



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 06:17 AM UTC

PDB ID : 6FTG / pdb_00006ftg
EMDB ID : EMD-4315
Title : Subtomogram average of OST-containing ribosome-translocon complexes from canine rough microsomal membranes
Authors : Pfeffer, S.; Foerster, F.
Deposited on : 2018-02-22
Resolution : 9.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

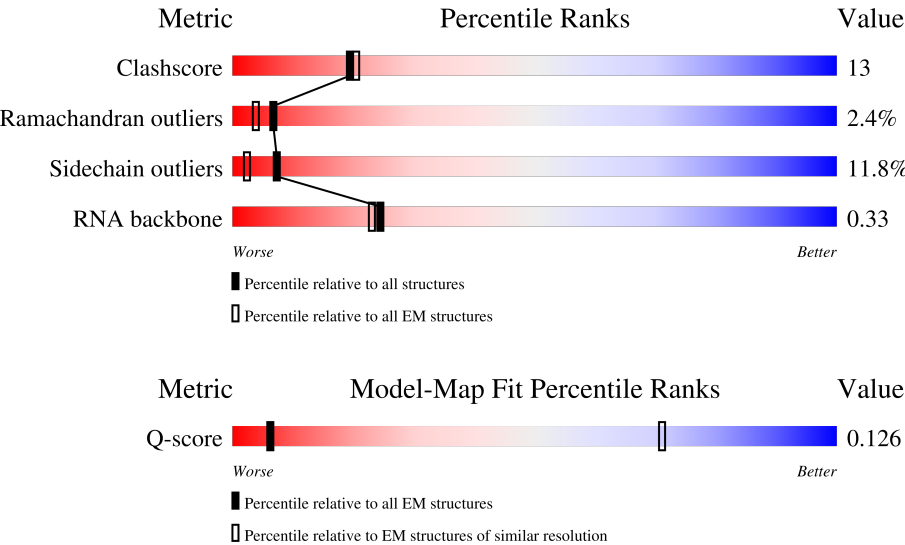
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 9.10 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	244 (8.60 - 9.60)

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

Mol	Chain	Length	Quality of chain
1	A	244	42% 75% 18% 6%
2	B	394	30% 72% 23%
3	C	362	38% 70% 28%

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Mol	Chain	Length	Quality of chain
4	D	292	
5	E	248	
6	F	225	
7	G	241	
8	H	190	
9	I	213	
10	J	169	
11	L	210	
12	M	138	
13	N	203	
14	O	199	
15	P	153	
16	Q	187	
17	R	180	
18	S	175	
19	T	159	
20	U	99	
21	V	131	
22	W	63	
23	X	119	
24	Y	134	
25	Z	135	
26	a	147	
27	b	75	
28	c	94	

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Mol	Chain	Length	Quality of chain
29	d	107	
30	e	128	
31	f	109	
32	g	114	
33	h	122	
34	i	102	
35	j	86	
36	k	69	
37	l	50	
38	m	52	
39	n	23	
40	o	104	
41	p	91	
42	r	136	
43	s	198	
44	t	163	
45	u	3662	
46	v	120	
47	w	156	
48	x	461	
49	y	62	
50	z	29	
51	1	162	
52	2	60	
53	3	120	

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Mol	Chain	Length	Quality of chain
54	4	34	
55	5	705	
56	6	97	
57	7	25	
58	8	80	
59	K	8	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	ZN	o	201	-	-	X	-
62	9UB	5	801	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 152114 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1868	1171	382	309	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3148	2007	591	537	13		

- Molecule 3 is a protein called Ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2884	1814	578	478	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	362	LYS	-	expression tag	UNP G1SVW5
C	363	SER	-	expression tag	UNP G1SVW5

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	292	Total	C	N	O	S	0	0
			2386	1509	437	426	14		

- Molecule 5 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	236	Total	C	N	O	S	0	0
			1898	1215	362	318	3		

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	175	ALA	THR	conflict	UNP G1SV32
F	185	GLY	ASN	conflict	UNP G1SV32
F	202	ARG	HIS	conflict	UNP G1SV32
F	233	GLU	GLY	conflict	UNP G1SV32

