125:G:C6	1:1:1126:A:N6	2.82	0.47
1:1:1426:G:O2'	1:1:1572:A:N6	2.40	0.47
2:2:108:G:H5'	2:2:109:A:H5"	1.95	0.47
2:2:664:G:H22	2:2:741:G:H1	1.62	0.47
15:M:38:LEU:HB3	15:M:39:PRO:HD3	1.95	0.47
36:h:170:TRP:CD2	36:h:186:PRO:HB3	2.49	0.47
1:1:77:G:O3'	26:X:7:ARG:NH2	2.47	0.47
1:1:282:A:C6	1:1:359:G:C6	3.02	0.47
1:1:322:A:P	7:E:162:ARG:HH11	2.37	0.47
1:1:571:U:C5	1:1:2030:6MZ:H9	2.49	0.47
1:1:1053:C:H2'	1:1:1054:A:H8	1.79	0.47
1:1:2540:C:O2'	1:1:2740:A:N3	2.44	0.47
2:2:496:A:O2'	2:2:497:G:C8	2.65	0.47
2:2:1032:G:N2	2:2:1033:G:C1'	2.77	0.47
10:H:50:ARG:HB2	10:H:51:ARG:HD2	1.96	0.47
10:H:58:LEU:HA	10:H:61:VAL:HG12	1.96	0.47
10:H:122:LEU:HD22	10:H:122:LEU:N	2.30	0.47
25:W:6:GLN:O	25:W:74:ARG:NH2	2.45	0.47
25:W:51:VAL:HG22	25:W:52:SER:O	2.14	0.47
43:o:16:VAL:HG13	43:o:79:ILE:HG12	1.97	0.47
54:z:31:G:H1	54:z:41:U:H3	1.61	0.47
1:1:704:G:O2'	1:1:726:G:N2	2.44	0.47
1:1:1000:A:N6	1:1:1155:A:C8	2.83	0.47
1:1:2795:C:H2'	1:1:2796:U:C6	2.50	0.47
2:2:1223:C:OP1	51:w:78:ARG:NH1	2.47	0.47
10:H:40:THR:O	10:H:44:ILE:HG12	2.15	0.47
21:S:10:VAL:HG13	21:S:38:ALA:HB2	1.96	0.47
52:x:32:ILE:HG12	52:x:54:MET:CE	2.45	0.47
1:1:601:C:O5'	1:1:601:C:H6	1.98	0.47
1:1:1059:G:P	1:1:1060:U:H3'	2.55	0.47
1:1:1538:G:H2'	1:1:1539:U:C6	2.50	0.47
1:1:1799:G:N2	5:C:154:LEU:HD23	2.30	0.47
1:1:2109:U:H2'	1:1:2110:G:C8	2.49	0.47
1:1:2328:A:H2'	1:1:2329:U:C6	2.49	0.47
1:1:2880:C:O2'	15:M:90:ARG:NH2	2.36	0.47
2:2:280:C:N4	49:u:41:THR:OG1	2.47	0.47
2:2:309:A:H2'	2:2:310:G:H8	1.80	0.47
2:2:857:C:H2'	2:2:858:G:O4'	2.15	0.47
3:3:48:U:P	16:N:30:ARG:HH22	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:132:MET:HG2	5:C:135:ILE:HD12	1.97	0.47
8:F:53:ALA:HA	8:F:150:ARG:HE	1.78	0.47
20:R:80:PRO:O	20:R:100:THR:OG1	2.32	0.47
34:f:218:ALA:HA	34:f:221:VAL:HG22	1.97	0.47
35:g:160:ALA:HB3	35:g:164:ARG:HH22	1.80	0.47
36:h:27:ALA:HB3	36:h:30:THR:HG23	1.95	0.47
41:m:15:SER:OG	41:m:78:ALA:HB2	2.14	0.47
45:q:49:SER:OG	45:q:52:GLN:HG3	2.15	0.47
51:w:13:LEU:HD23	51:w:14:HIS:H	1.78	0.47
53:y:69:ARG:C	53:y:70:LEU:HD22	2.40	0.47
54:z:52:C:H4'	54:z:53:A:OP1	2.14	0.47
1:1:12:U:H2'	1:1:13:A:H5'	1.96	0.47
1:1:2190:G:H2'	1:1:2191:A:H8	1.80	0.47
1:1:2636:C:H2'	1:1:2637:U:C6	2.50	0.47
1:1:2804:U:H2'	1:1:2805:C:C6	2.50	0.47
7:E:1:MET:HB3	7:E:14:VAL:HG23	1.97	0.47
36:h:143:VAL:HG23	36:h:143:VAL:O	2.14	0.47
1:1:137:U:C2'	1:1:138:U:H5'	2.44	0.47
1:1:1057:A:C2	1:1:1082:U:C5	3.03	0.47
1:1:1077:A:N6	1:1:1078:U:O2	2.47	0.47
1:1:1169:A:H62	1:1:1180:U:H3	1.62	0.47
1:1:1754:A:O2'	17:O:103:ARG:NH2	2.48	0.47
1:1:2150:C:H2'	1:1:2151:U:N1	2.30	0.47
1:1:2519:U:O4'	1:1:2542:A:N6	2.48	0.47
1:1:2523:G:HO2'	1:1:2764:A:HO2'	1.55	0.47
2:2:1280:A:OP1	42:n:9:ARG:NH1	2.46	0.47
2:2:1417:G:O2'	2:2:1483:A:N6	2.45	0.47
3:3:48:U:OP1	16:N:30:ARG:NH2	2.41	0.47
11:I:89:PHE:O	11:I:93:ILE:HG12	2.14	0.47
40:l:54:ASP:OD1	40:l:54:ASP:N	2.46	0.47
44:p:87:VAL:CG1	44:p:90:LEU:HD12	2.40	0.47
53:y:4:ILE:HD12	53:y:19:PHE:CD1	2.38	0.47
1:1:856:G:H2'	1:1:857:G:C8	2.50	0.47
1:1:1196:C:H2'	1:1:1197:G:O4'	2.15	0.47
1:1:1418:G:N2	1:1:1579:A:C8	2.83	0.47
1:1:2190:G:H2'	1:1:2191:A:C8	2.50	0.47
2:2:686:U:O4	2:2:703:G:O2'	2.27	0.47
10:H:116:ARG:NH1	10:H:133:GLN:HB3	2.30	0.47
22:T:33:LYS:HE2	22:T:66:GLN:OE1	2.15	0.47
35:g:19:ASN:OD1	35:g:54:ARG:NE	2.45	0.47
45:q:46:SER:C	45:q:47:GLU:HG3	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B:1:FME:C	55:B:3:GLY:N	2.78	0.47
1:1:1051:G:C5	1:1:1052:C:C5	3.03	0.46
1:1:2128:G:C2	1:1:2173:A:O2'	2.67	0.46
1:1:2532:G:O2'	1:1:2657:A:N1	2.48	0.46
1:1:2780:G:OP2	11:I:120:ARG:NE	2.36	0.46
2:2:355:C:C4	2:2:356:A:N7	2.83	0.46
2:2:489:C:H2'	2:2:490:C:H6	1.80	0.46
2:2:844:G:N1	2:2:846:G:H1'	2.30	0.46
6:D:64:GLU:HG2	6:D:68:PHE:HE2	1.80	0.46
54:z:42:G:O2'	54:z:43:U:H5'	2.15	0.46
1:1:952:G:C6	1:1:966:G:C6	3.02	0.46
1:1:1796:U:H2'	1:1:1797:G:H8	1.80	0.46
1:1:2178:C:H2'	1:1:2179:C:C6	2.50	0.46
1:1:2183:A:H2'	1:1:2184:A:C8	2.50	0.46
1:1:2766:A:C5	1:1:2767:C:C5	3.04	0.46
2:2:1345:U:OP1	41:m:122:ARG:NH1	2.47	0.46
8:F:122:PHE:O	8:F:123:ASP:OD1	2.32	0.46
10:H:66:ASN:OD1	10:H:66:ASN:C	2.56	0.46
10:H:76:GLU:O	10:H:143:ILE:HG12	2.14	0.46
10:H:125:THR:HA	10:H:146:VAL:HG23	1.97	0.46
13:K:127:VAL:HG12	13:K:128:THR:O	2.15	0.46
15:M:12:ARG:O	15:M:17:ARG:NH2	2.48	0.46
35:g:11:ARG:NH2	35:g:177:THR:O	2.35	0.46
36:h:3:ARG:HD2	36:h:115:ARG:HE	1.80	0.46
1:1:2195:U:O2'	1:1:2196:C:H5'	2.15	0.46
9:G:18:LYS:HG2	9:G:25:THR:HB	1.96	0.46
30:b:28:ARG:N	30:b:28:ARG:HD2	2.30	0.46
45:q:22:ILE:HB	45:q:25:VAL:HG22	1.96	0.46
52:x:31:PHE:O	52:x:35:VAL:HG23	2.15	0.46
1:1:364:C:H2'	1:1:365:U:C6	2.51	0.46
1:1:546:U:H3'	1:1:548:G:C6	2.50	0.46
1:1:1061:U:O3'	1:1:1070:A:H4'	2.15	0.46
1:1:1095:A:O2'	1:1:1096:A:O4'	2.33	0.46
1:1:1217:U:OP1	18:P:15:LYS:NZ	2.41	0.46
1:1:2591:C:H2'	1:1:2592:G:C8	2.50	0.46
2:2:792:A:O2'	2:2:794:A:N7	2.42	0.46
3:3:37:C:N3	3:3:48:U:O2'	2.48	0.46
7:E:5:LEU:HD22	7:E:122:GLU:OE2	2.15	0.46
8:F:142:ASP:OD1	8:F:143:TYR:N	2.48	0.46
35:g:157:LEU:HB2	35:g:164:ARG:CZ	2.46	0.46
39:k:74:GLU:HG2	39:k:91:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:n:28:THR:CG2	42:n:87:LEU:HD21	2.45	0.46
52:x:35:VAL:HG11	52:x:79:LEU:HD13	1.97	0.46
54:z:56:G:C2	54:z:57:U:C6	3.03	0.46
1:1:1153:C:H2'	1:1:1154:G:O4'	2.16	0.46
1:1:2204:G:OP2	5:C:147:LYS:NZ	2.38	0.46
2:2:515:G:H3'	2:2:516:PSU:O4	2.15	0.46
11:I:34:ARG:NH2	11:I:40:HIS:HB3	2.31	0.46
19:Q:52:PRO:O	19:Q:53:PHE:CD2	2.68	0.46
22:T:99:ASN:C	22:T:99:ASN:OD1	2.58	0.46
47:s:21:ASP:O	47:s:23:GLY:N	2.49	0.46
48:t:46:LYS:N	48:t:46:LYS:HD2	2.31	0.46
54:z:54:A:H2'	54:z:54:A:N3	2.31	0.46
1:1:201:C:OP1	25:W:18:ARG:NH1	2.49	0.46
1:1:563:A:C2'	18:P:37:GLN:HE21	2.28	0.46
1:1:980:A:N7	1:1:1136:G:H5'	2.31	0.46
2:2:68:G:N7	2:2:69:G:C8	2.83	0.46
2:2:270:A:C6	2:2:271:C:C4	3.03	0.46
2:2:979:C:O5'	2:2:979:C:C6	2.69	0.46
6:D:153:GLY:O	6:D:154:LYS:HB3	2.14	0.46
7:E:200:LEU:HD12	7:E:200:LEU:N	2.29	0.46
40:l:121:LEU:HD12	40:l:121:LEU:O	2.15	0.46
42:n:82:LYS:HA	42:n:85:ASP:OD1	2.15	0.46
1:1:2144:G:O2'	1:1:2147:A:N6	2.49	0.46
2:2:74:A:C4	2:2:75:G:C8	3.04	0.46
2:2:556:C:H2'	2:2:557:G:O4'	2.14	0.46
2:2:1309:G:P	45:q:87:ARG:HH11	2.38	0.46
24:V:10:THR:HG22	24:V:11:ARG:N	2.31	0.46
26:X:18:LEU:HD23	26:X:18:LEU:C	2.40	0.46
34:f:66:LYS:O	34:f:159:ASP:OD1	2.34	0.46
34:f:68:LEU:HD11	34:f:92:VAL:HG23	1.98	0.46
34:f:130:THR:CG2	34:f:133:GLU:HB3	2.45	0.46
34:f:196:VAL:HB	34:f:199:VAL:HG22	1.98	0.46
43:o:70:CYS:O	43:o:74:VAL:HG22	2.16	0.46
49:u:61:ILE:HA	49:u:75:LEU:HA	1.98	0.46
1:1:1485:U:H2'	1:1:1486:U:C6	2.50	0.46
2:2:1130:A:O2'	41:m:5:GLN:NE2	2.48	0.46
2:2:1145:A:O2'	2:2:1146:A:O5'	2.33	0.46
2:2:1270:G:HO2'	2:2:1313:U:HO2'	1.61	0.46
5:C:205:LEU:N	5:C:205:LEU:HD12	2.31	0.46
37:i:39:VAL:HG12	37:i:40:GLY:N	2.31	0.46
38:j:4:TYR:HD1	38:j:91:ARG:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2798:U:H4'	1:1:2799:A:H5'	1.97	0.46
2:2:258:G:H2'	2:2:259:G:O4'	2.15	0.46
2:2:580:C:H2'	2:2:581:G:O4'	2.16	0.46
2:2:869:G:O5'	2:2:869:G:H8	1.99	0.46
2:2:1032:G:H3'	2:2:1032:G:N3	2.31	0.46
5:C:80:ARG:NE	5:C:82:GLU:OE2	2.44	0.46
9:G:103:ILE:CD1	9:G:117:LEU:HD21	2.44	0.46
10:H:8:LYS:HA	10:H:14:SER:HA	1.98	0.46
10:H:117:LEU:HD22	10:H:120:GLY:HA2	1.96	0.46
28:Z:58:ASP:OD1	28:Z:58:ASP:C	2.59	0.46
34:f:207:ILE:O	34:f:210:VAL:HG22	2.16	0.46
40:l:13:ARG:NH1	40:l:26:THR:O	2.49	0.46
45:q:106:ALA:HB3	45:q:110:LYS:CD	2.44	0.46
1:1:335:C:O2	22:T:68:SER:OG	2.34	0.46
1:1:545:U:HO2'	1:1:547:A:P	2.39	0.46
1:1:897:C:H2'	1:1:898:C:C6	2.51	0.46
1:1:1069:A:N1	1:1:1096:A:H5'	2.31	0.46
1:1:1099:G:C6	1:1:1100:C:C4	3.04	0.46
1:1:1824:G:OP1	5:C:52:ARG:HG3	2.15	0.46
1:1:2467:C:O2	14:L:123:LYS:NZ	2.50	0.46
2:2:41:G:H2'	2:2:42:G:H8	1.81	0.46
2:2:1288:A:N3	2:2:1352:C:O2'	2.45	0.46
3:3:1:U:O2'	3:3:2:G:H8	1.98	0.46
21:S:14:PRO:HA	21:S:32:LEU:HD23	1.98	0.46
35:g:8:ASN:O	35:g:12:LEU:HG	2.16	0.46
35:g:121:THR:HG23	35:g:189:ALA:CB	2.46	0.46
51:w:40:ILE:HD12	51:w:66:MET:O	2.15	0.46
1:1:445:C:O2'	1:1:449:A:N3	2.42	0.45
1:1:1278:C:H2'	1:1:1279:G:H8	1.81	0.45
1:1:1532:A:C6	1:1:1540:G:C6	3.03	0.45
5:C:91:ILE:HD12	5:C:103:TYR:CD1	2.51	0.45
10:H:115:VAL:CG1	10:H:117:LEU:HD11	2.44	0.45
13:K:19:LEU:HD23	13:K:31:GLY:HA3	1.98	0.45
18:P:50:ARG:O	18:P:54:LYS:NZ	2.50	0.45
38:j:9:MET:HG2	38:j:59:TYR:CE1	2.52	0.45
39:k:24:ALA:HA	39:k:27:VAL:HG22	1.96	0.45
39:k:69:VAL:HG23	39:k:100:ALA:HB1	1.98	0.45
42:n:52:LEU:HD23	42:n:62:ARG:HG2	1.98	0.45
47:s:21:ASP:OD1	47:s:22:THR:N	2.46	0.45
1:1:674:G:H5"	7:E:71:GLY:N	2.31	0.45
1:1:1048:A:N7	1:1:1111:A:C6	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2150:C:H2'	1:1:2151:U:C1'	2.46	0.45
2:2:247:G:C6	2:2:278:G:C2	3.04	0.45
2:2:269:C:H2'	2:2:270:A:H8	1.80	0.45
2:2:1328:C:H2'	2:2:1329:A:O4'	2.15	0.45
5:C:210:ALA:HA	5:C:213:TRP:CE3	2.51	0.45
8:F:54:ALA:HB1	8:F:65:PRO:HG2	1.98	0.45
14:L:21:ALA:HB2	14:L:97:GLN:HB2	1.99	0.45
28:Z:51:VAL:CG2	28:Z:52:ALA:H	2.28	0.45
42:n:57:VAL:O	42:n:57:VAL:HG13	2.16	0.45
43:o:42:LEU:HD22	43:o:77:TYR:CE2	2.52	0.45
54:z:51:G:O6	54:z:53:A:O4'	2.34	0.45
55:B:4:LYS:O	55:B:8:ILE:HG23	2.16	0.45
1:1:142:A:H2'	1:1:143:C:C6	2.52	0.45
1:1:1589:U:HO2'	1:1:1590:A:H8	1.61	0.45
2:2:707:U:OP1	43:o:87:LYS:NZ	2.29	0.45
2:2:945:G:C2	2:2:946:A:C8	3.03	0.45
2:2:1360:A:OP2	46:r:75:ARG:NH2	2.46	0.45
8:F:56:ASP:HB3	8:F:141:ILE:HD11	1.99	0.45
9:G:155:GLU:HG2	9:G:157:TYR:H	1.80	0.45
10:H:121:VAL:HG13	10:H:122:LEU:N	2.31	0.45
21:S:25:GLU:HG3	21:S:26:LYS:HG3	1.98	0.45
36:h:163:GLU:OE2	36:h:167:LYS:NZ	2.43	0.45
37:i:39:VAL:CG1	37:i:40:GLY:N	2.79	0.45
41:m:46:MET:O	41:m:50:GLN:HG3	2.16	0.45
42:n:15:HIS:HA	42:n:18:ILE:HG22	1.98	0.45
47:s:3:LEU:HB2	47:s:35:GLN:OE1	2.17	0.45
48:t:19:VAL:HG22	48:t:37:GLY:C	2.41	0.45
1:1:137:U:H2'	1:1:138:U:H5'	1.98	0.45
1:1:878:A:H3'	1:1:879:G:H8	1.81	0.45
1:1:1791:A:C2	1:1:1829:A:H4'	2.51	0.45
1:1:2063:C:O2	1:1:2450:A:N1	2.49	0.45
1:1:2160:C:H6	1:1:2160:C:O5'	1.99	0.45
2:2:878:A:P	40:l:80:ARG:HH11	2.39	0.45
5:C:261:LYS:HA	5:C:264:ASP:OD2	2.15	0.45
10:H:51:ARG:HB3	10:H:55:GLU:OE2	2.17	0.45
18:P:80:ILE:O	18:P:84:LYS:HG2	2.16	0.45
21:S:8:LEU:HD23	21:S:50:LEU:HD21	1.97	0.45
24:V:59:LEU:HD13	24:V:80:ILE:HD12	1.99	0.45
27:Y:17:LEU:HD12	27:Y:20:HIS:CE1	2.52	0.45
8:F:37:ASN:HB3	8:F:153:ASP:OD1	2.16	0.45
15:M:85:PRO:HA	15:M:88:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:15:THR:OG1	22:T:69:ASN:OD1	2.33	0.45
34:f:63:ARG:O	34:f:64:LYS:HG2	2.15	0.45
37:i:46:VAL:O	37:i:72:ILE:N	2.44	0.45
37:i:99:ALA:CB	37:i:103:THR:HG21	2.47	0.45
38:j:12:PRO:HB2	38:j:44:ARG:NH1	2.32	0.45
54:z:64:G:C2	54:z:75:C:O2	2.70	0.45
1:1:400:G:N7	25:W:57:ARG:NH1	2.65	0.45
1:1:891:G:C2	1:1:892:A:C8	3.05	0.45
1:1:1536:C:O2	1:1:1537:G:N2	2.50	0.45
1:1:2097:A:C6	1:1:2193:G:C6	3.05	0.45
2:2:41:G:C6	2:2:402:G:C6	3.04	0.45
2:2:511:C:C2	2:2:512:U:C5	3.05	0.45
2:2:978:A:C4	2:2:1319:A:C2	3.04	0.45
2:2:979:C:O5'	2:2:979:C:H6	2.00	0.45
6:D:34:VAL:HB	6:D:92:VAL:O	2.16	0.45
9:G:101:ASN:OD1	9:G:117:LEU:HB2	2.16	0.45
22:T:83:VAL:HG22	22:T:103:ILE:HD11	1.99	0.45
43:o:64:GLN:O	43:o:68:GLU:HG3	2.16	0.45
51:w:63:THR:HG22	51:w:64:ASP:OD1	2.17	0.45
54:z:1:G:H2'	54:z:2:G:O4'	2.17	0.45
54:z:56:G:O2'	54:z:57:U:H5'	2.16	0.45
1:1:138:U:H1'	1:1:141:G:O6	2.17	0.45
1:1:2300:C:O2'	1:1:2301:C:H5'	2.17	0.45
1:1:2619:C:O2	6:D:161:MET:HE1	2.17	0.45
2:2:459:A:C6	2:2:474:G:C6	3.05	0.45
2:2:981:U:OP1	46:r:9:ARG:NH1	2.50	0.45
2:2:1048:G:O6	2:2:1210:C:N4	2.50	0.45
2:2:1256:A:N1	2:2:1277:C:N4	2.64	0.45
5:C:130:LEU:O	5:C:135:ILE:HD11	2.17	0.45
6:D:4:LEU:HD23	6:D:29:VAL:HG11	1.98	0.45
18:P:66:ASN:OD1	18:P:70:ARG:NE	2.50	0.45
22:T:98:SER:O	22:T:99:ASN:OD1	2.35	0.45
27:Y:13:ALA:O	27:Y:21:LYS:HE2	2.16	0.45
37:i:153:VAL:HG21	40:l:99:LEU:HD22	1.98	0.45
39:k:23:LEU:O	39:k:27:VAL:HG13	2.17	0.45
1:1:414:C:H2'	1:1:415:A:C8	2.52	0.45
1:1:1071:G:H2'	1:1:1072:C:C6	2.52	0.45
2:2:94:G:N1	2:2:98:A:C2	2.85	0.45
2:2:1028:C:O2	2:2:1034:G:C2	2.69	0.45
8:F:98:GLU:OE1	28:Z:9:TYR:OH	2.25	0.45
34:f:207:ILE:HA	34:f:210:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:113:ALA:O	37:i:117:VAL:HG22	2.17	0.45
37:i:153:VAL:HG23	37:i:164:ILE:HD13	1.98	0.45