- Molecule 7 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	241	Total	C	N	O	S	0	0
			1934	1233	371	326	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 9 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1655	1051	319	272	13		

- Molecule 10 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	210	Total	C	N	O	S	0	0
			1703	1065	354	280	4		

- Molecule 12 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	199	Total	C	N	O	S	0	0
			1638	1056	321	256	5		

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	54	GLN	LYS	conflict	UNP G1TVT6

- Molecule 16 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	187	Total	C	N	O	S	0	0
			1506	941	311	249	5		

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	175	Total	C	N	O	S	0	0
			1454	925	284	235	10		

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 21 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 22 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 24 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 25 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 26 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 27 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	75	Total	C	N	O	S	0	0
			609	378	130	98	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 30 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 31 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 32 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 33 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 34 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 35 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 36 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 38 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 39 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 40 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 41 is a protein called Ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	136	Total	C	N	O	S	0	0
			1094	676	229	183	6		

- Molecule 43 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	198	Total	C	N	O	S	0	0
			1523	969	265	280	9		

- Molecule 44 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	163	Total	C	N	O	S	0	0
			1238	773	230	230	5		

- Molecule 45 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	u	3662	Total	C	N	O	P	0	0
			78486	34947	14363	25515	3661		

- Molecule 46 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 47 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 48 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	426	Total	C	N	O	S	0	0
			3313	2181	535	576	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	145	SER	ALA	conflict	UNP P38377

- Molecule 49 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	y	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 50 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	29	Total	C	N	O	S	0	0
			229	157	36	34	2		

- Molecule 51 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1,RPN1.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	1	162	Total	C	N	O	0	0
			885	553	165	167		

- Molecule 52 is a protein called TMEM258.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	2	60	Total	C	N	O	0	0
			300	180	60	60		

- Molecule 53 is a protein called Oligosaccharyltransferase complex subunit OSTC.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	120	Total	C	N	O	S	0	0
			802	529	130	136	7		

- Molecule 54 is a protein called OST4.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	34	Total	C	N	O	S	0	0
			268	180	41	45	2		

- Molecule 55 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	5	644	Total	C	N	O	S	0	0
			5090	3331	819	904	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	88	LEU	ILE	conflict	UNP F1PJP5

- Molecule 56 is a protein called DAD1.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	6	97	Total	C	N	O	0	0
			485	291	97	97		

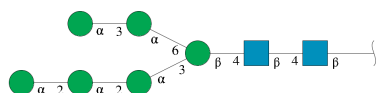
- Molecule 57 is a protein called OST48.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	7	25	Total	C	N	O	0	0
			125	75	25	25		

- Molecule 58 is a protein called RPN2.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	8	80	Total	C	N	O	0	0
			400	240	80	80		

- Molecule 59 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
59	K	8	Total	C	N	O	0	0
			94	52	2	40		

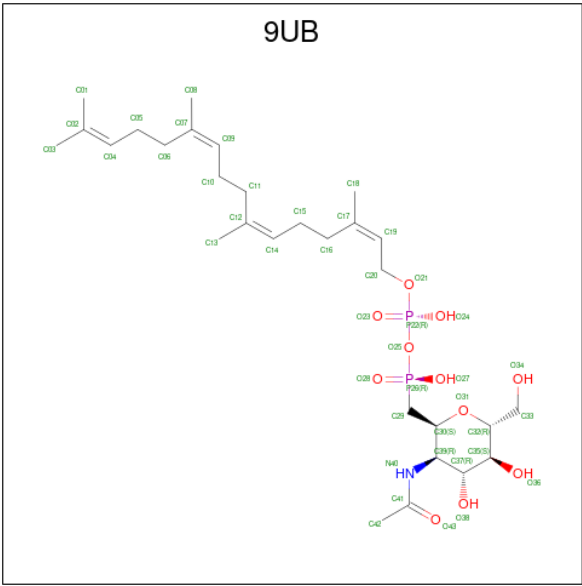
- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	B	1	Total	Mg	0
			1	1	
60	C	1	Total	Mg	0
			1	1	
60	I	1	Total	Mg	0
			1	1	
60	P	1	Total	Mg	0
			1	1	
60	V	1	Total	Mg	0
			1	1	
60	g	1	Total	Mg	0
			1	1	
60	u	146	Total	Mg	0
			146	146	
60	v	5	Total	Mg	0
			5	5	
60	w	2	Total	Mg	0
			2	2	

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	g	1	Total	Zn	0
			1	1	
61	j	1	Total	Zn	0
			1	1	
61	m	1	Total	Zn	0
			1	1	
61	o	1	Total	Zn	0
			1	1	
61	p	1	Total	Zn	0
			1	1	

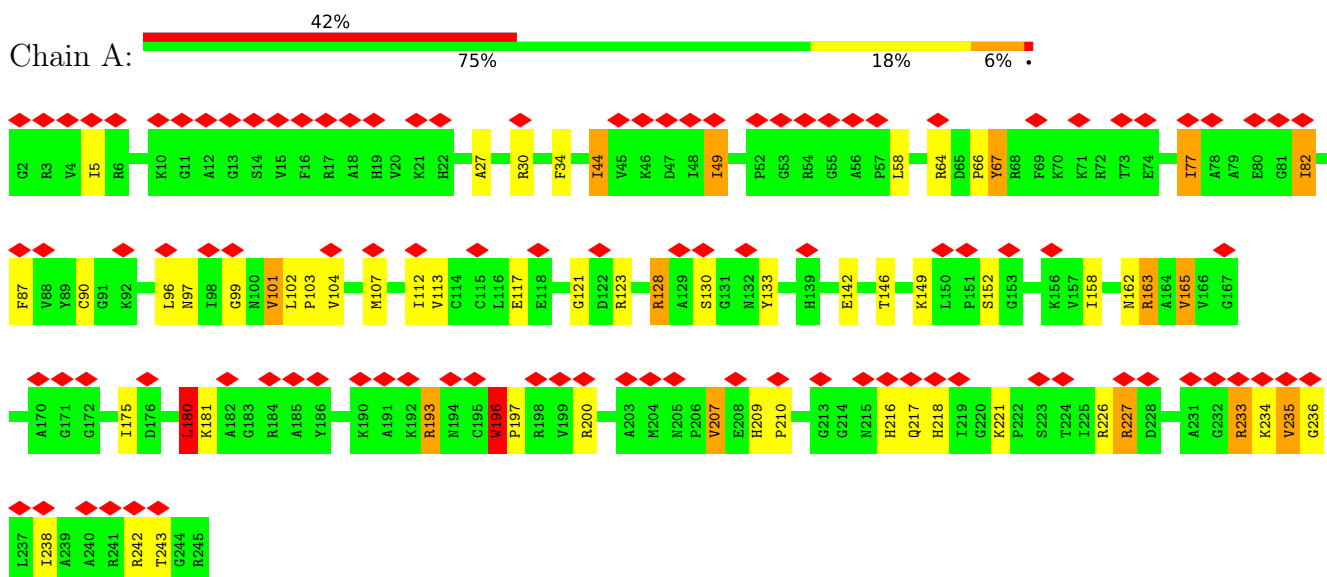
- Molecule 62 is [(2 {S},3 {R},4 {R},5 {S},6 {R})-3-acetamido-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl]methyl-[oxidanyl-[(2 {Z},6 {Z},10 {Z})-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenoxy]phosphoryl]oxy-phosphinic acid (CCD ID: 9UB) (formula: C₂₉H₅₁NO₁₁P₂).