45:q:27:LYS:O	45:q:31:LYS:HG3	2.16	0.45
54:z:9:G:H22	54:z:13:G:H1	1.65	0.45
1:1:1138:G:N2	11:I:108:MET:HE2	2.32	0.45
1:1:1341:G:OP2	1:1:1394:U:O2'	2.28	0.45
1:1:2314:A:H1'	8:F:155:THR:HG21	1.98	0.45
2:2:214:C:C2	2:2:215:C:C5	3.05	0.45
2:2:218:U:H2'	2:2:219:U:O4'	2.16	0.45
2:2:335:C:H2'	2:2:336:A:H8	1.82	0.45
2:2:404:G:O2'	2:2:498:A:N1	2.47	0.45
5:C:161:TYR:HB3	5:C:194:GLU:HG2	1.99	0.45
8:F:10:ASP:OD1	8:F:11:GLU:N	2.50	0.45
12:J:52:VAL:C	12:J:53:LYS:HG2	2.41	0.45
13:K:124:GLY:C	13:K:125:LEU:HD12	2.41	0.45
39:k:57:SER:HB3	39:k:60:GLU:OE1	2.17	0.45
54:z:88:A:O3'	55:B:27:SER:OG	2.32	0.45
1:1:403:U:O5'	1:1:403:U:H6	1.99	0.45
1:1:1062:G:C2	1:1:1063:G:C5	3.05	0.45
1:1:1722:A:H2'	1:1:1723:G:H8	1.82	0.45
1:1:2751:G:H5'	1:1:2752:C:C5	2.52	0.45
1:1:2799:A:C6	1:1:2801:G:C5	3.05	0.45
2:2:513:C:H2'	2:2:514:C:H6	1.82	0.45
2:2:1151:A:O2'	2:2:1152:A:O4'	2.35	0.45
16:N:27:VAL:HG21	16:N:40:ILE:HD12	1.99	0.45
24:V:56:ASP:CG	24:V:58:THR:HG1	2.21	0.45
29:a:3:VAL:HG22	29:a:4:GLN:N	2.31	0.45
34:f:9:MET:HB3	34:f:14:VAL:HB	1.99	0.45
35:g:7:PRO:O	35:g:11:ARG:HD3	2.17	0.45
40:l:5:ASP:CG	40:l:77:ARG:HH12	2.25	0.45
46:r:46:LEU:HD12	51:w:13:LEU:HB3	1.99	0.45
1:1:116:C:H2'	1:1:117:G:O4'	2.17	0.44
1:1:848:C:H2'	1:1:849:A:C8	2.52	0.44
1:1:2145:C:O2	1:1:2145:C:O2'	2.35	0.44
1:1:2747:G:O2'	9:G:67:THR:HG23	2.18	0.44
2:2:58:C:O2'	2:2:388:G:N7	2.34	0.44
2:2:343:U:O3'	2:2:344:A:H8	1.99	0.44
10:H:116:ARG:HD2	10:H:133:GLN:HB2	1.98	0.44
34:f:130:THR:O	34:f:133:GLU:N	2.51	0.44
36:h:146:ARG:HG3	36:h:147:GLU:H	1.82	0.44
38:j:21:MET:HG2	38:j:24:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:k:66:LEU:O	39:k:70:ARG:HG3	2.17	0.44
45:q:77:ILE:HG22	45:q:81:MET:HE3	1.98	0.44
54:z:63:G:C4	54:z:64:G:C8	3.04	0.44
1:1:875:G:C6	1:1:876:C:N4	2.85	0.44
1:1:2521:C:C2	1:1:2545:G:N2	2.85	0.44
2:2:279:A:H5"	2:2:280:C:H3'	1.98	0.44
2:2:1243:C:H2'	2:2:1244:G:H8	1.82	0.44
2:2:1244:G:H2'	2:2:1245:C:C6	2.52	0.44
9:G:101:ASN:O	9:G:116:GLN:NE2	2.50	0.44
10:H:70:GLU:HG3	10:H:140:ALA:HB2	1.99	0.44
10:H:81:ALA:HA	10:H:147:VAL:CG2	2.48	0.44
15:M:65:LEU:O	15:M:69:ARG:HG3	2.17	0.44
24:V:18:ALA:O	24:V:20:ARG:HD2	2.17	0.44
35:g:181:ASP:HB2	35:g:207:ILE:HD11	1.98	0.44
54:z:4:G:O6	54:z:5:A:N6	2.50	0.44
54:z:56:G:N1	54:z:57:U:C4	2.85	0.44
1:1:549:G:H2'	1:1:550:C:C6	2.53	0.44
1:1:711:G:C6	1:1:721:A:C6	3.05	0.44
1:1:1096:A:H2'	1:1:1097:U:O4'	2.18	0.44
1:1:1197:G:H2'	1:1:1198:U:H6	1.81	0.44
1:1:2030:6MZ:H2	1:1:2499:C:H5"	1.99	0.44
1:1:2052:A:O2'	6:D:148:GLN:O	2.31	0.44
2:2:552:U:C2	2:2:553:A:C8	3.05	0.44
2:2:1055:A:C6	2:2:1206:G:C5	3.05	0.44
5:C:271:ARG:O	5:C:272:SER:CB	2.65	0.44
19:Q:37:GLU:OE1	19:Q:37:GLU:HA	2.16	0.44
23:U:51:GLN:OE1	23:U:57:TYR:OH	2.28	0.44
42:n:65:TYR:HB3	46:r:96:LEU:HD11	2.00	0.44
44:p:7:LEU:HD22	44:p:12:ARG:HG2	2.00	0.44
51:w:36:ARG:NH2	51:w:72:GLY:O	2.50	0.44
52:x:35:VAL:HG22	52:x:50:ALA:CB	2.47	0.44
1:1:510:C:OP1	1:1:512:G:O6	2.35	0.44
1:1:634:C:O5'	1:1:634:C:H6	2.00	0.44
1:1:1070:A:C8	1:1:1096:A:O2'	2.68	0.44
1:1:1353:A:O3'	5:C:36:LYS:NZ	2.50	0.44
1:1:2192:U:H2'	1:1:2193:G:O4'	2.17	0.44
2:2:608:A:H2'	2:2:609:A:O4'	2.17	0.44
2:2:1004:A:H2'	2:2:1005:A:O4'	2.18	0.44
2:2:1027:C:C5	2:2:1034:G:N1	2.85	0.44
2:2:1338:G:N2	54:z:42:G:HO2'	2.15	0.44
7:E:171:ASP:OD1	7:E:172:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:57:LYS:HD2	10:H:57:LYS:C	2.43	0.44
10:H:88:GLY:HA2	10:H:125:THR:HG22	1.99	0.44
28:Z:59:ARG:O	28:Z:63:ARG:HG3	2.17	0.44
34:f:87:CYS:HB2	34:f:221:VAL:HG23	1.99	0.44
45:q:29:ARG:O	45:q:33:ILE:HG12	2.18	0.44
1:1:273:G:N1	1:1:365:U:N3	2.66	0.44
1:1:1321:A:C4	1:1:1322:A:C8	3.06	0.44
1:1:2064:C:H2'	1:1:2065:C:C6	2.52	0.44
1:1:2102:G:C8	1:1:2102:G:C5'	2.99	0.44
2:2:460:A:H2'	2:2:461:A:H8	1.81	0.44
2:2:505:G:C2	2:2:506:G:C5	3.05	0.44
2:2:1027:C:C5	2:2:1034:G:C6	3.06	0.44
7:E:105:LEU:O	7:E:109:LEU:HD13	2.18	0.44
9:G:137:ASP:OD2	9:G:140:VAL:HG23	2.17	0.44
13:K:74:THR:HG22	13:K:107:PHE:HB2	2.00	0.44
20:R:86:MET:SD	20:R:87:PRO:HD2	2.57	0.44
35:g:24:ALA:HB1	35:g:28:GLU:CG	2.46	0.44
36:h:168:PRO:CG	36:h:171:LEU:HD12	2.48	0.44
40:l:7:ILE:O	40:l:11:LEU:HG	2.18	0.44
43:o:89:PRO:HB3	53:y:29:LEU:HD23	2.00	0.44
1:1:553:G:C5	1:1:554:U:C5	3.06	0.44
1:1:720:U:H2'	1:1:721:A:H8	1.82	0.44
1:1:1521:G:OP2	1:1:1522:A:O2'	2.26	0.44
1:1:1629:U:C4	1:1:1630:A:N7	2.86	0.44
1:1:2333:A:OP2	24:V:77:ARG:NH2	2.44	0.44
1:1:2698:U:H2'	1:1:2699:C:C6	2.51	0.44
2:2:109:A:C6	2:2:327:A:C6	3.05	0.44
2:2:542:G:P	36:h:10:LYS:HZ1	2.40	0.44
2:2:1029:U:O2	2:2:1033:G:C6	2.70	0.44
2:2:1339:A:HO2'	54:z:41:U:HO2'	1.60	0.44
3:3:46:A:C5	3:3:47:C:C5	3.05	0.44
3:3:66:A:O4'	3:3:108:A:N6	2.48	0.44
14:L:111:GLU:HG2	14:L:112:LEU:N	2.32	0.44
15:M:114:GLU:OE1	15:M:118:ARG:NE	2.50	0.44
27:Y:24:LEU:HD11	27:Y:54:MET:CE	2.48	0.44
39:k:71:PRO:O	39:k:96:ARG:HG2	2.17	0.44
41:m:128:SER:OG	41:m:130:ARG:OXT	2.28	0.44
45:q:117:LYS:HZ3	54:z:47:U:P	2.40	0.44
46:r:54:ASP:HA	46:r:59:ARG:HD3	1.98	0.44
53:y:47:ARG:NH1	53:y:47:ARG:HB3	2.32	0.44
1:1:278:A:C6	1:1:362:A:C8	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:835:C:C2	1:1:836:G:C8	3.06	0.44
1:1:851:C:O2'	27:Y:43:ALA:O	2.34	0.44
1:1:1020:A:C2	1:1:1141:U:C2	3.05	0.44
1:1:1143:A:OP1	11:I:27:ARG:NH2	2.50	0.44
1:1:2297:A:N1	1:1:2321:U:H5	2.14	0.44
2:2:1005:A:N6	2:2:1024:G:O2'	2.50	0.44
2:2:1175:G:N3	2:2:1176:A:C8	2.86	0.44
2:2:1309:G:OP2	45:q:98:ARG:CZ	2.66	0.44
3:3:39:A:C2	3:3:44:G:N3	2.86	0.44
35:g:46:GLU:HB2	35:g:47:LEU:HD12	1.99	0.44
40:l:10:MET:HG3	40:l:27:MET:HE1	1.99	0.44
1:1:388:G:O6	1:1:390:U:O2'	2.27	0.44
1:1:1413:A:C5	1:1:1414:C:C5	3.05	0.44
1:1:1863:G:H2'	1:1:1864:U:H6	1.82	0.44
2:2:258:G:H1	2:2:268:U:H3	1.66	0.44
2:2:337:G:C2	2:2:338:A:C5	3.06	0.44
2:2:1436:U:H2'	2:2:1437:A:H8	1.81	0.44
8:F:111:ILE:HB	8:F:114:PHE:HB2	1.99	0.44
31:c:22:MET:SD	31:c:31:LEU:HD12	2.57	0.44
42:n:51:VAL:HB	46:r:81:ARG:HB2	1.99	0.44
49:u:20:SER:OG	49:u:71:LYS:NZ	2.36	0.44
54:z:38:A:H2'	54:z:39:A:O4'	2.17	0.44
1:1:1585:C:H2'	1:1:1586:A:O4'	2.17	0.44
1:1:1799:G:H8	5:C:180:GLU:OE1	2.00	0.44
1:1:2162:G:H2'	1:1:2164:C:C4	2.52	0.44
2:2:439:U:O2	36:h:120:HIS:CD2	2.71	0.44
2:2:1039:G:H2'	2:2:1040:U:H6	1.82	0.44
7:E:176:ASP:OD1	7:E:176:ASP:N	2.50	0.44
29:a:53:LYS:HE2	29:a:55:ILE:O	2.18	0.44
36:h:100:ASN:OD1	36:h:111:ARG:NH1	2.50	0.44
36:h:140:ASN:N	36:h:182:PHE:O	2.51	0.44
1:1:221:A:N1	1:1:265:A:O2'	2.51	0.43
1:1:1870:C:C6	1:1:1870:C:OP1	2.71	0.43
1:1:2079:U:O2'	25:W:23:ASN:OD1	2.29	0.43
1:1:2140:G:C6	1:1:2141:G:N1	2.85	0.43
1:1:2788:C:H2'	1:1:2789:C:C6	2.53	0.43
2:2:222:C:H2'	2:2:223:A:H8	1.83	0.43
2:2:451:A:H4'	2:2:452:A:O4'	2.17	0.43
2:2:1244:G:H2'	2:2:1245:C:H6	1.83	0.43
2:2:1518:MA6:C6	2:2:1519:MA6:H93	2.47	0.43
3:3:31:C:O5'	3:3:31:C:H6	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:3:VAL:CG2	10:H:36:ALA:HB1	2.48	0.43
28:Z:47:LYS:O	28:Z:50:ASP:OD1	2.36	0.43
44:p:55:VAL:HG21	44:p:80:ILE:HD11	1.98	0.43
1:1:880:G:C2	1:1:881:G:C8	3.06	0.43
1:1:1358:G:N1	1:1:1372:U:OP2	2.29	0.43
1:1:1416:G:C4	1:1:1417:C:C5	3.07	0.43
1:1:1563:U:H2'	1:1:1564:C:C6	2.53	0.43
1:1:2047:C:H2'	1:1:2048:G:H8	1.83	0.43
1:1:2138:G:N1	1:1:2152:G:O6	2.51	0.43
1:1:2646:C:OP2	1:1:2732:G:O2'	2.36	0.43
2:2:1530:G:H2'	2:2:1531:A:H8	1.83	0.43
40:l:26:THR:HG22	40:l:27:MET:N	2.32	0.43
51:w:40:ILE:HB	51:w:66:MET:O	2.18	0.43
51:w:47:LEU:O	51:w:62:VAL:HG23	2.18	0.43
54:z:36:G:H2'	54:z:37:A:O4'	2.18	0.43
54:z:83:C:O2'	54:z:84:C:H5'	2.17	0.43
54:z:87:C:H5"	54:z:88:A:OP2	2.18	0.43
55:B:8:ILE:HG13	55:B:9:VAL:N	2.32	0.43
1:1:1349:C:O5'	1:1:1349:C:H6	2.01	0.43
1:1:2118:U:O4	1:1:2143:C:O2	2.35	0.43
1:1:2129:C:C5	1:1:2130:U:C5	3.06	0.43
1:1:2387:U:O4'	24:V:41:ARG:NH1	2.51	0.43
2:2:41:G:H2'	2:2:42:G:C8	2.53	0.43
2:2:73:C:H5"	2:2:73:C:H6	1.82	0.43
17:O:78:SER:OG	17:O:80:VAL:HG12	2.19	0.43
34:f:115:LYS:CE	34:f:152:LYS:O	2.67	0.43
36:h:146:ARG:CG	36:h:147:GLU:H	2.32	0.43
1:1:875:G:C2	1:1:903:C:C2	3.06	0.43
1:1:1060:U:H1'	1:1:1062:G:OP2	2.19	0.43
1:1:1486:U:H2'	1:1:1487:U:H6	1.84	0.43
1:1:2127:G:OP2	1:1:2162:G:N2	2.51	0.43
2:2:110:C:H2'	2:2:111:G:O4'	2.19	0.43
2:2:1048:G:C6	2:2:1210:C:N4	2.86	0.43
54:z:1:G:C4	54:z:2:G:C8	3.07	0.43
55:B:21:ILE:O	55:B:21:ILE:HG22	2.18	0.43
1:1:499:U:H5"	22:T:43:LYS:HE2	1.99	0.43
1:1:1630:A:N6	1:1:1637:A:N6	2.66	0.43
1:1:1870:C:H2'	1:1:1871:A:C8	2.53	0.43
2:2:375:U:C2	2:2:376:G:C8	3.06	0.43
2:2:1144:G:N2	2:2:1146:A:H62	2.16	0.43
2:2:1323:G:H2'	2:2:1324:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:123:ASP:OD2	8:F:127:ASN:HB2	2.18	0.43
9:G:94:TYR:HA	9:G:106:SER:O	2.18	0.43
21:S:50:LEU:HD23	26:X:26:PHE:CE2	2.54	0.43
28:Z:44:PHE:HD2	28:Z:45:THR:HG23	1.79	0.43
34:f:69:PHE:HB3	34:f:80:VAL:CG2	2.47	0.43
34:f:93:ASN:OD1	34:f:94:HIS:N	2.51	0.43
40:l:77:ARG:NE	40:l:79:SER:O	2.51	0.43
41:m:113:ARG:NH2	41:m:114:LYS:O	2.50	0.43
41:m:130:ARG:HD2	54:z:36:G:OP1	2.18	0.43
43:o:96:THR:CG2	43:o:97:ILE:N	2.81	0.43
47:s:4:SER:O	47:s:8:THR:HG23	2.18	0.43
1:1:2:G:C2	1:1:2902:C:C2	3.07	0.43
1:1:894:U:H1’	1:1:895:U:O5’	2.18	0.43
1:1:1231:U:H2’	1:1:1232:G:H8	1.83	0.43
1:1:1653:G:O6	15:M:11:ASN:N	2.48	0.43
1:1:2108:A:C2	1:1:2181:U:O2	2.72	0.43
1:1:2162:G:H2’	1:1:2164:C:C5	2.53	0.43
2:2:181:A:N6	2:2:195:A:C8	2.87	0.43
2:2:383:A:C5	2:2:384:G:H1’	2.53	0.43
2:2:1060:U:C5	35:g:2:GLY:HA3	2.53	0.43
2:2:1107:C:C4	2:2:1108:G:C8	3.06	0.43
2:2:1356:G:H2’	2:2:1357:A:C8	2.53	0.43
2:2:1414:U:H2’	2:2:1415:G:H8	1.83	0.43
8:F:119:ALA:HB1	8:F:167:ARG:HE	1.83	0.43
41:m:47:VAL:HG12	41:m:50:GLN:OE1	2.18	0.43
1:1:5:A:H2’	1:1:6:A:C8	2.53	0.43
1:1:45:G:H5”	1:1:46:G:H5’	2.01	0.43
1:1:172:A:H2’	1:1:173:A:C8	2.54	0.43
1:1:558:U:OP1	11:I:113:PRO:HD2	2.18	0.43
1:1:1534:U:H2’	1:1:1534:U:O2	2.19	0.43
2:2:439:U:O2	2:2:439:U:O4’	2.35	0.43
2:2:1057:G:H2’	2:2:1058:G:O4’	2.19	0.43
2:2:1294:G:C2	2:2:1295:U:C2	3.07	0.43
8:F:80:ARG:NH2	54:z:18:G:C6	2.87	0.43
10:H:93:SER:CB	10:H:121:VAL:HG23	2.48	0.43
28:Z:37:CYS:SG	28:Z:39:LYS:HB3	2.57	0.43
28:Z:44:PHE:HA	28:Z:48:GLN:HE22	1.83	0.43
38:j:90:MET:HE1	50:v:61:ARG:NE	2.34	0.43
45:q:46:SER:O	45:q:47:GLU:HG3	2.19	0.43
45:q:57:ARG:O	45:q:60:VAL:HG12	2.19	0.43
53:y:28:VAL:HG23	53:y:29:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:184:C:H2'	1:1:185:G:H8	1.83	0.43
1:1:1141:U:H4'	1:1:1142:A:O4'	2.19	0.43
2:2:750:C:O2'	47:s:21:ASP:O	2.24	0.43
2:2:1315:U:H2'	2:2:1316:G:O4'	2.18	0.43
20:R:34:ASP:HB3	29:a:28:LEU:HD11	2.00	0.43
52:x:28:MET:HE1	52:x:67:ILE:HG21	1.99	0.43
54:z:49:C:H5'	54:z:50:G:P	2.58	0.43
54:z:57:U:H2'	54:z:58:A:O4'	2.19	0.43
54:z:72:U:OP1	54:z:73:C:N4	2.47	0.43
55:B:16:LYS:O	55:B:16:LYS:HD2	2.19	0.43
1:1:323:C:H2'	7:E:163:ASN:OD1	2.19	0.43
1:1:588:U:O4	1:1:670:A:H1'	2.18	0.43
1:1:1715:G:N2	1:1:1744:A:OP2	2.39	0.43
1:1:2364:C:H2'	1:1:2365:G:O4'	2.19	0.43
2:2:1124:G:OP1	42:n:38:GLY:HA3	2.19	0.43
2:2:1148:U:H2'	2:2:1149:C:O4'	2.19	0.43
2:2:1496:C:H2'	2:2:1497:G:O4'	2.19	0.43
33:e:30:GLU:HG3	33:e:32:LYS:H	1.84	0.43
37:i:120:VAL:HG11	37:i:123:VAL:HG13	2.00	0.43
54:z:23:A:H3'	54:z:24:G:C8	2.53	0.43
1:1:494:G:H4'	20:R:6:LYS:HB2	2.01	0.43
1:1:1799:G:OP1	5:C:258:ARG:NE	2.48	0.43
2:2:414:A:C2	2:2:415:A:C4	3.06	0.43
2:2:475:C:H2'	2:2:476:U:C6	2.53	0.43
2:2:518:C:C2'	2:2:530:G:H21	2.31	0.43
7:E:106:LYS:HG3	7:E:200:LEU:HD23	2.01	0.43
23:U:21:ARG:HE	23:U:87:GLN:HA	1.84	0.43
24:V:9:SER:O	24:V:10:THR:OG1	2.33	0.43
26:X:44:LYS:O	26:X:48:ARG:HD2	2.19	0.43
34:f:18:HIS:ND1	34:f:188:ASP:OD2	2.52	0.43
34:f:120:GLN:O	34:f:126:PHE:HB2	2.19	0.43
36:h:95:GLU:HA	36:h:100:ASN:HD22	1.84	0.43
36:h:129:VAL:HB	36:h:146:ARG:NH2	2.34	0.43
37:i:154:ALA:HB2	37:i:164:ILE:HD12	2.01	0.43
43:o:15:GLN:NE2	43:o:78:GLY:O	2.52	0.43
43:o:53:ARG:HH21	43:o:57:LYS:HE2	1.83	0.43
54:z:48:A:H61	54:z:58:A:N6	2.17	0.43
1:1:910:A:H2	1:1:2264:C:O2	2.02	0.42
1:1:1048:A:C5	1:1:1049:C:C5	3.07	0.42
1:1:1074:G:C2	1:1:1075:C:N4	2.87	0.42
1:1:1092:C:H2'	1:1:1093:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1095:A:O2'	1:1:1096:A:C8	2.66	0.42
1:1:1227:G:OP2	18:P:16:LYS:NZ	2.52	0.42
1:1:1429:G:H2'	1:1:1430:G:H8	1.84	0.42
1:1:2050:C:H2'	1:1:2051:A:O4'	2.19	0.42
1:1:2246:G:H2'	1:1:2247:A:C8	2.54	0.42