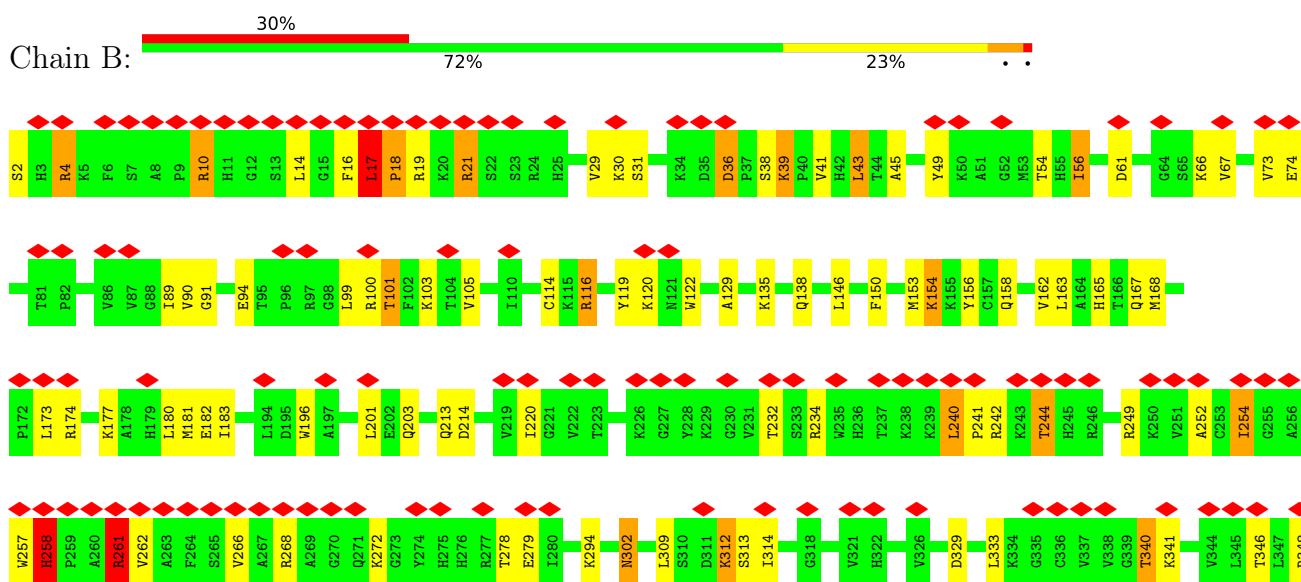
3 Residue-property plots

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

• Molecule 1: uL2

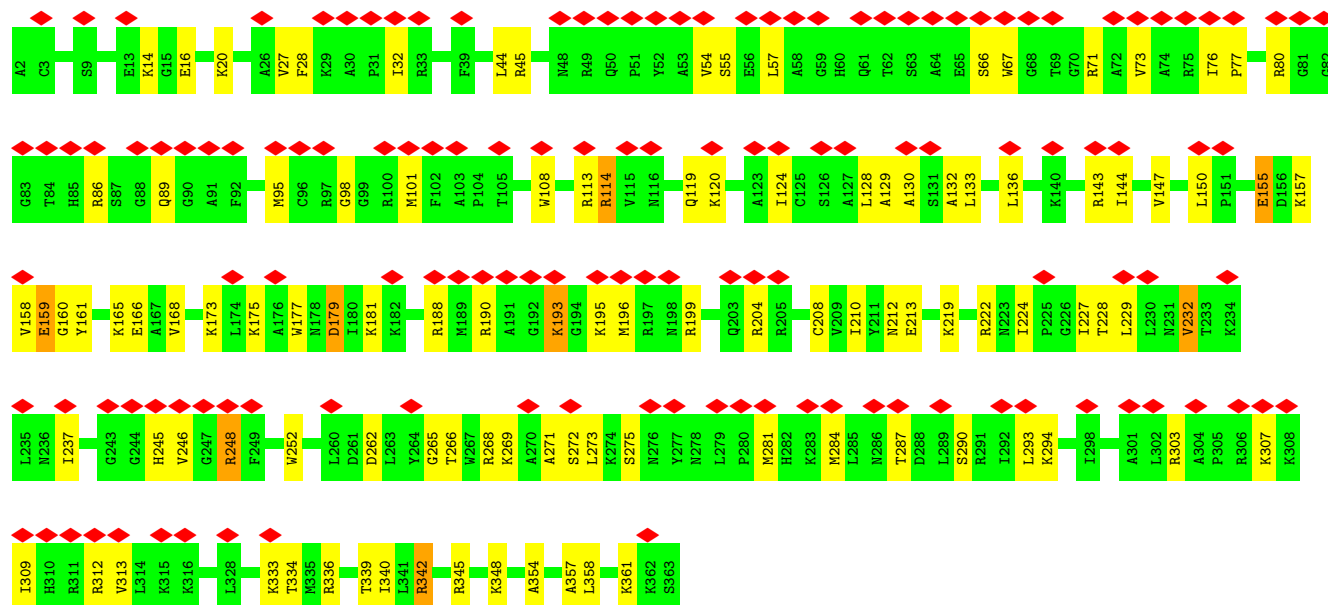
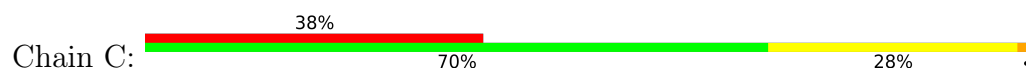


• Molecule 2: uL3

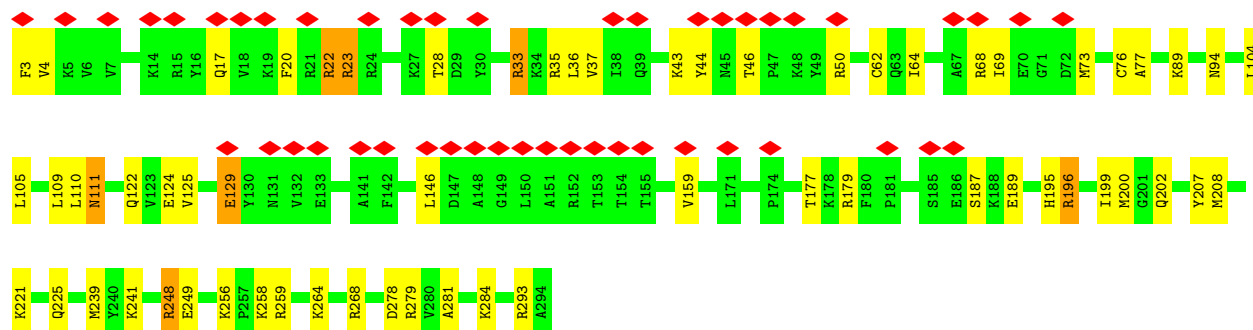
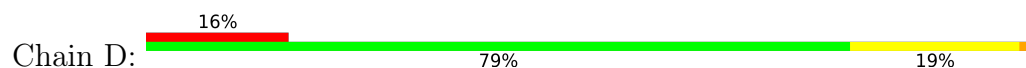