1:1:2322:A:H2'	1:1:2323:G:O4'	2.19	0.42
2:2:235:C:H2'	2:2:236:A:C8	2.54	0.42
2:2:475:C:H2'	2:2:476:U:H6	1.84	0.42
2:2:622:A:C8	2:2:623:C:C6	3.07	0.42
2:2:1014:A:C2	2:2:1219:A:H1'	2.53	0.42
2:2:1055:A:O2'	35:g:161:GLU:O	2.30	0.42
2:2:1160:G:C2	2:2:1161:C:C6	3.06	0.42
9:G:35:ARG:NH1	9:G:75:MET:SD	2.92	0.42
17:O:29:LYS:HB2	17:O:83:SER:OG	2.18	0.42
18:P:36:PHE:O	18:P:40:ILE:HG12	2.19	0.42
36:h:145:ILE:O	36:h:150:LYS:HE3	2.18	0.42
1:1:359:G:C6	1:1:360:U:C4	3.07	0.42
1:1:553:G:C6	1:1:554:U:C4	3.08	0.42
1:1:1073:A:N7	1:1:1074:G:C5	2.87	0.42
1:1:1584:U:H5'	1:1:1585:C:C6	2.54	0.42
1:1:1588:G:C2	1:1:1589:U:C4	3.07	0.42
1:1:1849:G:H2'	1:1:1850:G:H8	1.83	0.42
1:1:1922:G:C6	1:1:1923:U:C4	3.07	0.42
1:1:2053:G:O6	1:1:2614:A:C2	2.72	0.42
1:1:2698:U:H2'	1:1:2699:C:H6	1.84	0.42
1:1:2794:C:C2	1:1:2803:G:C2	3.07	0.42
2:2:215:C:H2'	2:2:216:U:O4'	2.20	0.42
2:2:844:G:C6	2:2:846:G:H1'	2.54	0.42
2:2:1040:U:H2'	2:2:1041:G:H8	1.84	0.42
2:2:1158:C:N3	2:2:1160:G:C8	2.88	0.42
6:D:104:VAL:HG12	6:D:105:LYS:N	2.34	0.42
35:g:47:LEU:HD11	35:g:87:LEU:HD11	2.01	0.42
35:g:123:GLN:HB3	35:g:128:VAL:CG2	2.49	0.42
37:i:46:VAL:HG22	37:i:118:ALA:HA	2.01	0.42
54:z:64:G:C2	54:z:65:G:C4	3.07	0.42
1:1:45:G:H2'	1:1:215:G:C5	2.54	0.42
1:1:138:U:O2'	1:1:139:U:O2	2.26	0.42
1:1:1266:G:OP2	29:a:17:ARG:NH2	2.52	0.42
1:1:1359:A:OP2	1:1:1371:G:N1	2.40	0.42
1:1:1386:C:H2'	1:1:1387:A:C8	2.54	0.42
1:1:2191:A:H2'	1:1:2192:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1133:G:C2	2:2:1142:G:C2	3.06	0.42
3:3:8:C:O2'	16:N:40:ILE:HD13	2.20	0.42
7:E:150:THR:HG22	7:E:152:GLU:H	1.83	0.42
34:f:20:THR:O	34:f:23:TRP:CD1	2.72	0.42
38:j:45:ARG:HD3	38:j:59:TYR:CE2	2.54	0.42
42:n:35:GLN:HB3	42:n:78:GLU:OE1	2.18	0.42
1:1:284:U:N3	1:1:285:G:N7	2.67	0.42
1:1:293:U:C4	1:1:345:A:C6	3.08	0.42
1:1:771:G:OP2	31:c:11:LYS:HE2	2.20	0.42
1:1:1413:A:N6	1:1:1590:A:N6	2.67	0.42
1:1:2531:A:C4	1:1:2532:G:C8	3.07	0.42
2:2:513:C:H2'	2:2:514:C:C6	2.54	0.42
2:2:1033:G:H2'	2:2:1034:G:C8	2.54	0.42
2:2:1061:G:OP2	35:g:2:GLY:O	2.37	0.42
5:C:232:HIS:CG	5:C:240:PHE:CE1	3.08	0.42
10:H:101:ASP:C	10:H:104:THR:HG22	2.43	0.42
34:f:72:THR:HA	34:f:93:ASN:O	2.20	0.42
37:i:45:ARG:HA	37:i:72:ILE:O	2.19	0.42
43:o:65:VAL:O	43:o:69:ARG:HG3	2.19	0.42
46:r:46:LEU:HD12	51:w:13:LEU:CB	2.49	0.42
1:1:281:C:H2'	1:1:282:A:H8	1.83	0.42
1:1:1061:U:O4'	1:1:1070:A:H1'	2.20	0.42
1:1:1291:C:C4	1:1:1292:G:N7	2.88	0.42
1:1:1407:G:H3'	1:1:1408:G:H5"	2.00	0.42
1:1:1775:U:O4	1:1:1789:A:H2	2.03	0.42
1:1:2687:U:H2'	1:1:2688:G:O4'	2.20	0.42
2:2:263:A:OP1	52:x:74:ARG:NE	2.51	0.42
2:2:524:G:H2'	2:2:525:C:C6	2.54	0.42
2:2:1032:G:N2	2:2:1033:G:O4'	2.52	0.42
2:2:1106:G:H5"	35:g:172:ARG:HB3	2.02	0.42
2:2:1241:G:H2'	2:2:1242:G:H8	1.84	0.42
10:H:77:THR:HA	10:H:143:ILE:O	2.20	0.42
26:X:31:GLN:HG3	26:X:36:GLN:HB2	2.00	0.42
34:f:43:LEU:HA	34:f:46:THR:HB	2.01	0.42
34:f:167:ASP:OD1	34:f:168:HIS:N	2.53	0.42
35:g:40:ARG:O	35:g:44:THR:HG23	2.19	0.42
35:g:42:TYR:O	35:g:45:LYS:HG2	2.19	0.42
39:k:107:ALA:O	39:k:111:ARG:HG3	2.20	0.42
41:m:51:PRO:O	41:m:55:VAL:HG22	2.20	0.42
42:n:84:VAL:HG13	42:n:85:ASP:N	2.35	0.42
44:p:43:LYS:HB2	44:p:89:0TD:SB	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:z:26:A:C5	54:z:27:G:C8	3.06	0.42
1:1:829:A:N7	1:1:2247:A:O2'	2.53	0.42
1:1:2107:G:C6	1:1:2108:A:C5	3.08	0.42
2:2:84:U:H2'	2:2:86:G:C2	2.54	0.42
2:2:381:C:H2'	2:2:382:A:O4'	2.20	0.42
7:E:149:ILE:HG22	7:E:170:ARG:HB2	2.01	0.42
32:d:15:LYS:HB2	32:d:23:LYS:HE2	2.02	0.42
35:g:181:ASP:HB2	35:g:207:ILE:CD1	2.50	0.42
38:j:20:GLY:O	38:j:24:ARG:HG3	2.18	0.42
42:n:17:LEU:CD2	42:n:96:VAL:HG23	2.49	0.42
54:z:69:G:H2'	54:z:70:U:H5'	2.02	0.42
54:z:81:C:H2'	54:z:82:A:H8	1.84	0.42
1:1:155:A:H2'	1:1:156:A:C8	2.55	0.42
1:1:270:A:H5'	1:1:271:G:H5"	2.01	0.42
1:1:603:A:O5'	1:1:655:A:N6	2.46	0.42
1:1:711:G:C4	1:1:712:G:C8	3.07	0.42
1:1:1913:A:N1	2:2:1492:A:H2'	2.33	0.42
1:1:2142:A:N7	1:1:2143:C:N4	2.68	0.42
2:2:413:G:H21	2:2:428:G:H1'	1.85	0.42
2:2:414:A:P	2:2:428:G:H22	2.43	0.42
2:2:663:A:H5'	2:2:836:G:OP1	2.19	0.42
2:2:692:U:H1'	2:2:695:A:N7	2.35	0.42
2:2:1237:C:O3'	2:2:1300:G:N2	2.52	0.42
7:E:149:ILE:HD11	7:E:188:MET:HE3	2.02	0.42
10:H:125:THR:O	10:H:125:THR:HG23	2.18	0.42
12:J:90:ASN:OD1	12:J:91:SER:N	2.48	0.42
1:1:1779:U:OP2	1:1:1784:A:N6	2.39	0.42
1:1:1850:G:C6	1:1:1851:U:C4	3.08	0.42
1:1:2118:U:O4'	1:1:2147:A:C2	2.73	0.42
2:2:204:G:H2'	2:2:205:A:C8	2.55	0.42
2:2:537:G:H5"	44:p:110:ARG:NH1	2.34	0.42
2:2:1157:A:C2	2:2:1181:G:C4	3.07	0.42
2:2:1338:G:H21	54:z:42:G:C2'	2.32	0.42
3:3:39:A:C2	3:3:44:G:C2	3.08	0.42
5:C:174:LEU:O	5:C:181:MET:HA	2.19	0.42
8:F:128:TYR:O	8:F:156:ILE:N	2.42	0.42
29:a:9:THR:HG22	29:a:10:ARG:N	2.34	0.42
1:1:282:A:N6	1:1:359:G:O6	2.53	0.42
1:1:640:C:H2'	1:1:641:U:H6	1.84	0.42
1:1:1445:G:C5	1:1:1446:C:C5	3.07	0.42
1:1:1863:G:H2'	1:1:1864:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2189:U:C2	1:1:2190:G:C8	3.08	0.42
2:2:297:G:N2	2:2:300:A:OP2	2.52	0.42
2:2:436:C:C2	2:2:437:U:C5	3.08	0.42
2:2:604:G:C6	2:2:635:A:C6	3.08	0.42
2:2:950:U:OP2	45:q:101:ARG:NH2	2.53	0.42
2:2:1040:U:H2'	2:2:1041:G:C8	2.54	0.42
2:2:1216:A:C2	2:2:1217:C:C5	3.08	0.42
2:2:1244:G:C6	2:2:1294:G:N1	2.88	0.42
10:H:3:VAL:HG22	10:H:36:ALA:HB1	2.01	0.42
12:J:105:ARG:O	12:J:108:ARG:HG2	2.20	0.42
34:f:184:PHE:HD1	34:f:198:PHE:HB2	1.84	0.42
36:h:48:LEU:HD23	36:h:53:VAL:HG12	2.02	0.42
47:s:70:LEU:HD21	47:s:77:ARG:HB2	2.01	0.42
49:u:29:VAL:HG22	49:u:30:LYS:N	2.35	0.42
1:1:271:G:C4	1:1:272:A:C8	3.08	0.42
1:1:301:G:C4	1:1:302:C:C5	3.08	0.42
1:1:510:C:H2'	1:1:511:U:H5'	2.02	0.42
1:1:593:U:H2'	1:1:594:U:C6	2.55	0.42
1:1:893:C:O2'	1:1:894:U:H5'	2.19	0.42
1:1:971:G:H2'	1:1:972:A:O4'	2.20	0.42
1:1:1907:G:C2	1:1:1924:C:C2	3.08	0.42
1:1:2294:G:OP1	16:N:10:ARG:HD3	2.20	0.42
2:2:67:C:H2'	2:2:68:G:C8	2.54	0.42
2:2:270:A:C5	2:2:271:C:C5	3.08	0.42
2:2:373:A:C2	2:2:482:A:N6	2.88	0.42
2:2:708:C:H2'	2:2:709:U:H6	1.85	0.42
2:2:1120:C:H2'	2:2:1121:U:C6	2.54	0.42
2:2:1509:C:C2	2:2:1510:C:C5	3.08	0.42
6:D:25:THR:HG21	6:D:193:VAL:HG22	2.02	0.42
12:J:80:ASP:OD2	17:O:62:ARG:NH1	2.48	0.42
35:g:47:LEU:N	35:g:47:LEU:CD1	2.77	0.42
37:i:111:MET:HG2	37:i:115:LEU:HD12	2.01	0.42
39:k:150:ALA:HB1	43:o:59:THR:HG21	2.02	0.42
1:1:1326:U:H2'	1:1:1327:A:H8	1.84	0.41
1:1:1407:G:H2'	1:1:1408:G:O4'	2.19	0.41
1:1:1808:A:H3'	1:1:1809:A:C8	2.54	0.41
1:1:2233:U:H2'	1:1:2234:G:C8	2.55	0.41
1:1:2637:U:O4	1:1:2776:A:N7	2.53	0.41
2:2:202:G:O2'	2:2:468:A:H2'	2.20	0.41
2:2:604:G:H2'	2:2:605:U:O4'	2.20	0.41
2:2:1278:G:H4'	2:2:1279:G:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:40:ARG:O	32:d:44:LEU:HG	2.20	0.41
43:o:29:ASN:OD1	43:o:30:THR:N	2.53	0.41
54:z:5:A:N1	54:z:81:C:C4	2.88	0.41
54:z:6:G:N2	54:z:80:U:C2	2.88	0.41
54:z:30:C:C2	54:z:31:G:C8	3.08	0.41
1:1:1802:A:H2'	1:1:1803:A:C8	2.55	0.41
1:1:2079:U:C4	1:1:2080:A:N7	2.89	0.41
1:1:2190:G:C6	1:1:2191:A:C6	3.08	0.41
1:1:2314:A:H2'	1:1:2315:G:C8	2.55	0.41
1:1:2412:A:H2'	1:1:2413:G:O4'	2.20	0.41
1:1:2635:A:O2'	6:D:49:GLN:NE2	2.51	0.41
2:2:201:G:N1	2:2:217:C:N3	2.69	0.41
2:2:736:C:OP1	50:v:61:ARG:NH2	2.53	0.41
2:2:837:U:H2'	2:2:838:G:H8	1.85	0.41
2:2:891:U:H2'	2:2:892:A:H8	1.85	0.41
2:2:1304:G:N1	2:2:1332:A:OP2	2.52	0.41
10:H:3:VAL:HG23	10:H:37:VAL:C	2.45	0.41
10:H:81:ALA:HA	10:H:147:VAL:HG23	2.01	0.41
11:I:116:ARG:O	11:I:120:ARG:HG3	2.20	0.41
20:R:10:ALA:HB3	20:R:101:SER:HB2	2.02	0.41
21:S:31:VAL:HG22	21:S:84:TYR:CD1	2.55	0.41
26:X:59:GLU:O	26:X:63:ALA:HB3	2.19	0.41
32:d:31:HIS:N	32:d:31:HIS:CD2	2.88	0.41
34:f:63:ARG:C	34:f:64:LYS:HG2	2.45	0.41
42:n:22:THR:HG23	42:n:23:ALA:N	2.34	0.41
46:r:74:LEU:HD12	46:r:84:VAL:HG21	2.02	0.41
48:t:67:ILE:HG22	48:t:68:SER:O	2.20	0.41
54:z:52:C:O2	54:z:53:A:N3	2.53	0.41
1:1:414:C:H2'	1:1:415:A:H8	1.85	0.41
1:1:604:G:C6	1:1:625:G:N1	2.89	0.41
1:1:811:U:C2	1:1:1251:C:C5	3.08	0.41
1:1:885:C:N3	1:1:892:A:C6	2.89	0.41
1:1:1446:C:H2'	1:1:1447:C:C6	2.55	0.41
1:1:2496:C:H2'	1:1:2497:A:O4'	2.20	0.41
2:2:137:U:H2'	2:2:138:G:H8	1.83	0.41
2:2:440:C:C2	2:2:441:A:C8	3.08	0.41
2:2:911:U:H2'	2:2:912:C:C6	2.55	0.41
2:2:1006:G:N2	2:2:1024:G:H1'	2.35	0.41
2:2:1228:C:H2'	2:2:1229:A:H8	1.86	0.41
2:2:1326:U:H2'	2:2:1327:C:H6	1.84	0.41
3:3:15:A:O4'	3:3:109:A:C8	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:37:ASN:OD1	8:F:38:MET:N	2.53	0.41
9:G:101:ASN:OD1	9:G:117:LEU:CB	2.68	0.41
29:a:46:ASP:O	29:a:53:LYS:HE3	2.20	0.41
36:h:152:GLN:HB2	36:h:155:VAL:HG23	2.02	0.41
39:k:142:HIS:O	39:k:146:GLU:OE1	2.38	0.41
47:s:69:TYR:OH	47:s:73:LYS:NZ	2.41	0.41
49:u:29:VAL:O	49:u:38:ILE:N	2.41	0.41
50:v:11:CYS:HB3	50:v:14:THR:OG1	2.20	0.41
1:1:278:A:H3'	1:1:278:A:N3	2.35	0.41
1:1:323:C:C4	1:1:333:G:C8	3.09	0.41
1:1:373:U:H2'	1:1:374:A:H8	1.85	0.41
1:1:1680:U:H2'	1:1:1681:G:O4'	2.20	0.41
1:1:1955:U:C5	1:1:2552:OMU:H1'	2.55	0.41
1:1:2285:C:OP2	30:b:6:ARG:NH1	2.53	0.41
2:2:489:C:C2	2:2:490:C:C5	3.08	0.41
7:E:108:ILE:HG21	7:E:108:ILE:HD13	1.79	0.41
8:F:105:THR:HG21	28:Z:22:MET:SD	2.61	0.41
10:H:4:ILE:HA	10:H:17:ASP:O	2.20	0.41
20:R:7:HIS:CD2	20:R:10:ALA:HB2	2.56	0.41
21:S:29:THR:HG23	21:S:85:VAL:C	2.46	0.41
22:T:98:SER:C	22:T:100:SER:H	2.27	0.41
34:f:101:LEU:HB3	34:f:179:LEU:CD1	2.50	0.41
34:f:207:ILE:C	34:f:210:VAL:HG22	2.46	0.41
35:g:6:HIS:CE1	35:g:8:ASN:HB3	2.54	0.41
50:v:57:ARG:HG2	50:v:61:ARG:NH2	2.36	0.41
1:1:469:G:O6	31:c:37:LYS:HE2	2.21	0.41
1:1:967:U:H2'	1:1:968:C:C6	2.56	0.41
1:1:1068:G:C2	1:1:1095:A:N3	2.88	0.41
1:1:1174:U:O2	1:1:1174:U:O4'	2.38	0.41
1:1:1790:C:H2'	1:1:1791:A:C5	2.54	0.41
1:1:1867:G:H2'	1:1:1868:C:O4'	2.20	0.41
1:1:2630:G:C5	1:1:2894:G:C6	3.08	0.41
1:1:2803:G:H2'	1:1:2804:U:H6	1.85	0.41
2:2:64:G:C4	2:2:99:C:N4	2.89	0.41
2:2:100:G:C4	2:2:101:A:C8	3.08	0.41
2:2:176:C:H2'	2:2:177:G:N3	2.36	0.41
2:2:1003:G:N2	2:2:1005:A:O5'	2.52	0.41
2:2:1109:C:C5'	2:2:1109:C:C3'	2.99	0.41
2:2:1120:C:H2'	2:2:1121:U:H6	1.86	0.41
6:D:13:ARG:HD2	6:D:21:SER:OG	2.21	0.41
9:G:80:THR:HG23	9:G:81:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:63:ALA:O	10:H:66:ASN:CG	2.64	0.41
19:Q:34:GLU:HG2	19:Q:60:LYS:HG2	2.02	0.41
19:Q:37:GLU:OE1	19:Q:53:PHE:CG	2.74	0.41
34:f:68:LEU:HB3	34:f:161:LEU:HD12	2.03	0.41
35:g:112:ASP:HB3	35:g:115:LEU:HD12	2.01	0.41
48:t:38:PHE:CE1	48:t:51:ARG:HB3	2.56	0.41
54:z:50:G:C2	54:z:51:G:C2	3.08	0.41
1:1:638:G:C6	1:1:639:U:C4	3.09	0.41
1:1:877:A:C6	1:1:899:A:C6	3.08	0.41
1:1:922:C:H1'	24:V:26:PHE:CD2	2.56	0.41
1:1:2570:G:H2'	1:1:2571:U:O4'	2.20	0.41
2:2:779:C:H2'	2:2:780:A:O4'	2.21	0.41
2:2:1082:A:C6	2:2:1083:U:C4	3.08	0.41
2:2:1460:C:H2'	2:2:1461:G:O4'	2.21	0.41
36:h:107:PHE:CE1	36:h:159:LEU:HD21	2.56	0.41
37:i:81:LEU:HG	37:i:147:MET:SD	2.61	0.41
41:m:6:TYR:CD2	41:m:90:TYR:HD1	2.39	0.41
41:m:63:LEU:HD12	41:m:63:LEU:N	2.36	0.41
44:p:114:ARG:HB3	44:p:119:VAL:HB	2.02	0.41
54:z:69:G:C2'	54:z:70:U:H5'	2.50	0.41
1:1:5:A:H2'	1:1:6:A:H8	1.86	0.41
1:1:1086:A:O2'	1:1:1103:A:N1	2.46	0.41
1:1:1156:A:P	18:P:55:ARG:HH21	2.43	0.41
1:1:1198:U:H2'	1:1:1199:U:C6	2.55	0.41
1:1:2195:U:H2'	1:1:2196:C:H6	1.84	0.41
1:1:2301:C:H2'	1:1:2302:U:C6	2.55	0.41
2:2:34:C:H2'	2:2:35:G:H8	1.85	0.41
2:2:214:C:H2'	2:2:215:C:C6	2.54	0.41
2:2:283:U:C4	2:2:284:C:C4	3.08	0.41
2:2:460:A:H2'	2:2:461:A:C8	2.55	0.41
34:f:164:ILE:O	34:f:186:ILE:HB	2.19	0.41
37:i:57:PRO:O	37:i:60:ILE:HG13	2.21	0.41
37:i:92:SER:OG	37:i:130:SER:O	2.28	0.41
38:j:1:MET:SD	38:j:1:MET:N	2.84	0.41
40:l:75:ILE:O	40:l:75:ILE:HG23	2.19	0.41
45:q:54:ASP:OD1	45:q:57:ARG:NH1	2.54	0.41
49:u:14:SER:HA	49:u:55:ILE:HD12	2.01	0.41
54:z:9:G:H22	54:z:13:G:H22	1.69	0.41
1:1:233:A:H61	1:1:429:A:N6	2.19	0.41
1:1:567:U:OP2	13:K:29:LYS:NZ	2.54	0.41
1:1:1026:G:OP1	1:1:1134:A:O2'	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1062:G:C8	1:1:1088:A:C8	3.09	0.41
1:1:1186:G:H2'	1:1:1187:G:O4'	2.20	0.41
1:1:1445:G:C6	1:1:1446:C:C4	3.09	0.41
1:1:1539:U:H2'	1:1:1540:G:H8	1.86	0.41
1:1:2139:U:O2	1:1:2140:G:N7	2.54	0.41
2:2:415:A:C4	2:2:416:G:C8	3.08	0.41
2:2:433:G:C6	2:2:434:U:C4	3.09	0.41
2:2:606:G:H5"	2:2:607:A:H5'	2.03	0.41
2:2:644:U:C2	2:2:645:G:C8	3.09	0.41
2:2:950:U:P	45:q:101:ARG:HH21	2.43	0.41
2:2:1041:G:C2	2:2:1042:A:C5	3.08	0.41
23:U:64:VAL:HG22	23:U:69:GLU:HG3	2.02	0.41
24:V:56:ASP:OD1	24:V:58:THR:OG1	2.28	0.41
43:o:84:VAL:HG23	43:o:107:ILE:HD11	2.02	0.41
44:p:3:THR:HB	44:p:6:GLN:HG3	2.02	0.41
51:w:11:ILE:HG13	51:w:38:SER:HB3	2.02	0.41
55:B:17:GLY:H	55:B:18:PHE:HD1	1.69	0.41
1:1:143:C:C6	1:1:143:C:O5'	2.74	0.41
1:1:565:C:P	19:Q:80:ARG:H	2.44	0.41
1:1:901:C:C4	1:1:902:C:C4	3.08	0.41
1:1:931:U:O4	1:1:1166:G:N2	2.48	0.41
1:1:1056:G:C2'	1:1:1103:A:N6	2.84	0.41
1:1:1172:C:H5"	1:1:1173:U:C4	2.56	0.41
1:1:1548:A:H2'	1:1:1549:A:C8	2.56	0.41
1:1:1568:G:P	5:C:63:ARG:HH12	2.43	0.41
1:1:2116:G:N1	1:1:2164:C:C5	2.89	0.41
1:1:2206:C:C2	1:1:2207:C:C5	3.09	0.41
1:1:2425:A:H4'	1:1:2426:A:H5"	2.01	0.41
1:1:2581:G:OP2	1:1:2581:G:N2	2.54	0.41
1:1:2838:G:C4	1:1:2839:G:C8	3.08	0.41
2:2:155:A:N6	2:2:167:A:N6	2.69	0.41
2:2:259:G:N2	2:2:268:U:C2	2.89	0.41
2:2:272:C:C2	2:2:273:U:C5	3.09	0.41
2:2:413:G:O3'	2:2:428:G:N2	2.53	0.41
2:2:458:U:H2'	2:2:459:A:C8	2.56	0.41
2:2:490:C:H2'	2:2:491:G:H8	1.85	0.41
2:2:707:U:H2'	2:2:708:C:C6	2.56	0.41
2:2:1073:U:H2'	2:2:1074:G:O4'	2.21	0.41
2:2:1418:A:N6	2:2:1482:G:O2'	2.49	0.41
5:C:144:VAL:HB	5:C:154:LEU:HB2	2.01	0.41
6:D:13:ARG:HH11	17:O:56:HIS:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:175:PHE:HA	8:F:176:PRO:HD3	1.95	0.41
13:K:135:ILE:CG2	13:K:140:GLY:HA3	2.51	0.41
15:M:47:VAL:O	15:M:51:LEU:HD23	2.21	0.41
23:U:25:LYS:HD3	23:U:41:GLU:OE1	2.21	0.41
37:i:154:ALA:HB1	37:i:159:LYS:O	2.21	0.41
38:j:25:TYR:O	38:j:29:ILE:HG12	2.21	0.41
39:k:28:ASN:OD1	39:k:36:LYS:HE2	2.21	0.41
46:r:48:LEU:HD12	46:r:51:LEU:HD12	2.03	0.41
47:s:64:ARG:NH2	47:s:89:ARG:OXT	2.47	0.41
47:s:70:LEU:HD23	47:s:70:LEU:O	2.20	0.41
54:z:10:U:C2	54:z:11:C:C5	3.09	0.41
55:B:1:FME:O	55:B:4:LYS:HG2	2.21	0.41
1:1:48:G:H22	1:1:177:G:P	2.42	0.41
1:1:711:G:H2'	1:1:712:G:O4'	2.20	0.41
1:1:1684:G:O6	1:1:1705:A:N6	2.54	0.41
1:1:1722:A:N6	1:1:1738:G:H1'	2.36	0.41
1:1:2300:C:H2'	1:1:2301:C:H6	1.86	0.41
2:2:272:C:H2'	2:2:273:U:H6	1.85	0.41
2:2:469:C:H2'	2:2:470:C:C6	2.56	0.41
2:2:770:C:H1'	2:2:899:C:H42	1.86	0.41
8:F:17:MET:SD	8:F:22:TYR:HB2	2.61	0.41
9:G:156:PRO:O	9:G:172:LYS:N	2.53	0.41
24:V:11:ARG:O	24:V:11:ARG:HG2	2.21	0.41
28:Z:35:ASP:OD1	28:Z:35:ASP:C	2.64	0.41
39:k:12:ILE:HD11	39:k:28:ASN:HD22	1.82	0.41
39:k:78:ARG:HG2	39:k:80:VAL:HG23	2.02	0.41
49:u:11:ARG:HD2	49:u:58:VAL:HG22	2.02	0.41
54:z:56:G:C2'	54:z:57:U:H5'	2.50	0.41
1:1:28:A:H1'	1:1:513:A:C2	2.55	0.40
1:1:57:C:H2'	1:1:58:G:O4'	2.21	0.40
1:1:635:C:H6	1:1:635:C:O5'	2.04	0.40
1:1:720:U:H2'	1:1:721:A:C8	2.56	0.40
1:1:1059:G:H3'	1:1:1060:U:H2'	2.04	0.40
1:1:1093:G:H21	1:1:1098:A:H62	1.69	0.40
1:1:1818:U:OP2	5:C:156:ARG:NE	2.54	0.40
1:1:1996:C:H5	12:J:32:TYR:OH	2.03	0.40
1:1:2111:U:C4	1:1:2147:A:C2	3.09	0.40
1:1:2314:A:C1'	8:F:155:THR:HG21	2.51	0.40
1:1:2703:C:C2	1:1:2704:C:C5	3.09	0.40
2:2:293:G:C6	2:2:305:G:C2	3.09	0.40
2:2:312:C:H2'	2:2:313:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:555:U:H2'	2:2:556:C:C6	2.56	0.40
2:2:1356:G:C2	2:2:1357:A:C5	3.09	0.40
2:2:1377:A:C5	39:k:7:ILE:CD1	3.03	0.40
6:D:3:GLY:O	6:D:4:LEU:HD12	2.20	0.40
11:I:13:ARG:NH1	11:I:49:ASP:O	2.50	0.40
12:J:110:GLU:OE1	12:J:110:GLU:N	2.33	0.40
24:V:59:LEU:HA	24:V:59:LEU:HD23	1.86	0.40
39:k:5:ARG:NH1	39:k:7:ILE:HA	2.36	0.40
42:n:7:ARG:HD3	42:n:75:ASP:CG	2.46	0.40
54:z:17:OMG:HM21	54:z:18:G:C5	2.56	0.40
55:B:13:ASN:O	55:B:16:LYS:NZ	2.51	0.40
1:1:196:A:OP2	13:K:47:ARG:NH1	2.47	0.40
1:1:273:G:N2	1:1:365:U:C2	2.89	0.40
1:1:438:G:H2'	1:1:439:A:C8	2.57	0.40
1:1:1066:U:O2	1:1:1069:A:H8	2.03	0.40
1:1:1386:C:H2'	1:1:1387:A:H8	1.87	0.40
1:1:1391:U:C2	1:1:1394:U:O4	2.74	0.40
1:1:1532:A:C5	1:1:1533:C:C4	3.09	0.40
1:1:2070:A:H2'	1:1:2071:A:O4'	2.22	0.40
2:2:8:A:C4	37:i:112:ARG:NH2	2.89	0.40
2:2:376:G:H5"	48:t:5:ARG:HB2	2.03	0.40
2:2:542:G:H5"	36:h:10:LYS:NZ	2.36	0.40
2:2:696:A:N1	2:2:797:C:O2'	2.51	0.40
2:2:1060:U:H5"	42:n:53:ILE:HD12	2.03	0.40
2:2:1108:G:OP1	35:g:175:LEU:HB2	2.21	0.40
3:3:44:G:N2	3:3:48:U:C2	2.89	0.40
12:J:110:GLU:H	12:J:110:GLU:CD	2.25	0.40
22:T:7:ARG:O	22:T:25:VAL:O	2.39	0.40
27:Y:6:LYS:HB2	27:Y:58:GLU:HB3	2.03	0.40
37:i:64:MET:O	37:i:68:ARG:HG3	2.20	0.40
38:j:42:TRP:HZ2	38:j:61:LEU:HD22	1.87	0.40
42:n:59:LYS:HE2	42:n:62:ARG:NH2	2.36	0.40
54:z:27:G:C5	54:z:28:C:C5	3.09	0.40
1:1:1204:A:O4'	1:1:1206:G:C8	2.74	0.40
1:1:1614:A:C6	20:R:87:PRO:HB3	2.57	0.40
1:1:2170:A:C2	1:1:2171:A:C5	3.09	0.40
1:1:2220:U:H5'	10:H:112:LYS:NZ	2.36	0.40
1:1:2243:U:H2'	1:1:2244:U:C6	2.56	0.40
1:1:2528:U:H2'	1:1:2530:A:O5'	2.22	0.40
2:2:73:C:H2'	2:2:74:A:H5'	2.03	0.40
2:2:1062:U:H2'	2:2:1063:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1067:A:N6	2:2:1109:C:C5'	2.84	0.40
2:2:1338:G:H21	54:z:42:G:HO2'	1.68	0.40
2:2:1507:A:C2	2:2:1530:G:C4	3.10	0.40
3:3:66:A:C4	3:3:108:A:C6	3.10	0.40
39:k:25:LYS:O	39:k:29:ILE:HG13	2.22	0.40
40:l:113:ASP:OD1	40:l:113:ASP:N	2.54	0.40
54:z:37:A:C6	54:z:38:A:N7	2.89	0.40
1:1:11:C:C2'	1:1:12:U:H5'	2.51	0.40
1:1:61:C:C4	1:1:62:U:H5	2.40	0.40
1:1:1012:U:O4	11:I:30:THR:HG21	2.22	0.40
1:1:1106:G:C4	1:1:1107:G:C8	3.09	0.40
1:1:2832:U:C2	1:1:2834:G:C2	3.10	0.40
2:2:485:U:O2	2:2:485:U:H5'	2.21	0.40
2:2:489:C:H2'	2:2:490:C:C6	2.56	0.40
2:2:675:A:H1'	43:o:118:HIS:CD2	2.56	0.40
2:2:1438:G:H5"	52:x:33:LYS:NZ	2.36	0.40
8:F:7:TYR:O	8:F:10:ASP:OD1	2.38	0.40
10:H:73:ASN:OD1	10:H:108:VAL:HG21	2.21	0.40
16:N:4:LYS:O	16:N:8:ILE:HG13	2.21	0.40
19:Q:69:GLY:O	19:Q:90:ARG:NE	2.45	0.40
32:d:8:ARG:O	32:d:12:LYS:HG3	2.21	0.40
34:f:58:ASN:O	34:f:62:SER:HB3	2.21	0.40
35:g:11:ARG:HE	35:g:178:LEU:HA	1.86	0.40
44:p:102:LEU:N	44:p:102:LEU:HD12	2.37	0.40
54:z:54:A:N3	54:z:54:A:C2'	2.84	0.40
1:1:158:U:H2'	1:1:159:G:O4'	2.22	0.40
1:1:1443:U:C2	1:1:1444:G:C8	3.10	0.40
1:1:2032:G:C4	6:D:150:GLN:NE2	2.90	0.40
1:1:2149:U:C5	1:1:2150:C:N3	2.89	0.40
1:1:2514:U:H2'	1:1:2515:C:C6	2.57	0.40
1:1:2822:G:P	6:D:115:GLY:HA3	2.61	0.40
1:1:2829:A:C6	1:1:2830:C:C4	3.10	0.40
2:2:8:A:N3	37:i:112:ARG:NH2	2.70	0.40
2:2:8:A:C2	37:i:112:ARG:NH2	2.90	0.40
2:2:689:C:H2'	2:2:690:G:O4'	2.21	0.40
2:2:1181:G:O2'	2:2:1182:G:N7	2.50	0.40
2:2:1372:U:H2'	2:2:1373:G:O4'	2.21	0.40
11:I:41:LYS:NZ	11:I:50:THR:O	2.50	0.40
11:I:84:ILE:O	11:I:84:ILE:HG23	2.21	0.40
21:S:4:GLU:O	21:S:8:LEU:HG	2.21	0.40
34:f:87:CYS:CA	34:f:225:ARG:HH12	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:18:GLN:OE1	40:l:63:LEU:HD13	2.21	0.40
40:l:87:LYS:HG3	40:l:125:ILE:CD1	2.52	0.40
54:z:48:A:N6	54:z:49:C:N4	2.70	0.40
54:z:50:G:C8	54:z:53:A:C8	3.09	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	C	269/271 (99%)	256 (95%)	13 (5%)	0	100 100
6	D	207/209 (99%)	201 (97%)	3 (1%)	3 (1%)	9 39
7	E	199/201 (99%)	197 (99%)	2 (1%)	0	100 100
8	F	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	21 56
9	G	173/175 (99%)	161 (93%)	12 (7%)	0	100 100
10	H	147/149 (99%)	137 (93%)	10 (7%)	0	100 100
11	I	140/142 (99%)	137 (98%)	3 (2%)	0	100 100
12	J	121/123 (98%)	119 (98%)	2 (2%)	0	100 100
13	K	142/144 (99%)	138 (97%)	4 (3%)	0	100 100
14	L	134/136 (98%)	130 (97%)	4 (3%)	0	100 100
15	M	117/119 (98%)	114 (97%)	3 (3%)	0	100 100
16	N	114/116 (98%)	111 (97%)	3 (3%)	0	100 100
17	O	112/114 (98%)	111 (99%)	1 (1%)	0	100 100
18	P	115/117 (98%)	114 (99%)	1 (1%)	0	100 100
19	Q	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	6 31
20	R	108/110 (98%)	106 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
22	T	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
23	U	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	V	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
25	W	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
26	X	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
27	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
28	Z	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
29	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	b	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
31	c	44/46 (96%)	44 (100%)	0	0	100	100
32	d	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
33	e	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
34	f	223/225 (99%)	207 (93%)	16 (7%)	0	100	100
35	g	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
36	h	203/205 (99%)	201 (99%)	2 (1%)	0	100	100
37	i	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
38	j	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
39	k	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
40	l	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
41	m	125/127 (98%)	118 (94%)	7 (6%)	0	100	100
42	n	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
43	o	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
44	p	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
45	q	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
46	r	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
47	s	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
48	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
49	u	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
50	v	64/66 (97%)	64 (100%)	0	0	100	100
51	w	81/83 (98%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
52	x	84/86 (98%)	84 (100%)	0	0	100 100
53	y	68/70 (97%)	67 (98%)	1 (2%)	0	100 100
55	B	25/27 (93%)	13 (52%)	11 (44%)	1 (4%)	2 17
All	All	5637/5738 (98%)	5424 (96%)	206 (4%)	7 (0%)	49 79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	152	PRO
6	D	153	GLY
6	D	154	LYS
19	Q	52	PRO
19	Q	53	PHE
55	B	16	LYS
8	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
5	C	216/216 (100%)	216 (100%)	0	100 100
6	D	164/164 (100%)	163 (99%)	1 (1%)	78 84
7	E	165/165 (100%)	164 (99%)	1 (1%)	78 84
8	F	148/148 (100%)	148 (100%)	0	100 100
9	G	136/136 (100%)	136 (100%)	0	100 100
10	H	114/114 (100%)	112 (98%)	2 (2%)	51 74
11	I	116/116 (100%)	116 (100%)	0	100 100
12	J	104/104 (100%)	104 (100%)	0	100 100
13	K	103/103 (100%)	103 (100%)	0	100 100
14	L	109/109 (100%)	109 (100%)	0	100 100
15	M	99/99 (100%)	99 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	N	86/86 (100%)	85 (99%)	1 (1%)	63 79
17	O	99/99 (100%)	99 (100%)	0	100 100
18	P	89/89 (100%)	88 (99%)	1 (1%)	65 79
19	Q	84/84 (100%)	84 (100%)	0	100 100
20	R	93/93 (100%)	93 (100%)	0	100 100
21	S	81/81 (100%)	81 (100%)	0	100 100
22	T	84/84 (100%)	84 (100%)	0	100 100
23	U	78/78 (100%)	78 (100%)	0	100 100
24	V	59/59 (100%)	59 (100%)	0	100 100
25	W	67/67 (100%)	67 (100%)	0	100 100
26	X	54/54 (100%)	54 (100%)	0	100 100
27	Y	48/48 (100%)	48 (100%)	0	100 100
28	Z	59/59 (100%)	59 (100%)	0	100 100
29	a	47/47 (100%)	47 (100%)	0	100 100
30	b	47/47 (100%)	47 (100%)	0	100 100
31	c	38/38 (100%)	38 (100%)	0	100 100
32	d	51/51 (100%)	51 (100%)	0	100 100
33	e	34/34 (100%)	34 (100%)	0	100 100
34	f	187/187 (100%)	186 (100%)	1 (0%)	81 85
35	g	171/171 (100%)	171 (100%)	0	100 100
36	h	172/172 (100%)	171 (99%)	1 (1%)	78 84
37	i	119/119 (100%)	119 (100%)	0	100 100
38	j	91/91 (100%)	91 (100%)	0	100 100
39	k	124/124 (100%)	124 (100%)	0	100 100
40	l	104/104 (100%)	104 (100%)	0	100 100
41	m	105/105 (100%)	105 (100%)	0	100 100
42	n	86/86 (100%)	86 (100%)	0	100 100
43	o	90/90 (100%)	90 (100%)	0	100 100
44	p	102/102 (100%)	102 (100%)	0	100 100
45	q	94/94 (100%)	94 (100%)	0	100 100
46	r	83/83 (100%)	83 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	s	76/76 (100%)	76 (100%)	0	100 100
48	t	65/65 (100%)	65 (100%)	0	100 100
49	u	74/74 (100%)	74 (100%)	0	100 100
50	v	57/57 (100%)	57 (100%)	0	100 100
51	w	72/72 (100%)	72 (100%)	0	100 100
52	x	65/65 (100%)	65 (100%)	0	100 100
53	y	60/60 (100%)	59 (98%)	1 (2%)	53 75
55	B	20/20 (100%)	19 (95%)	1 (5%)	22 55
All	All	4689/4689 (100%)	4679 (100%)	10 (0%)	85 89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	151	THR
7	E	61	ARG
10	H	43	ASN
10	H	75	LEU
16	N	53	THR
18	P	78	LYS
34	f	129	LEU
36	h	138	SER
53	y	9	ASN
55	B	16	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
5	C	70	ASN
5	C	134	ASN
5	C	226	ASN
5	C	243	HIS
7	E	92	HIS
7	E	136	GLN
11	I	76	HIS
14	L	60	GLN
15	M	9	GLN
16	N	98	GLN
17	O	66	ASN