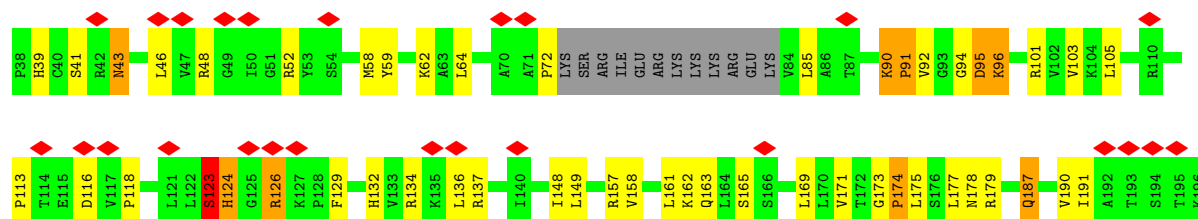
• Molecule 3: Ribosomal protein L4



• Molecule 4: 60S ribosomal protein L5

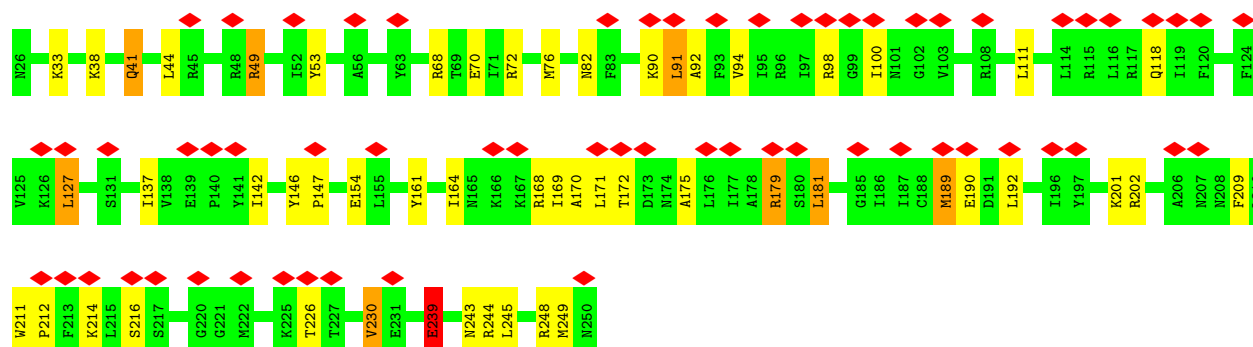
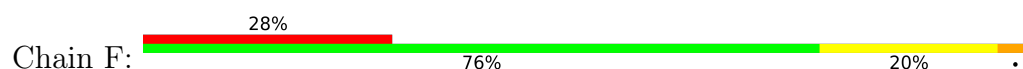


• Molecule 5: 60S ribosomal protein L6

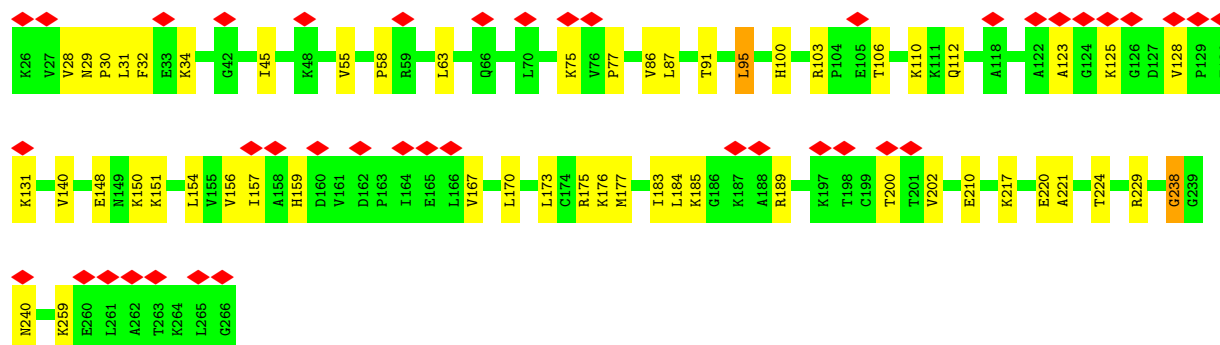
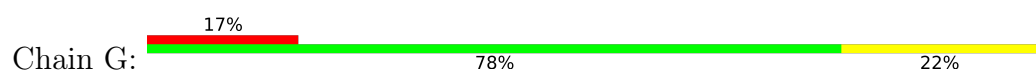




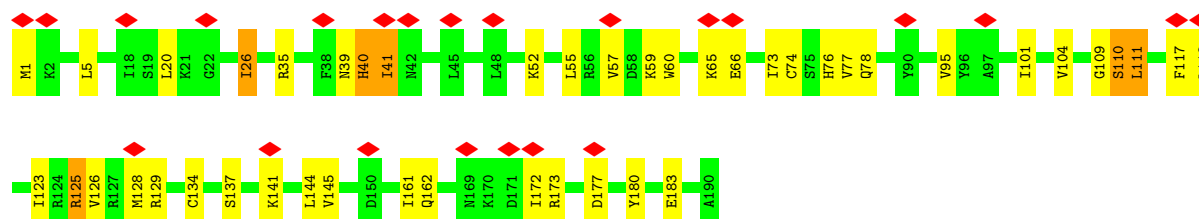
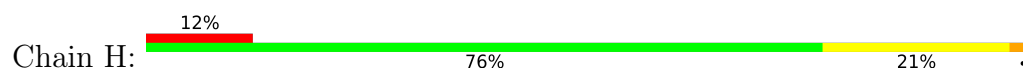
• Molecule 6: uL30