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Mol	Chain	Res	Type
17	O	115	ASN
21	S	70	HIS
23	U	87	GLN
24	V	46	HIS
25	W	36	HIS
27	Y	20	HIS
32	d	31	HIS
34	f	51	ASN
37	i	121	HIS
38	j	14	GLN
41	m	110	GLN
42	n	56	HIS
47	s	35	GLN
47	s	50	HIS
48	t	26	ASN
51	w	69	HIS
53	y	56	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2903 (99%)	495 (17%)	11 (0%)
2	2	1532/1534 (99%)	261 (17%)	4 (0%)
3	3	119/120 (99%)	15 (12%)	0
4	4	5/6 (83%)	1 (20%)	0
54	z	87/88 (98%)	41 (47%)	0
All	All	4645/4651 (99%)	813 (17%)	15 (0%)

All (813) 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

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Mol	Chain	Res	Type
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
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	222	A
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

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Mol	Chain	Res	Type
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
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	510	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	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	686	U
1	1	702	U

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Mol	Chain	Res	Type
1	1	709	U
1	1	710	U
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	893	C
1	1	894	U
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

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Mol	Chain	Res	Type
1	1	932	U
1	1	941	A
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	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

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Mol	Chain	Res	Type
1	1	1119	U
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	1136	G
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

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Mol	Chain	Res	Type
1	1	1352	U
1	1	1365	A
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	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

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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	1723	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	1802	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	1862	G
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

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Mol	Chain	Res	Type
1	1	1912	A
1	1	1914	C
1	1	1923	U
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	2103	C
1	1	2107	G
1	1	2110	G
1	1	2112	G
1	1	2113	U
1	1	2115	G

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Mol	Chain	Res	Type
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
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	2145	C
1	1	2146	C
1	1	2147	A
1	1	2151	U
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	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

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Mol	Chain	Res	Type
1	1	2243	U
1	1	2250	G
1	1	2278	A
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

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Mol	Chain	Res	Type
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU
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	2603	G
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

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Mol	Chain	Res	Type
1	1	2794	C
1	1	2797	U
1	1	2799	A
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
1	1	2903	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	71	A
2	2	72	A
2	2	73	C

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Mol	Chain	Res	Type
2	2	74	A
2	2	75	G
2	2	76	G
2	2	79	G
2	2	81	A
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	128	G
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

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Mol	Chain	Res	Type
2	2	332	G
2	2	347	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	372	C
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

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Mol	Chain	Res	Type
2	2	533	A
2	2	547	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	633	G
2	2	639	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	836	G
2	2	841	C

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Mol	Chain	Res	Type
2	2	843	U
2	2	844	G
2	2	845	A
2	2	846	G
2	2	884	U
2	2	885	G
2	2	887	G
2	2	914	A
2	2	934	C
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	982	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1004	A
2	2	1008	U
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	1044	A
2	2	1046	A
2	2	1065	U
2	2	1080	A

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Mol	Chain	Res	Type
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	1133	G
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1145	A
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	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	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A

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Mol	Chain	Res	Type
2	2	1277	C
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
2	2	1336	C
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	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	66	A

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Mol	Chain	Res	Type
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
4	4	2	G
54	z	2	G
54	z	7	G
54	z	8	U
54	z	10	U
54	z	13	G
54	z	14	A
54	z	15	G
54	z	16	U
54	z	17	OMG
54	z	19	C
54	z	20	U
54	z	21	G
54	z	22	A
54	z	23	A
54	z	24	G
54	z	36	G
54	z	37	A
54	z	45	U
54	z	46	A
54	z	48	A
54	z	49	C
54	z	50	G
54	z	51	G
54	z	53	A
54	z	54	A
54	z	55	C
54	z	56	G
54	z	59	U
54	z	61	G
54	z	65	G
54	z	66	5MU
54	z	68	C
54	z	71	A
54	z	72	U
54	z	73	C
54	z	76	C

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Mol	Chain	Res	Type
54	z	78	C
54	z	79	C
54	z	85	G
54	z	86	C
54	z	88	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	613	A
1	1	784	G
1	1	894	U
1	1	896	A
1	1	1379	U
1	1	2102	G
1	1	2146	C
1	1	2189	U
1	1	2602	A
1	1	2756	U
2	2	516	PSU
2	2	966	2MG
2	2	1109	C
2	2	1145	A

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

37 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	$\#\|Z\| > 2$
2	PSU	2	516	56,2	18,21,22	0.92	2 (11%)	22,30,33	1.77	4 (18%)
1	5MU	1	747	1	19,22,23	4.61	7 (36%)	28,32,35	3.73	9 (32%)
2	4OC	2	1402	2	20,23,24	2.85	8 (40%)	26,32,35	0.96	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MA	1	2503	56,1	22,25,26	3.59	10 (45%)	33,37,40	2.30	8 (24%)
1	PSU	1	2504	1	18,21,22	1.05	2 (11%)	22,30,33	1.89	5 (22%)
1	PSU	1	955	56,1	18,21,22	1.03	2 (11%)	22,30,33	1.97	5 (22%)
2	5MC	2	967	2	18,22,23	3.42	7 (38%)	26,32,35	1.00	2 (7%)
1	5MU	1	1939	56,1	19,22,23	4.54	7 (36%)	28,32,35	3.74	9 (32%)
1	OMG	1	2251	56,54,1	23,26,27	2.19	7 (30%)	33,38,41	1.72	7 (21%)
1	6MZ	1	1618	1	22,25,26	2.42	5 (22%)	30,36,39	3.38	11 (36%)
1	6MZ	1	2030	1	22,25,26	2.43	6 (27%)	30,36,39	3.31	13 (43%)
1	PSU	1	2580	1	18,21,22	1.07	2 (11%)	22,30,33	2.18	6 (27%)
55	FME	B	1	55	8,9,10	0.90	0	7,9,11	1.39	1 (14%)
54	5MU	z	66	54	19,22,23	4.90	7 (36%)	28,32,35	3.69	10 (35%)
1	OMC	1	2498	56,1	19,22,23	2.72	7 (36%)	26,31,34	0.91	1 (3%)
2	5MC	2	1407	2	18,22,23	3.28	7 (38%)	26,32,35	0.96	1 (3%)
1	1MG	1	745	1	22,26,27	2.92	7 (31%)	33,39,42	2.00	7 (21%)
2	2MG	2	1516	2	23,26,27	2.72	8 (34%)	32,38,41	2.07	9 (28%)
2	2MG	2	1207	2	23,26,27	2.69	8 (34%)	32,38,41	2.03	8 (25%)
1	PSU	1	2605	1	18,21,22	0.97	1 (5%)	22,30,33	2.01	5 (22%)
44	0TD	p	89	44	7,9,10	1.43	0	6,11,13	1.97	3 (50%)
2	MA6	2	1518	2	23,26,27	1.51	4 (17%)	34,38,41	3.13	11 (32%)
54	OMG	z	17	54	27,27,27	3.47	9 (33%)	40,41,41	6.53	15 (37%)
1	2MG	1	2445	1	23,26,27	2.64	8 (34%)	32,38,41	1.99	9 (28%)
1	OMU	1	2552	1	19,22,23	2.83	8 (42%)	26,31,34	1.71	6 (23%)
1	PSU	1	746	56,1	18,21,22	1.00	1 (5%)	22,30,33	1.70	3 (13%)
2	G7M	2	527	2	23,26,27	2.68	8 (34%)	35,39,42	2.33	11 (31%)
2	2MG	2	966	2	23,26,27	2.78	9 (39%)	32,38,41	2.12	8 (25%)
2	UR3	2	1498	2	19,22,23	2.56	7 (36%)	26,32,35	1.20	2 (7%)
1	PSU	1	1911	1	18,21,22	0.96	2 (11%)	22,30,33	1.94	4 (18%)
1	5MC	1	1962	1	18,22,23	3.35	7 (38%)	26,32,35	1.18	2 (7%)
1	PSU	1	2457	1	18,21,22	1.08	2 (11%)	22,30,33	2.08	6 (27%)
2	MA6	2	1519	2	23,26,27	1.52	5 (21%)	34,38,41	3.39	11 (32%)
1	PSU	1	1917	1	18,21,22	1.09	2 (11%)	22,30,33	1.97	6 (27%)
1	3TD	1	1915	1	18,22,23	3.97	7 (38%)	22,32,35	1.61	2 (9%)
1	2MG	1	1835	1	23,26,27	2.72	8 (34%)	32,38,41	1.99	7 (21%)
1	G7M	1	2069	1	23,26,27	2.69	10 (43%)	35,39,42	2.25	12 (34%)

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
2	PSU	2	516	56,2	-	2/7/25/26	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
1	2MA	1	2503	56,1	-	2/7/25/26	0/3/3/3
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	1	955	56,1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	56,1	-	0/7/25/26	0/2/2/2
1	OMG	1	2251	56,54,1	-	0/9/27/28	0/3/3/3
1	6MZ	1	1618	1	-	3/9/27/28	0/3/3/3
1	6MZ	1	2030	1	-	2/9/27/28	0/3/3/3
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
55	FME	B	1	55	-	3/7/9/11	-
54	5MU	z	66	54	-	6/7/25/26	0/2/2/2
1	OMC	1	2498	56,1	-	0/9/27/28	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/7/25/26	0/3/3/3
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
2	2MG	2	1207	2	-	0/9/27/28	0/3/3/3
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
44	0TD	p	89	44	-	2/7/12/14	-
2	MA6	2	1518	2	-	1/11/29/30	0/3/3/3
54	OMG	z	17	54	-	5/12/28/28	0/3/3/3
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	1	746	56,1	-	1/7/25/26	0/2/2/2
2	G7M	2	527	2	-	3/7/25/26	0/3/3/3
2	2MG	2	966	2	-	2/9/27/28	0/3/3/3
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	5/11/29/30	0/3/3/3
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	3TD	1	1915	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (207) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	11.52	1.48	1.35
1	1	2503	2MA	C4-N3	11.23	1.48	1.34
54	z	66	5MU	C6-N1	11.09	1.57	1.38
54	z	66	5MU	C2-N1	10.89	1.55	1.38
1	1	747	5MU	C2-N1	10.87	1.55	1.38
54	z	66	5MU	C4-C5	10.26	1.61	1.44
54	z	17	OMG	O6-C6	-10.17	1.04	1.23
1	1	1939	5MU	C2-N1	10.14	1.54	1.38
1	1	747	5MU	C6-N1	9.67	1.54	1.38
1	1	1939	5MU	C6-N1	9.63	1.54	1.38
1	1	1618	6MZ	C6-N6	9.33	1.44	1.34
1	1	1939	5MU	C4-C5	9.30	1.60	1.44
1	1	2030	6MZ	C6-N6	9.17	1.44	1.34
1	1	747	5MU	C4-C5	9.17	1.60	1.44
54	z	17	OMG	C4-N3	8.80	1.55	1.34
1	1	1915	3TD	C2-N1	8.66	1.48	1.37
2	2	967	5MC	C6-C5	8.65	1.48	1.34
2	2	1407	5MC	C6-C5	8.63	1.48	1.34
1	1	745	1MG	C2-N2	8.42	1.49	1.34
1	1	1962	5MC	C6-C5	8.16	1.48	1.34
54	z	17	OMG	C2-N3	8.01	1.52	1.33
1	1	1939	5MU	C4-N3	-7.60	1.24	1.38
2	2	966	2MG	C2-N3	7.56	1.46	1.31
1	1	747	5MU	C4-N3	-7.52	1.24	1.38
1	1	1835	2MG	C2-N3	7.43	1.46	1.31
2	2	1207	2MG	C2-N3	7.21	1.45	1.31
2	2	1516	2MG	C2-N3	7.06	1.45	1.31
54	z	66	5MU	C4-N3	-7.06	1.25	1.38
1	1	2445	2MG	C2-N3	6.94	1.45	1.31
1	1	2069	G7M	C5-N7	-6.82	1.31	1.39
1	1	1962	5MC	C4-N3	6.51	1.45	1.34
2	2	527	G7M	C5-N7	-6.40	1.31	1.39
1	1	2552	OMU	C2-N1	6.36	1.48	1.38
2	2	967	5MC	C4-N3	6.35	1.44	1.34
54	z	66	5MU	C6-C5	6.33	1.45	1.34
2	2	1498	UR3	C6-C5	6.32	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1402	4OC	C4-N3	6.26	1.43	1.32
1	1	2503	2MA	C2-N3	6.26	1.45	1.34
1	1	2552	OMU	C2-N3	6.23	1.49	1.38
2	2	966	2MG	C4-N3	6.15	1.48	1.34
1	1	1835	2MG	C4-N3	6.08	1.48	1.34
2	2	527	G7M	C4-N3	6.08	1.48	1.34
2	2	1207	2MG	C4-N3	6.05	1.48	1.34
1	1	1962	5MC	C2-N3	5.89	1.48	1.36
2	2	1516	2MG	C4-N3	5.88	1.48	1.34
2	2	967	5MC	C2-N3	5.81	1.48	1.36
1	1	745	1MG	C4-N3	5.81	1.48	1.34
2	2	1407	5MC	C4-N3	5.79	1.43	1.34
2	2	1402	4OC	C6-C5	5.74	1.48	1.35
1	1	2498	OMC	C2-N3	5.71	1.47	1.36
1	1	2445	2MG	C4-N3	5.70	1.47	1.34
1	1	747	5MU	C6-C5	5.64	1.43	1.34
1	1	2069	G7M	C4-N3	5.62	1.47	1.34
1	1	2251	OMG	C4-N3	5.59	1.47	1.34
2	2	1498	UR3	C2-N1	5.57	1.46	1.38
1	1	2503	2MA	C6-N1	5.57	1.43	1.35
1	1	1939	5MU	C6-C5	5.56	1.43	1.34
2	2	1402	4OC	C2-N3	5.53	1.47	1.36
2	2	1407	5MC	C2-N3	5.52	1.47	1.36
1	1	1915	3TD	C6-N1	5.47	1.45	1.36
1	1	2498	OMC	C6-C5	5.42	1.47	1.35
1	1	2552	OMU	C6-C5	5.34	1.47	1.35
1	1	745	1MG	C2-N3	5.32	1.44	1.34
2	2	527	G7M	C2-N3	5.26	1.45	1.33
54	z	17	OMG	C2-N1	5.07	1.50	1.37
2	2	1516	2MG	C2-N2	5.03	1.44	1.33
2	2	966	2MG	C2-N2	5.00	1.44	1.33
1	1	2251	OMG	C2-N3	4.99	1.45	1.33
2	2	1498	UR3	C2-N3	4.91	1.48	1.39
2	2	1207	2MG	C2-N2	4.82	1.44	1.33
1	1	1835	2MG	C2-N2	4.82	1.44	1.33
1	1	2503	2MA	C2-N1	4.77	1.42	1.34
1	1	2069	G7M	C2-N3	4.69	1.44	1.33
1	1	1915	3TD	C2-N3	4.67	1.48	1.38
1	1	2498	OMC	C4-N3	4.62	1.43	1.34
2	2	527	G7M	C2-N2	4.56	1.45	1.34
1	1	2498	OMC	C4-N4	4.54	1.44	1.33
2	2	1516	2MG	C2-N1	4.51	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2445	2MG	C2-N2	4.43	1.43	1.33
2	2	966	2MG	C2-N1	4.40	1.43	1.36
1	1	1962	5MC	C4-N4	4.34	1.45	1.34
2	2	967	5MC	C4-N4	4.31	1.45	1.34
2	2	1402	4OC	C4-N4	4.31	1.44	1.35
1	1	745	1MG	C5-N7	-4.19	1.31	1.39
1	1	2503	2MA	C5-C6	4.17	1.52	1.41
2	2	1207	2MG	C2-N1	4.15	1.43	1.36
1	1	2069	G7M	C2-N2	4.09	1.43	1.34
2	2	967	5MC	C6-N1	4.08	1.45	1.38
1	1	1835	2MG	C2-N1	3.99	1.43	1.36
1	1	1962	5MC	C2-N1	3.88	1.48	1.40
2	2	1407	5MC	C6-N1	3.86	1.44	1.38
1	1	2552	OMU	C4-N3	3.86	1.45	1.38
1	1	2445	2MG	C2-N1	3.84	1.42	1.36
2	2	1407	5MC	C4-N4	3.83	1.44	1.34
1	1	745	1MG	O6-C6	-3.81	1.15	1.23
1	1	2503	2MA	C6-N6	-3.79	1.24	1.34
54	z	17	OMG	C2-N2	3.71	1.43	1.34
2	2	967	5MC	C2-N1	3.68	1.48	1.40
1	1	2498	OMC	C2-N1	3.64	1.47	1.40
2	2	1407	5MC	C2-N1	3.62	1.47	1.40
2	2	1519	MA6	C5-C4	-3.60	1.32	1.39
1	1	1962	5MC	C6-N1	3.57	1.44	1.38
2	2	1402	4OC	C2-N1	3.56	1.47	1.40
1	1	2445	2MG	C5-N7	-3.56	1.32	1.39
1	1	1835	2MG	C5-N7	-3.48	1.32	1.39
2	2	1518	MA6	C5-C4	-3.46	1.32	1.39
1	1	2251	OMG	C5-N7	-3.29	1.32	1.39
1	1	2030	6MZ	C5-C4	-3.28	1.32	1.39
2	2	1516	2MG	C5-N7	-3.27	1.32	1.39
1	1	1618	6MZ	C5-C4	-3.24	1.33	1.39
1	1	2030	6MZ	C5-N7	-3.22	1.32	1.39
2	2	1402	4OC	C5-C4	3.21	1.47	1.40
2	2	527	G7M	C5-C6	3.18	1.52	1.43
54	z	17	OMG	C5-N7	-3.17	1.32	1.39
1	1	747	5MU	O4-C4	-3.17	1.17	1.23
54	z	17	OMG	C6-N1	3.16	1.44	1.38
1	1	2069	G7M	C5-C6	3.15	1.52	1.43
2	2	1207	2MG	C5-N7	-3.14	1.33	1.39
2	2	966	2MG	C5-N7	-3.12	1.33	1.39
1	1	2503	2MA	C4-N9	-3.05	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1939	5MU	O4-C4	-3.03	1.17	1.23
1	1	2498	OMC	O2-C2	-3.03	1.18	1.23
1	1	2251	OMG	C2-N2	3.03	1.41	1.34
1	1	2552	OMU	O4-C4	-2.98	1.18	1.24
2	2	967	5MC	O2-C2	-2.98	1.18	1.23
1	1	1618	6MZ	C5-N7	-2.98	1.33	1.39
2	2	1519	MA6	C8-N9	-2.98	1.32	1.37
1	1	1962	5MC	O2-C2	-2.96	1.18	1.23
1	1	2251	OMG	O6-C6	-2.95	1.18	1.23
2	2	1402	4OC	O2-C2	-2.94	1.18	1.23
2	2	1407	5MC	O2-C2	-2.91	1.18	1.23
2	2	1518	MA6	C6-N6	2.90	1.45	1.36
54	z	66	5MU	O4-C4	-2.86	1.18	1.23
1	1	1917	PSU	C6-C5	2.80	1.38	1.35
2	2	1518	MA6	C8-N9	-2.79	1.32	1.37
2	2	1519	MA6	C6-N6	2.79	1.45	1.36
1	1	745	1MG	C5-C6	2.75	1.52	1.45
1	1	2503	2MA	C5-N7	-2.75	1.33	1.39
2	2	527	G7M	O6-C6	-2.75	1.18	1.23
1	1	2445	2MG	O6-C6	-2.74	1.18	1.23
1	1	1939	5MU	O2-C2	-2.74	1.18	1.23
2	2	1519	MA6	C5-N7	-2.73	1.33	1.39
1	1	2069	G7M	C4-N9	-2.69	1.31	1.38
1	1	2069	G7M	O6-C6	-2.69	1.18	1.23
1	1	1835	2MG	O6-C6	-2.69	1.18	1.23
1	1	2030	6MZ	C8-N9	-2.68	1.32	1.37
1	1	2457	PSU	C6-C5	2.66	1.38	1.35
54	z	66	5MU	O2-C2	-2.63	1.18	1.23
1	1	1915	3TD	O2-C2	-2.63	1.18	1.23
2	2	1207	2MG	O6-C6	-2.62	1.18	1.23
2	2	1518	MA6	C5-N7	-2.61	1.34	1.39
2	2	1498	UR3	C6-N1	2.61	1.44	1.38
1	1	2504	PSU	C6-C5	2.61	1.38	1.35
54	z	17	OMG	C5-C6	2.61	1.54	1.44
1	1	2069	G7M	CN7-N7	-2.61	1.42	1.46
2	2	1516	2MG	O6-C6	-2.58	1.18	1.23
1	1	745	1MG	C4-N9	-2.58	1.31	1.38
1	1	2445	2MG	C4-N9	-2.57	1.31	1.38
1	1	2552	OMU	O2-C2	-2.55	1.18	1.23
1	1	747	5MU	O2-C2	-2.54	1.18	1.23
2	2	1402	4OC	C6-N1	2.53	1.44	1.38
1	1	2251	OMG	C4-N9	-2.50	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2030	6MZ	C6-N1	-2.48	1.31	1.35
2	2	966	2MG	C5-C6	2.47	1.53	1.44
1	1	2069	G7M	C2-N1	2.46	1.43	1.37
1	1	1915	3TD	O4-C4	-2.46	1.17	1.23
1	1	1618	6MZ	C8-N9	-2.44	1.33	1.37
2	2	527	G7M	C2-N1	2.44	1.43	1.37
2	2	966	2MG	O6-C6	-2.44	1.18	1.23
2	2	1516	2MG	C4-N9	-2.44	1.31	1.38
2	2	516	PSU	C6-C5	2.43	1.38	1.35
54	z	17	OMG	C4-N9	-2.42	1.31	1.38
1	1	1618	6MZ	C6-N1	-2.41	1.31	1.35
1	1	746	PSU	C6-C5	2.40	1.38	1.35
1	1	2580	PSU	C4-C5	-2.34	1.37	1.44
2	2	1207	2MG	C5-C6	2.34	1.53	1.44
1	1	2030	6MZ	C5-C6	-2.31	1.36	1.41
1	1	1915	3TD	C4-N3	2.29	1.45	1.40
1	1	1911	PSU	C6-C5	2.26	1.38	1.35
2	2	1516	2MG	C5-C6	2.25	1.52	1.44
1	1	2498	OMC	C6-N1	2.22	1.43	1.38
1	1	2457	PSU	C4-C5	-2.21	1.37	1.44
2	2	966	2MG	C6-N1	2.21	1.42	1.38
1	1	1835	2MG	C4-N9	-2.21	1.32	1.38
2	2	1207	2MG	C4-N9	-2.20	1.32	1.38
1	1	1835	2MG	C5-C6	2.20	1.52	1.44
1	1	955	PSU	C4-C5	-2.19	1.37	1.44
2	2	527	G7M	C4-N9	-2.16	1.32	1.38
1	1	1917	PSU	C4-C5	-2.16	1.38	1.44
1	1	2605	PSU	C4-C5	-2.16	1.38	1.44
1	1	2445	2MG	C5-C6	2.15	1.52	1.44
1	1	2552	OMU	C6-N1	2.14	1.43	1.38
2	2	516	PSU	C4-C5	-2.14	1.38	1.44
1	1	2069	G7M	C6-N1	2.13	1.42	1.38
1	1	955	PSU	C6-C5	2.12	1.37	1.35
1	1	2552	OMU	C5-C4	2.12	1.48	1.43
1	1	2504	PSU	C4-C5	-2.12	1.38	1.44
1	1	2503	2MA	C5-C4	-2.11	1.35	1.39
2	2	966	2MG	C4-N9	-2.11	1.32	1.38
1	1	2251	OMG	C5-C6	2.10	1.52	1.44
2	2	1498	UR3	O2-C2	-2.10	1.18	1.22
2	2	1498	UR3	C4-N3	2.07	1.45	1.40
2	2	1498	UR3	C3U-N3	-2.04	1.43	1.47
1	1	1911	PSU	C4-C5	-2.04	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1519	MA6	C4-N9	-2.03	1.33	1.37
1	1	2503	2MA	C8-N9	-2.01	1.33	1.37
1	1	2580	PSU	C6-C5	2.01	1.37	1.35

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	z	17	OMG	O6-C6-N1	-30.05	62.50	120.12
54	z	17	OMG	O6-C6-C5	-23.72	63.67	126.60
2	2	1519	MA6	N1-C6-N6	-13.99	101.79	117.08
1	1	747	5MU	C5-C4-N3	12.56	126.03	115.31
2	2	1518	MA6	N1-C6-N6	-12.30	103.63	117.08
54	z	66	5MU	C5-C4-N3	12.27	125.78	115.31
1	1	1939	5MU	C5-C4-N3	12.18	125.71	115.31
1	1	1939	5MU	C5-C6-N1	-9.91	113.15	123.34
1	1	747	5MU	C5-C6-N1	-9.57	113.50	123.34
54	z	66	5MU	C5-C6-N1	-8.89	114.19	123.34
1	1	1618	6MZ	C4-N9-C1'	-8.81	105.60	126.59
1	1	1618	6MZ	C1'-N9-C8	8.73	146.85	127.14
1	1	2030	6MZ	C4-N9-C1'	-8.46	106.44	126.59
1	1	2030	6MZ	C1'-N9-C8	8.07	145.35	127.14
1	1	2030	6MZ	C5-C4-N3	-6.67	118.05	126.75
2	2	1519	MA6	C5-C6-N6	6.66	136.89	125.30
1	1	2503	2MA	C1'-N9-C8	-6.43	112.62	127.14
1	1	1618	6MZ	C5-C4-N3	-6.31	118.52	126.75
1	1	747	5MU	O4-C4-C5	-6.01	117.93	124.90
2	2	966	2MG	C2-N3-C4	5.94	119.40	112.04
2	2	527	G7M	CN7-N7-C5	5.88	134.07	126.77
54	z	17	OMG	OP3-P-OP1	-5.87	87.70	110.68
2	2	1516	2MG	C2-N3-C4	5.80	119.23	112.04
1	1	2503	2MA	N9-C8-N7	-5.68	106.14	113.91
2	2	1207	2MG	C2-N3-C4	5.65	119.05	112.04
1	1	745	1MG	C1'-N9-C4	-5.64	109.74	126.50
2	2	1518	MA6	C5-C6-N6	5.62	135.09	125.30
1	1	1835	2MG	C2-N3-C4	5.61	119.00	112.04
1	1	747	5MU	C4-N3-C2	-5.50	120.23	127.35
1	1	1939	5MU	C4-N3-C2	-5.41	120.34	127.35
2	2	1519	MA6	N1-C2-N3	-5.41	120.14	128.60
1	1	2069	G7M	CN7-N7-C5	5.38	133.45	126.77
54	z	66	5MU	C5M-C5-C4	5.37	124.67	118.77
54	z	17	OMG	OP3-P-O5'	-5.35	92.51	106.73
1	1	1618	6MZ	C9-N6-C6	-5.32	118.29	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2445	2MG	C2-N3-C4	5.29	118.60	112.04
1	1	2580	PSU	N1-C2-N3	5.29	121.12	115.13
2	2	966	2MG	C5-C4-N3	-5.25	119.94	128.46
2	2	1518	MA6	N1-C2-N3	-5.23	120.42	128.60
1	1	1618	6MZ	N1-C2-N3	-5.23	120.42	128.60
1	1	1939	5MU	O4-C4-C5	-5.21	118.86	124.90
1	1	2605	PSU	C4-N3-C2	-5.20	118.85	126.34
1	1	1835	2MG	C5-C4-N3	-5.18	120.06	128.46
1	1	2457	PSU	N1-C2-N3	5.14	120.95	115.13
1	1	2457	PSU	C4-N3-C2	-5.14	118.94	126.34
1	1	2030	6MZ	C4-C5-C6	5.14	120.79	116.81
1	1	1911	PSU	C4-N3-C2	-5.13	118.95	126.34
1	1	2580	PSU	C4-N3-C2	-5.12	118.96	126.34
54	z	17	OMG	OP3-P-OP2	-5.12	88.07	107.64
54	z	17	OMG	C5-C6-N1	5.11	126.17	113.19
1	1	2552	OMU	C4-N3-C2	-5.11	119.84	126.58
1	1	745	1MG	C1'-N9-C8	5.10	141.21	126.70
2	2	527	G7M	CN7-N7-C8	-5.08	117.00	124.84
1	1	2069	G7M	CN7-N7-C8	-5.06	117.03	124.84
54	z	17	OMG	OP2-P-OP1	5.03	130.36	110.68
54	z	66	5MU	C4-N3-C2	-5.02	120.86	127.35
2	2	1519	MA6	C5-C4-N3	-5.01	120.21	126.75
54	z	17	OMG	C2-N1-C6	-5.01	115.97	125.10
2	2	1207	2MG	C5-C4-N3	-5.01	120.34	128.46
1	1	745	1MG	C5-C4-N3	-5.00	120.36	128.46
1	1	1917	PSU	C4-N3-C2	-4.99	119.14	126.34
2	2	1518	MA6	C5-C4-N3	-4.99	120.24	126.75
1	1	2030	6MZ	N3-C4-N9	4.98	135.29	127.08
1	1	955	PSU	C4-N3-C2	-4.97	119.17	126.34
54	z	66	5MU	O4-C4-C5	-4.97	119.14	124.90
1	1	1915	3TD	N1-C2-N3	4.94	120.03	116.14
1	1	2030	6MZ	N1-C2-N3	-4.92	120.90	128.60
2	2	516	PSU	C4-N3-C2	-4.90	119.28	126.34
54	z	66	5MU	N3-C2-N1	4.90	121.39	114.89
1	1	2445	2MG	C5-C4-N3	-4.86	120.58	128.46
1	1	2504	PSU	N1-C2-N3	4.84	120.62	115.13
1	1	955	PSU	N1-C2-N3	4.82	120.59	115.13
1	1	2605	PSU	N1-C2-N3	4.81	120.58	115.13
2	2	1516	2MG	C5-C4-N3	-4.78	120.71	128.46
1	1	746	PSU	C4-N3-C2	-4.77	119.47	126.34
1	1	2504	PSU	C4-N3-C2	-4.74	119.52	126.34
1	1	1939	5MU	N3-C2-N1	4.71	121.14	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1911	PSU	N1-C2-N3	4.70	120.46	115.13
1	1	2503	2MA	C4-N9-C8	4.70	110.82	105.73
1	1	1917	PSU	N1-C2-N3	4.70	120.45	115.13
54	z	66	5MU	C5M-C5-C6	-4.63	116.67	122.85
1	1	2251	OMG	C5-C4-N3	-4.59	121.01	128.46
1	1	747	5MU	N3-C2-N1	4.54	120.92	114.89
1	1	1939	5MU	C5M-C5-C6	-4.54	116.78	122.85
1	1	1939	5MU	C5M-C5-C4	4.50	123.72	118.77
2	2	966	2MG	C2-N1-C6	-4.49	119.31	124.48
1	1	2445	2MG	C2-N1-C6	-4.47	119.33	124.48
2	2	527	G7M	C1'-N9-C8	-4.46	111.67	126.74
2	2	1518	MA6	N9-C8-N7	-4.42	107.87	113.91
2	2	1519	MA6	N9-C8-N7	-4.42	107.87	113.91
1	1	2503	2MA	C5-C4-N3	-4.35	122.30	127.19
2	2	1516	2MG	C2-N1-C6	-4.35	119.47	124.48
2	2	527	G7M	C1'-N9-C4	4.28	139.23	126.50
2	2	1207	2MG	C2-N1-C6	-4.27	119.56	124.48
2	2	516	PSU	N1-C2-N3	4.26	119.96	115.13
1	1	746	PSU	N1-C2-N3	4.26	119.95	115.13
1	1	1915	3TD	C4-N3-C2	-4.26	119.99	124.61
2	2	1498	UR3	C4-N3-C2	-4.20	120.61	124.56
1	1	2503	2MA	C4-N9-C1'	4.18	136.56	126.59
1	1	1835	2MG	C2-N1-C6	-4.15	119.70	124.48
2	2	527	G7M	C5-C4-N3	-4.12	120.24	128.15
1	1	1618	6MZ	N3-C4-N9	4.05	133.75	127.08
1	1	2030	6MZ	N9-C8-N7	-3.96	108.50	113.91
1	1	1618	6MZ	C2-N3-C4	3.96	121.10	111.75
1	1	1618	6MZ	C4-C5-C6	3.91	119.84	116.81
2	2	527	G7M	C2-N3-C4	3.91	119.27	112.30
1	1	2069	G7M	C2-N3-C4	3.89	119.23	112.30
1	1	747	5MU	C5M-C5-C6	-3.81	117.77	122.85
2	2	1518	MA6	N3-C4-N9	3.79	133.32	127.08
1	1	2030	6MZ	C2-N3-C4	3.75	120.61	111.75
1	1	2069	G7M	C5-C4-N3	-3.71	121.04	128.15
2	2	1519	MA6	N3-C4-N9	3.66	133.12	127.08
1	1	1618	6MZ	N9-C8-N7	-3.65	108.92	113.91
1	1	747	5MU	C5M-C5-C4	3.65	122.78	118.77
1	1	2580	PSU	O2-C2-N1	-3.64	118.78	122.79
2	2	1407	5MC	C5-C6-N1	-3.62	119.61	123.34
1	1	2069	G7M	C1'-N9-C8	-3.58	114.67	126.74
2	2	527	G7M	C5-C6-N1	3.57	119.24	111.79
1	1	2069	G7M	C5-C6-N1	3.55	119.20	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	p	89	0TD	OD2-CG-CB	3.53	120.77	113.15
1	1	2069	G7M	O6-C6-C5	-3.53	120.11	128.06
1	1	2251	OMG	C2-N3-C4	3.51	118.55	112.30
1	1	1618	6MZ	C5-C6-N1	3.49	121.92	118.20
1	1	745	1MG	N9-C4-N3	3.46	132.88	125.94
1	1	2580	PSU	C6-C5-C4	3.44	120.60	118.20
2	2	527	G7M	O6-C6-C5	-3.42	120.34	128.06
2	2	1519	MA6	C2-N3-C4	3.42	119.84	111.75
1	1	1835	2MG	N9-C4-N3	3.42	132.80	125.94
2	2	1518	MA6	C4-C5-C6	3.39	119.67	115.88
2	2	527	G7M	N9-C4-N3	3.37	132.71	125.94
2	2	1518	MA6	C4-N9-C8	3.36	109.36	105.73
1	1	2552	OMU	N3-C2-N1	3.34	119.32	114.89
2	2	1519	MA6	C4-N9-C8	3.27	109.27	105.73
1	1	2552	OMU	C5-C4-N3	3.27	119.72	114.84
2	2	1518	MA6	C2-N3-C4	3.25	119.44	111.75
2	2	966	2MG	N9-C4-N3	3.24	132.45	125.94
2	2	1519	MA6	C4-C5-C6	3.24	119.50	115.88
1	1	2251	OMG	C2-N1-C6	-3.20	119.26	125.10
54	z	66	5MU	O2-C2-N1	-3.18	118.56	122.79
2	2	967	5MC	C5-C6-N1	-3.17	120.08	123.34
1	1	2069	G7M	C1'-N9-C4	3.16	135.90	126.50
1	1	2605	PSU	C6-C5-C4	3.13	120.39	118.20
1	1	2069	G7M	C2-N1-C6	-3.12	119.40	125.10
55	B	1	FME	C-CA-N	3.11	115.34	109.73
1	1	2457	PSU	O2-C2-N1	-3.10	119.38	122.79
1	1	2030	6MZ	C5-C6-N1	3.10	121.50	118.20
54	z	17	OMG	C6-C5-N7	3.09	136.00	130.25
2	2	1519	MA6	C2-N1-C6	3.07	118.99	111.75
1	1	2030	6MZ	C9-N6-C6	-3.06	120.23	122.87
1	1	1911	PSU	O2-C2-N1	-3.06	119.43	122.79
1	1	2251	OMG	N9-C8-N7	-3.05	107.64	113.39
2	2	1518	MA6	C2-N1-C6	3.05	118.95	111.75
54	z	17	OMG	O5'-P-OP1	3.03	114.97	106.47
1	1	2503	2MA	C5-N7-C8	3.03	107.81	103.51
1	1	745	1MG	C2-N3-C4	3.03	118.78	111.98
1	1	1917	PSU	C6-C5-C4	3.01	120.30	118.20
1	1	955	PSU	C6-C5-C4	3.00	120.30	118.20
54	z	17	OMG	OP2-P-O5'	2.96	114.61	106.73
1	1	1939	5MU	O2-C2-N1	-2.96	118.85	122.79
2	2	1207	2MG	N9-C4-N3	2.92	131.79	125.94
2	2	1516	2MG	N9-C8-N7	-2.90	107.93	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2457	PSU	C6-C5-C4	2.89	120.22	118.20
1	1	2445	2MG	N9-C4-N3	2.88	131.72	125.94
1	1	1917	PSU	O2-C2-N1	-2.88	119.62	122.79
1	1	2580	PSU	C6-N1-C2	-2.86	119.75	122.68
1	1	2552	OMU	O4-C4-C5	-2.86	120.14	125.16
1	1	2503	2MA	N3-C4-N9	2.86	130.95	126.99
1	1	2504	PSU	O2-C2-N1	-2.81	119.70	122.79
2	2	1516	2MG	N9-C4-N3	2.80	131.57	125.94
2	2	1207	2MG	N9-C8-N7	-2.79	108.13	113.39
2	2	527	G7M	C2-N1-C6	-2.78	120.03	125.10
1	1	2030	6MZ	C5-N7-C8	2.75	107.42	103.51
1	1	746	PSU	O2-C2-N1	-2.74	119.78	122.79
2	2	1498	UR3	C3U-N3-C4	2.73	121.78	117.89
1	1	2445	2MG	N9-C8-N7	-2.71	108.28	113.39
1	1	955	PSU	O2-C2-N1	-2.71	119.81	122.79
1	1	1911	PSU	C6-C5-C4	2.71	120.09	118.20
1	1	2605	PSU	O2-C2-N1	-2.71	119.81	122.79
1	1	745	1MG	N9-C8-N7	-2.70	108.31	113.39
1	1	2251	OMG	N9-C4-N3	2.69	131.33	125.94
2	2	966	2MG	N9-C8-N7	-2.65	108.40	113.39
1	1	2503	2MA	N3-C2-N1	-2.65	120.85	125.72
54	z	17	OMG	C5-C4-N3	-2.64	124.19	128.46
54	z	66	5MU	O4-C4-N3	-2.63	115.08	120.12
1	1	1835	2MG	N9-C8-N7	-2.62	108.46	113.39
2	2	1207	2MG	CM2-N2-C2	-2.62	118.08	123.86
1	1	2457	PSU	C6-N1-C2	-2.61	120.02	122.68
1	1	1618	6MZ	C5-N7-C8	2.57	107.15	103.51
1	1	747	5MU	O2-C2-N1	-2.55	119.40	122.79
2	2	1516	2MG	C5-C6-N1	2.51	119.58	113.19
1	1	2069	G7M	N9-C4-N3	2.51	130.99	125.94
1	1	2445	2MG	CM2-N2-C2	-2.51	118.31	123.86
1	1	2504	PSU	C6-N1-C2	-2.51	120.12	122.68
2	2	966	2MG	C5-C6-N1	2.49	119.52	113.19
1	1	2251	OMG	C5-C6-N1	2.48	119.49	113.19
2	2	966	2MG	CM2-N2-C2	-2.47	118.41	123.86
2	2	1516	2MG	O6-C6-C5	-2.46	120.08	126.60
1	1	1962	5MC	C5-C6-N1	-2.45	120.82	123.34
1	1	1939	5MU	O4-C4-N3	-2.45	115.43	120.12
2	2	1207	2MG	C5-C6-N1	2.44	119.40	113.19
1	1	2498	OMC	CM2-O2'-C2'	-2.44	108.12	114.52
1	1	1835	2MG	C5-C6-N1	2.44	119.38	113.19
2	2	516	PSU	O2-C2-N1	-2.44	120.11	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	966	2MG	O6-C6-C5	-2.43	120.14	126.60
1	1	2069	G7M	N9-C8-N7	-2.43	106.20	112.21
1	1	2445	2MG	C5-C6-N1	2.42	119.34	113.19
1	1	2504	PSU	C6-C5-C4	2.40	119.88	118.20
1	1	2069	G7M	N2-C2-N1	2.40	121.82	116.71
1	1	1835	2MG	O6-C6-C5	-2.38	120.29	126.60
2	2	1519	MA6	C5-N7-C8	2.37	106.88	103.51
1	1	2580	PSU	O4'-C1'-C2'	2.37	108.49	105.14
1	1	2251	OMG	O6-C6-C5	-2.36	120.33	126.60
1	1	1962	5MC	C1'-N1-C6	-2.36	117.19	121.12
1	1	2445	2MG	O6-C6-C5	-2.34	120.41	126.60
1	1	2552	OMU	CM2-O2'-C2'	-2.33	108.41	114.52
2	2	1516	2MG	C1'-N9-C4	-2.32	119.61	126.50
2	2	1518	MA6	C5-N7-C8	2.30	106.78	103.51
54	z	17	OMG	N9-C8-N7	-2.28	109.09	113.39
1	1	2030	6MZ	C6-C5-N7	-2.27	129.94	132.39
1	1	2457	PSU	O4'-C1'-C2'	2.26	108.34	105.14
1	1	2030	6MZ	C4-N9-C8	2.25	108.16	105.73
2	2	967	5MC	CM5-C5-C6	-2.23	119.87	122.85
2	2	1402	4OC	C6-C5-C4	2.20	119.65	116.96
2	2	1207	2MG	O6-C6-C5	-2.17	120.84	126.60
44	p	89	0TD	OD1-CG-CB	-2.17	117.90	122.44
54	z	17	OMG	C6-C5-C4	-2.16	115.45	118.77
54	z	66	5MU	C6-N1-C2	-2.14	119.13	121.30
1	1	747	5MU	O4-C4-N3	-2.13	116.03	120.12
2	2	527	G7M	N9-C8-N7	-2.11	106.99	112.21
1	1	745	1MG	C5-C6-N1	2.10	118.96	114.91
2	2	516	PSU	C6-N1-C2	-2.09	120.54	122.68
1	1	1917	PSU	C6-N1-C2	-2.09	120.55	122.68
1	1	955	PSU	C6-N1-C2	-2.08	120.56	122.68
2	2	1516	2MG	N1-C2-N3	-2.05	120.77	123.95
1	1	2445	2MG	C1'-N9-C4	-2.05	120.42	126.50
44	p	89	0TD	CSB-SB-CB	2.05	106.15	102.44
1	1	2552	OMU	O2-C2-N1	-2.03	120.08	122.79
1	1	1917	PSU	O4'-C1'-C2'	2.03	108.01	105.14
54	z	17	OMG	N9-C4-N3	2.02	130.00	125.94
1	1	2605	PSU	C6-N1-C2	-2.00	120.64	122.68

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
55	B	1	FME	O-C-CA-CB
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
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'
54	z	17	OMG	C5'-O5'-P-OP2
54	z	17	OMG	C5'-O5'-P-OP3
54	z	17	OMG	C1'-C2'-O2'-CM2
54	z	66	5MU	C2'-C1'-N1-C2
54	z	66	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	527	G7M	O4'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
2	2	1519	MA6	N1-C6-N6-C10
54	z	17	OMG	C3'-C2'-O2'-CM2
55	B	1	FME	N-CA-CB-CG
2	2	966	2MG	C3'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
54	z	66	5MU	O4'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C10
2	2	1519	MA6	C5-C6-N6-C9
54	z	66	5MU	O4'-C1'-N1-C2
54	z	66	5MU	O4'-C1'-N1-C6
1	1	2503	2MA	C3'-C4'-C5'-O5'
54	z	66	5MU	C3'-C4'-C5'-O5'
44	p	89	0TD	CG-CB-SB-CSB
44	p	89	0TD	SB-CB-CG-OD1
2	2	527	G7M	C4'-C5'-O5'-P
1	1	1618	6MZ	N1-C6-N6-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	2	1402	4OC	C3'-C4'-C5'-O5'
55	B	1	FME	C-CA-CB-CG
1	1	746	PSU	O4'-C1'-C5-C6
1	1	2069	G7M	O4'-C4'-C5'-O5'
54	z	17	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	516	PSU	3	0
1	1	955	PSU	1	0
1	1	2030	6MZ	2	0
1	1	2580	PSU	1	0
55	B	1	FME	2	0
54	z	66	5MU	1	0
2	2	1516	2MG	1	0
44	p	89	0TD	1	0
2	2	1518	MA6	3	0
54	z	17	OMG	7	0
1	1	2445	2MG	1	0
1	1	2552	OMU	1	0
2	2	966	2MG	2	0
1	1	1962	5MC	2	0
1	1	2457	PSU	1	0
2	2	1519	MA6	4	0
1	1	1915	3TD	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 402 ligands modelled in this entry, 402 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.

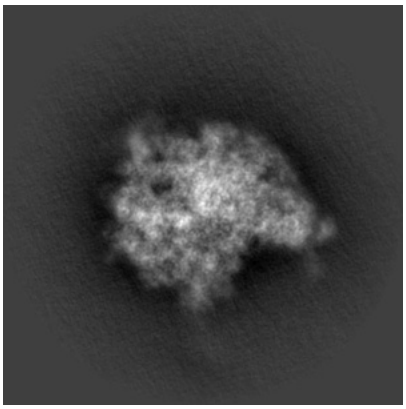
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12929. These allow visual inspection of the internal detail of the map and identification of artifacts.

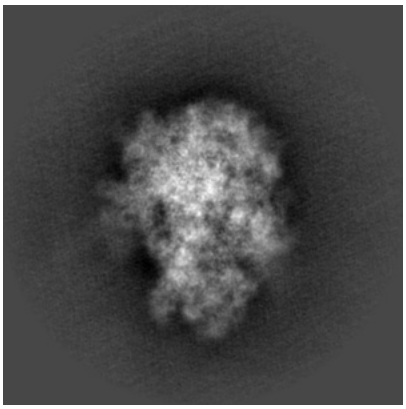
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

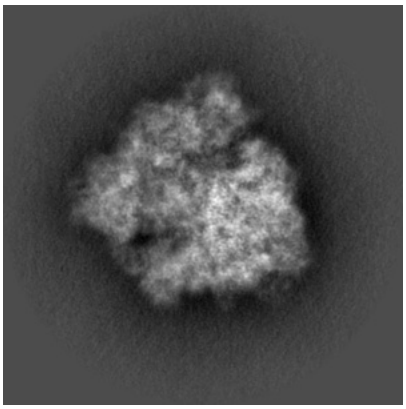
6.1.1 Primary map



X

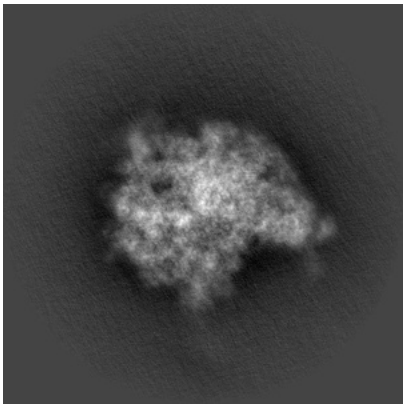


Y

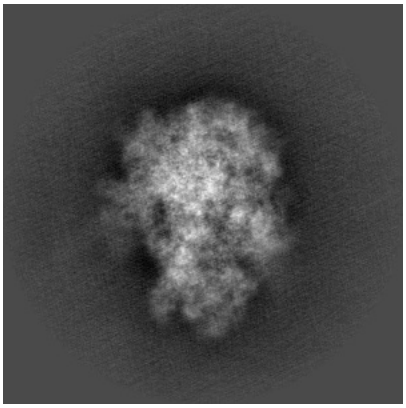


Z

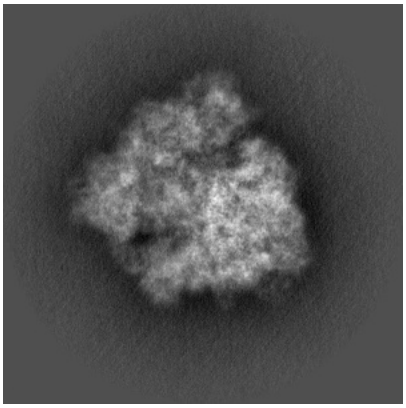
6.1.2 Raw map



X



Y

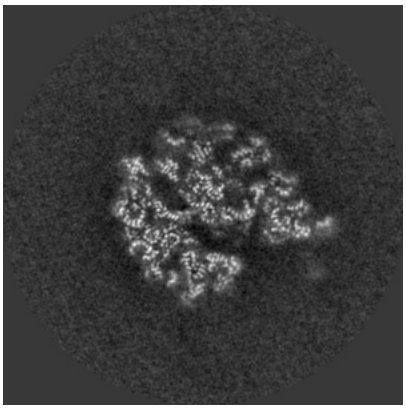


Z

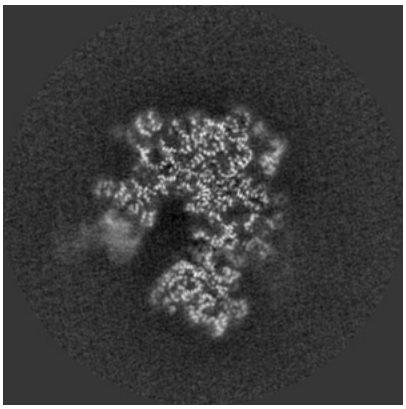
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

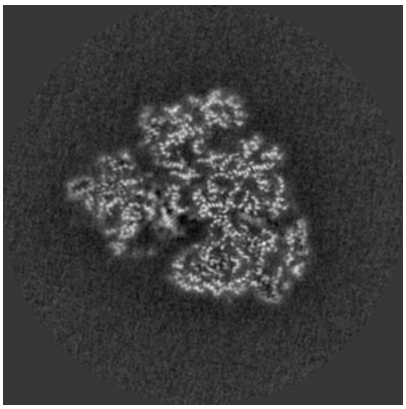
6.2.1 Primary map



X Index: 200

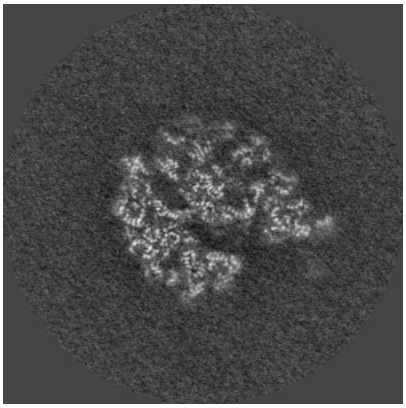


Y Index: 200

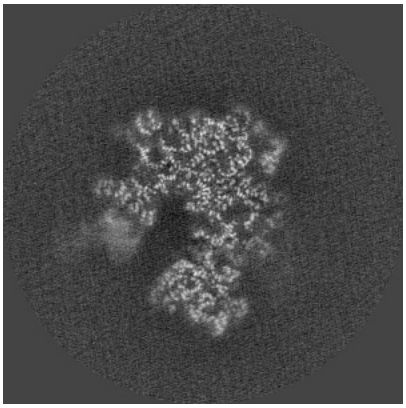


Z Index: 200

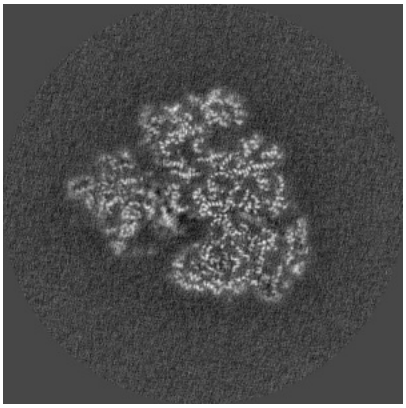
6.2.2 Raw map



X Index: 200



Y Index: 200

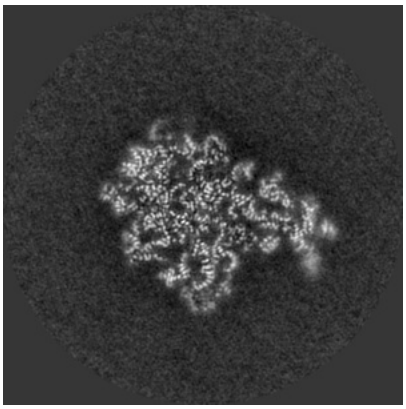


Z Index: 200

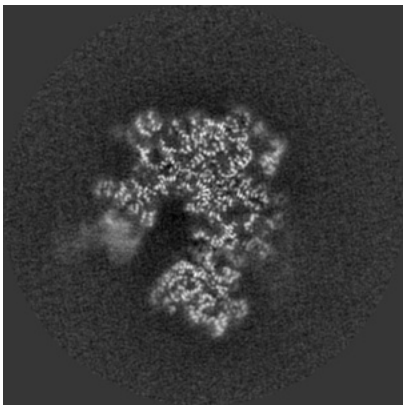
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

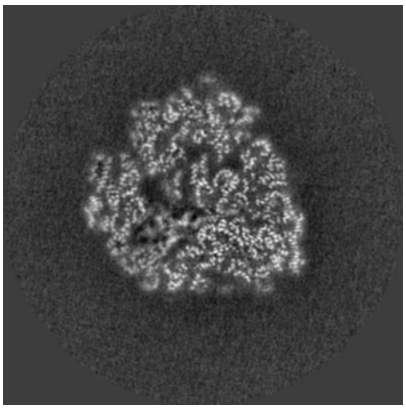
6.3.1 Primary map



X Index: 217

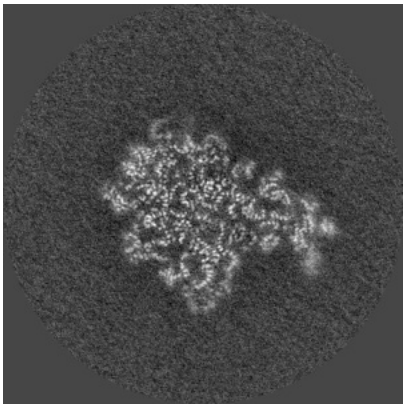


Y Index: 200

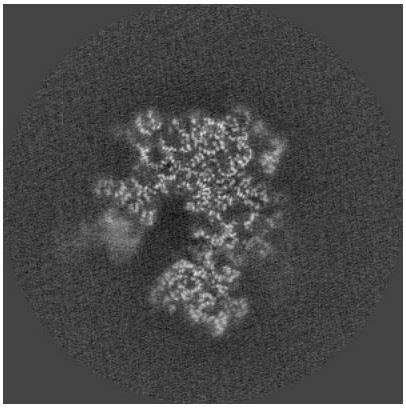


Z Index: 188

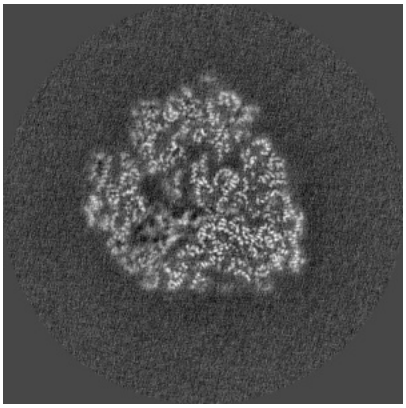
6.3.2 Raw map



X Index: 216



Y Index: 200

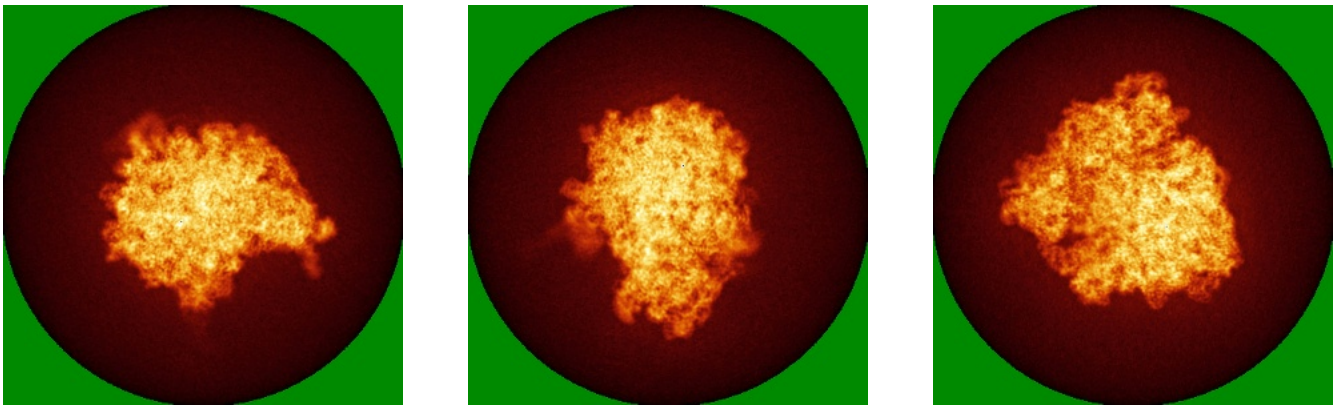


Z Index: 188

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

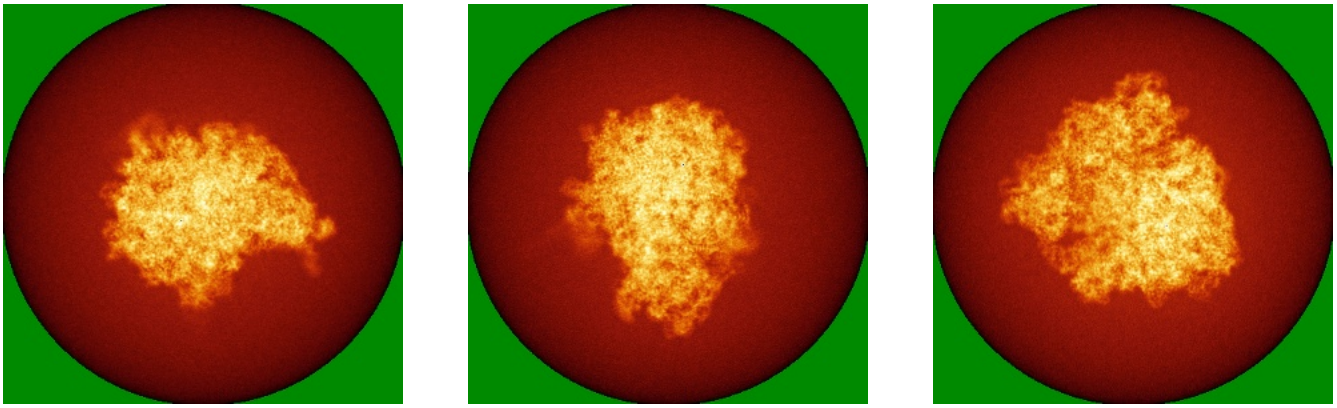
6.4 Orthogonal standard-deviation projections (False-color) (i)

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)

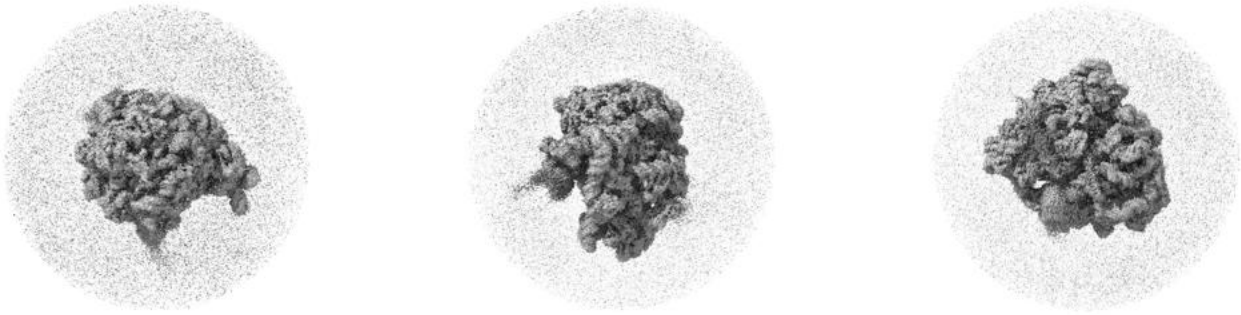
6.5.1 Primary map



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.

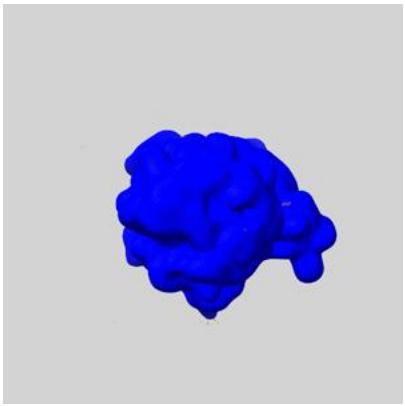
6.6 Mask visualisation

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

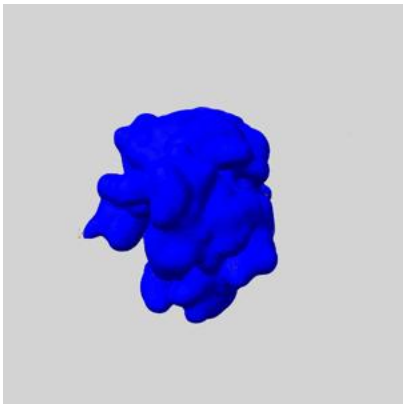
A mask typically either:

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

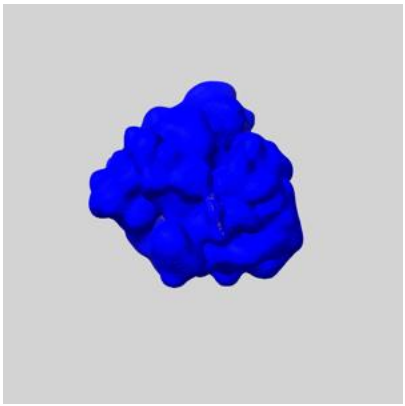
6.6.1 emd_12929_msk_1.map



X



Y

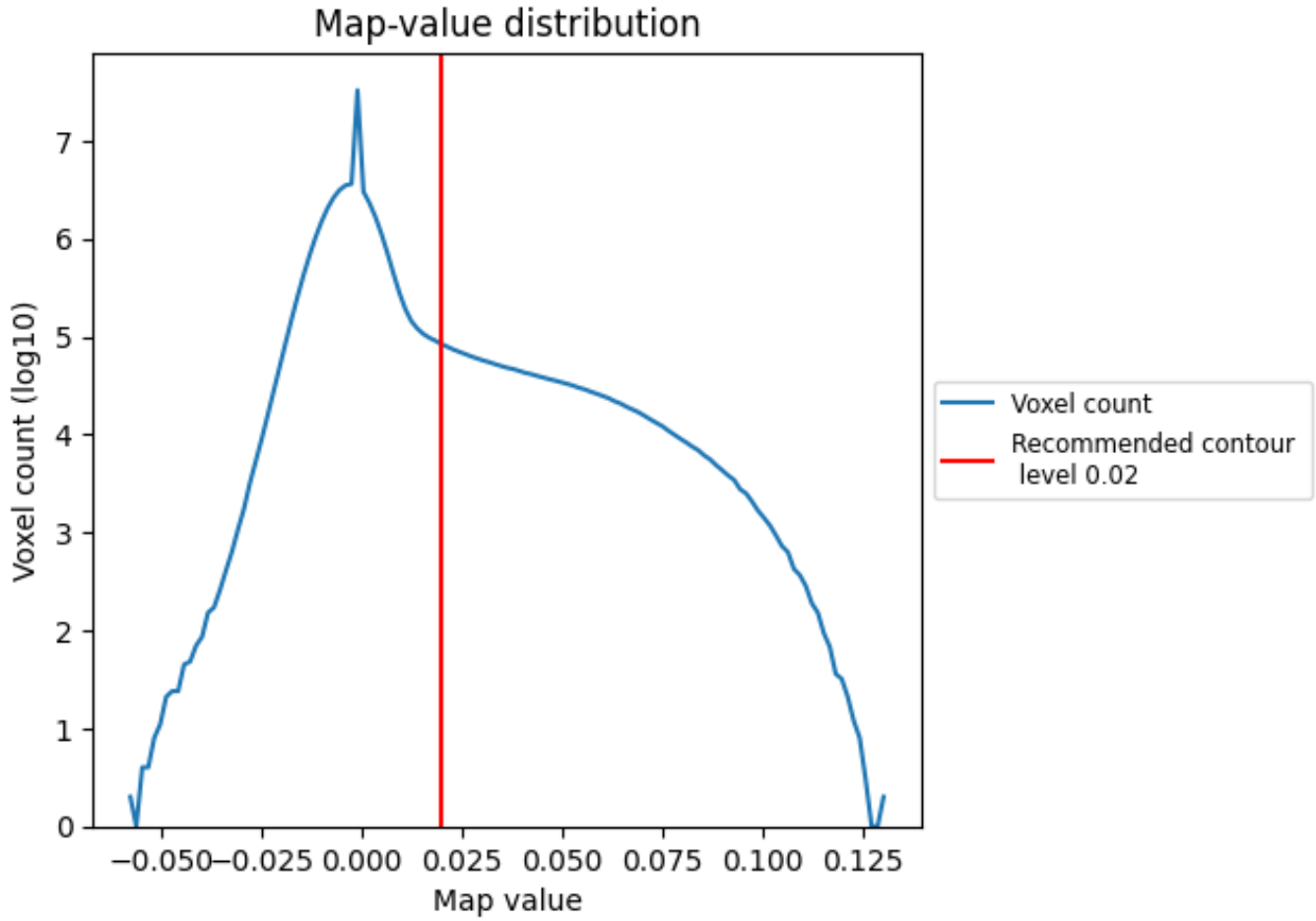


Z

7 Map analysis

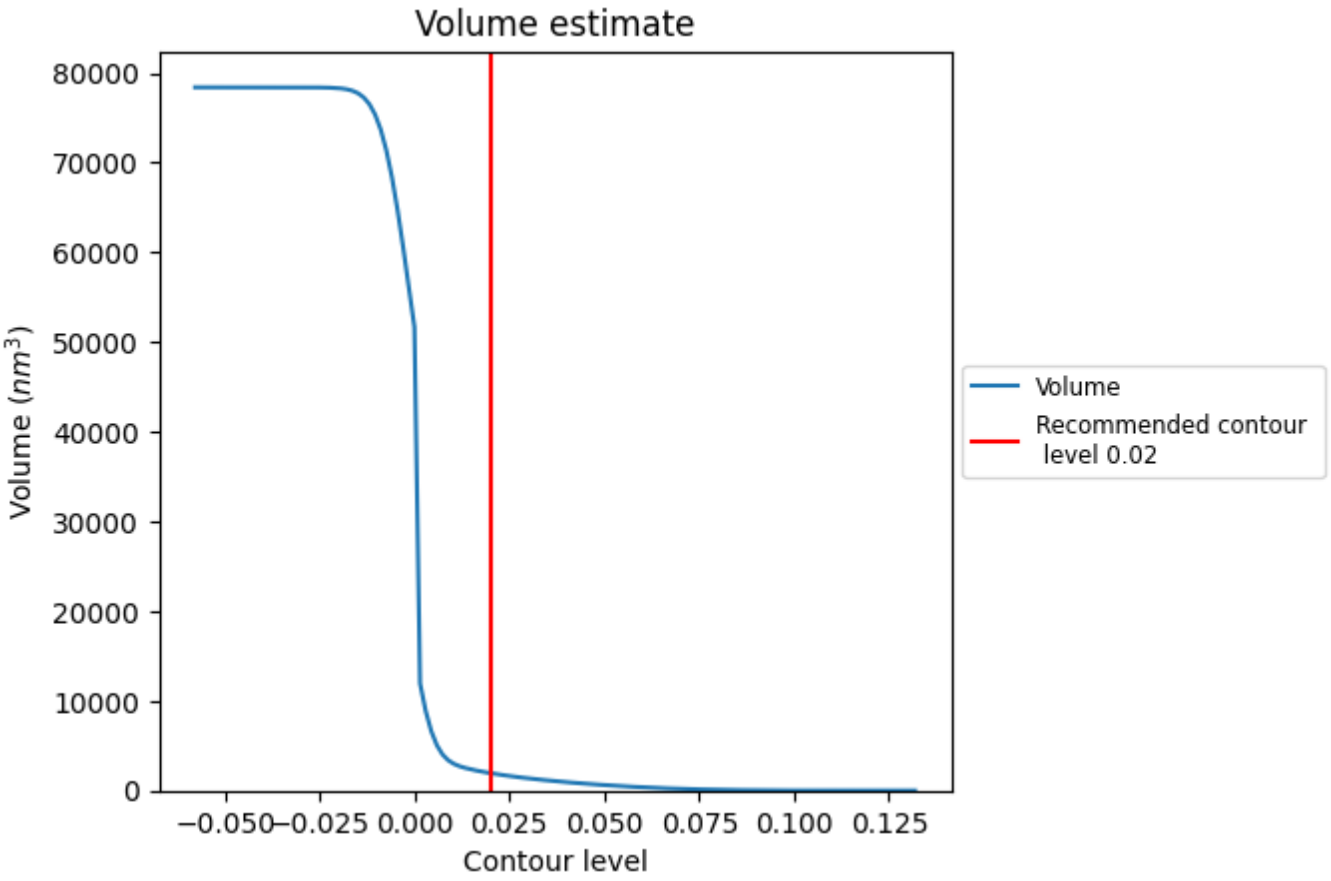
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

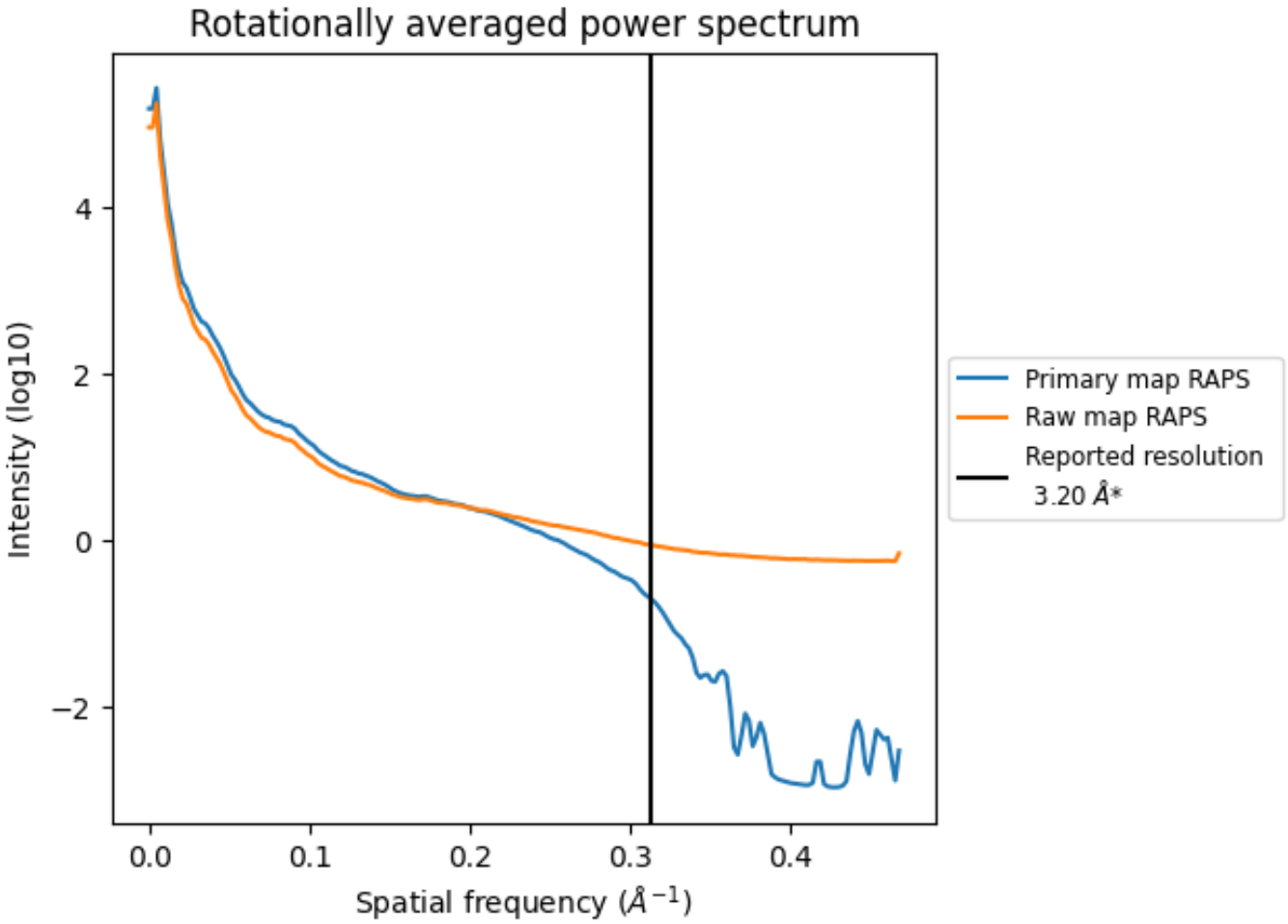
7.2 Volume estimate



The volume at the recommended contour level is 1943 nm^3; this corresponds to an approximate mass of 1755 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 (i)

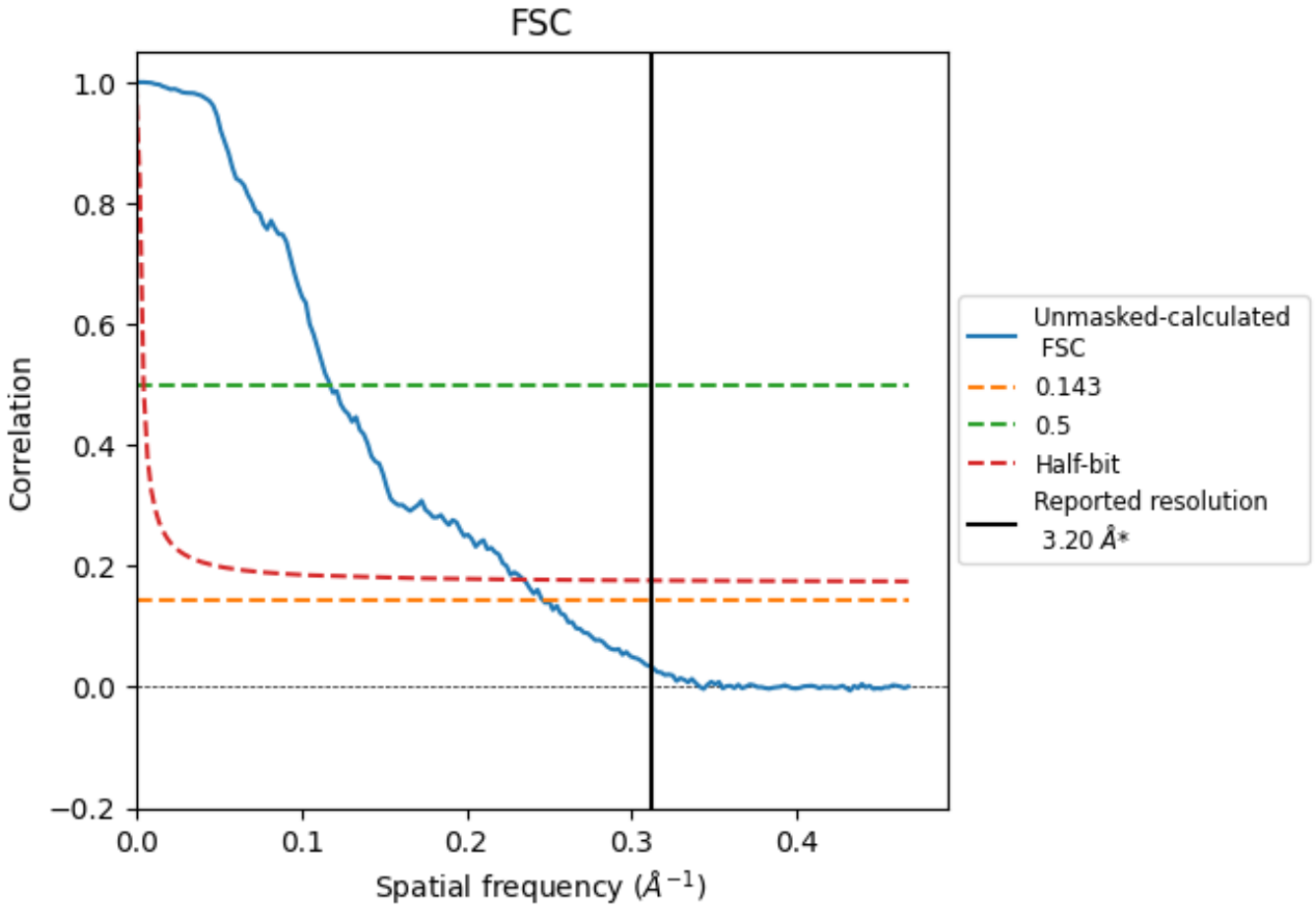


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

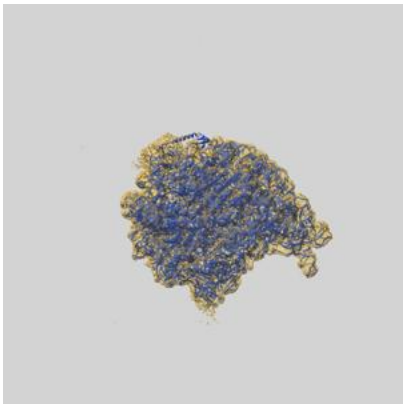
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	8.52	4.27

*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 4.06 differs from the reported value 3.2 by more than 10 %

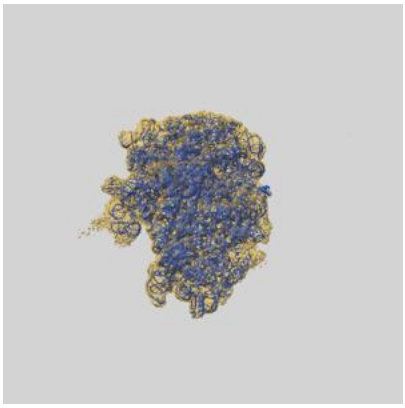
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12929 and PDB model 7OIG. Per-residue inclusion information can be found in section 3 on page 15.

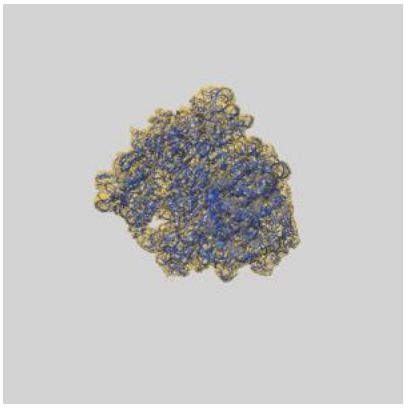
9.1 Map-model overlay



X



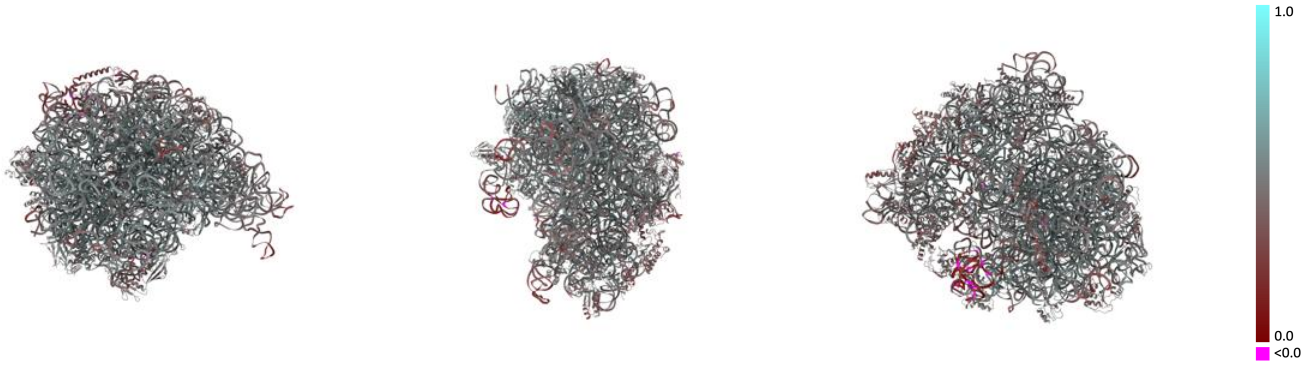
Y



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.

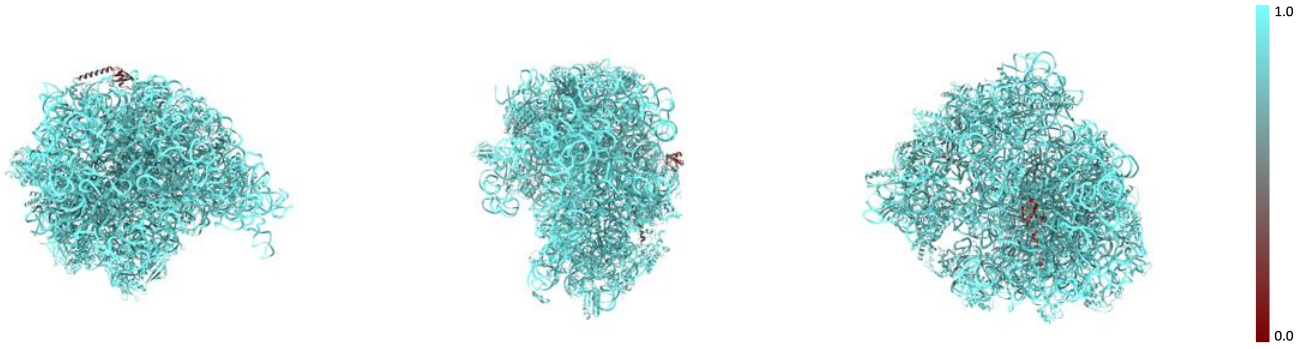
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

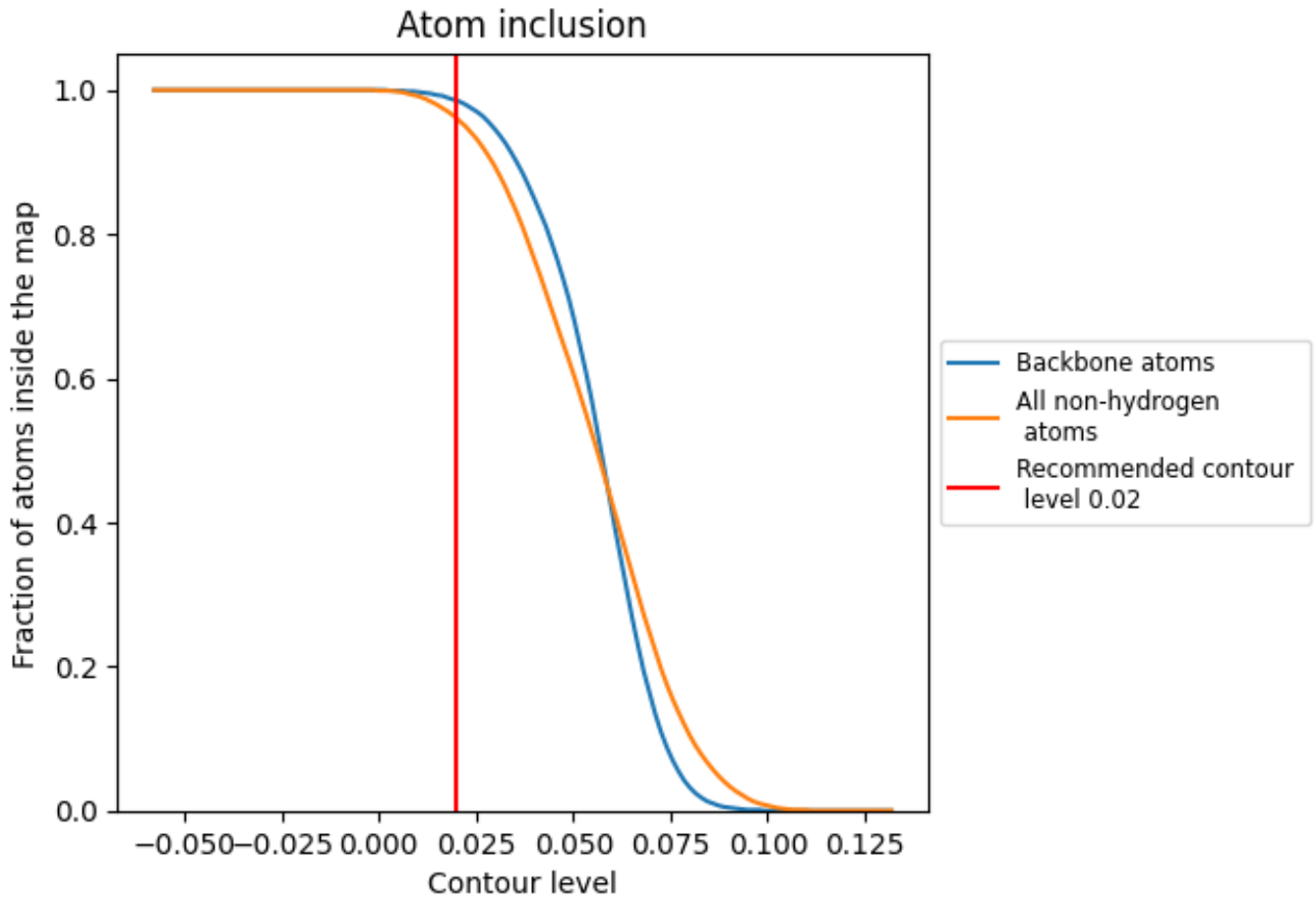
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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	0.9610	0.4740
1	0.9890	0.4850
2	0.9950	0.4790
3	0.9960	0.4770
4	0.9690	0.4430
B	0.7300	0.3290
C	0.9090	0.5200
D	0.9220	0.5130
E	0.9140	0.4730
F	0.8910	0.4110
G	0.9300	0.4410
H	0.4260	0.3480
I	0.9050	0.4920
J	0.8660	0.5010
K	0.9290	0.4960
L	0.9020	0.4920
M	0.9390	0.5020
N	0.9410	0.4550
O	0.8990	0.5020
P	0.9410	0.4950
Q	0.9160	0.5020
R	0.8910	0.4960
S	0.8960	0.4720
T	0.9100	0.4640
U	0.9120	0.4670
V	0.8960	0.5070
W	0.9250	0.4970
X	0.9000	0.4190
Y	0.9080	0.4820
Z	0.9040	0.3890
a	0.9000	0.4910
b	0.8570	0.4880
c	0.9100	0.5120
d	0.9350	0.5380
e	0.9280	0.4990



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.8690	0.3970
g	0.8910	0.4430
h	0.9030	0.4390
i	0.9210	0.4680
j	0.9180	0.4390
k	0.8790	0.4040
l	0.9060	0.4630
m	0.9300	0.4350
n	0.8670	0.4200
o	0.9160	0.4570
p	0.8680	0.4870
q	0.8980	0.4230
r	0.9410	0.4500
s	0.8970	0.4370
t	0.9430	0.4730
u	0.8730	0.4580
v	0.9120	0.4450
w	0.9330	0.4410
x	0.9200	0.4330
y	0.7530	0.3840
z	0.9630	0.3940