• Molecule 7: eL8

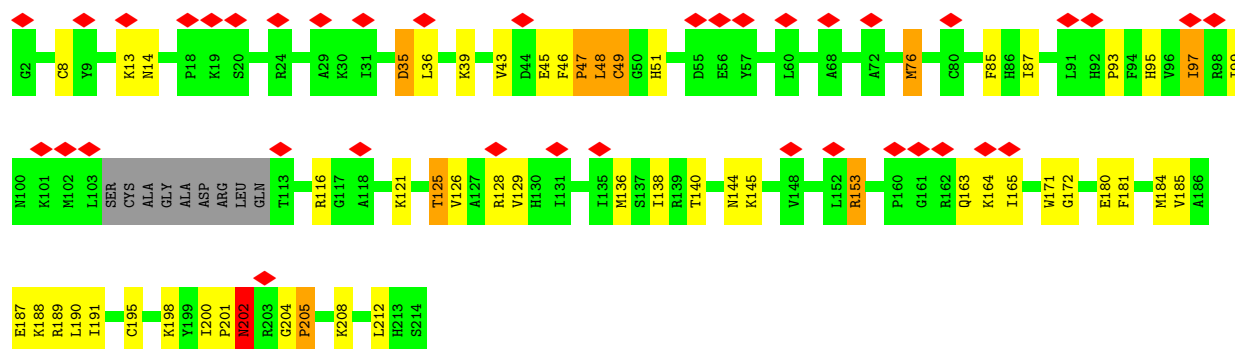


• Molecule 8: uL6

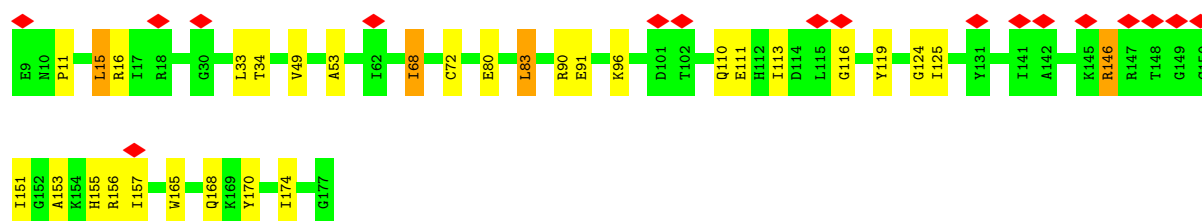
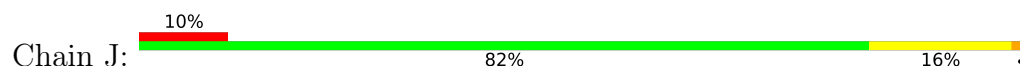


• Molecule 9: Ribosomal protein L10 (Predicted)

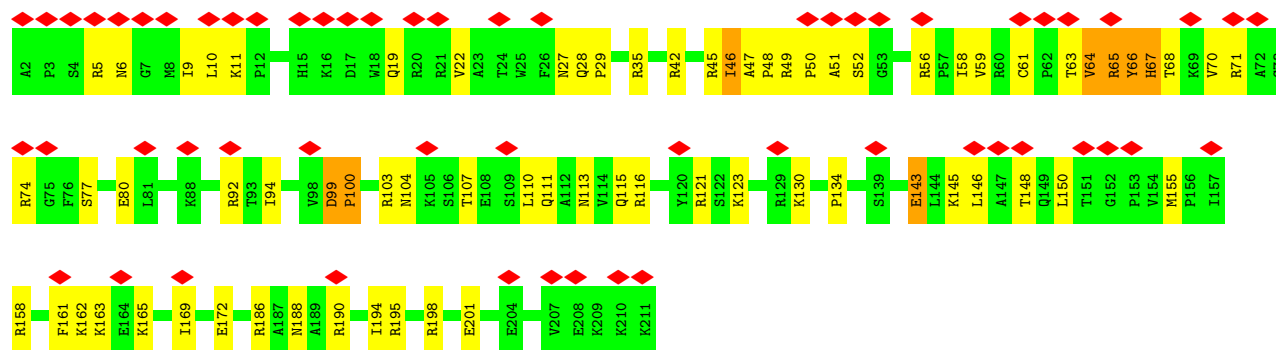




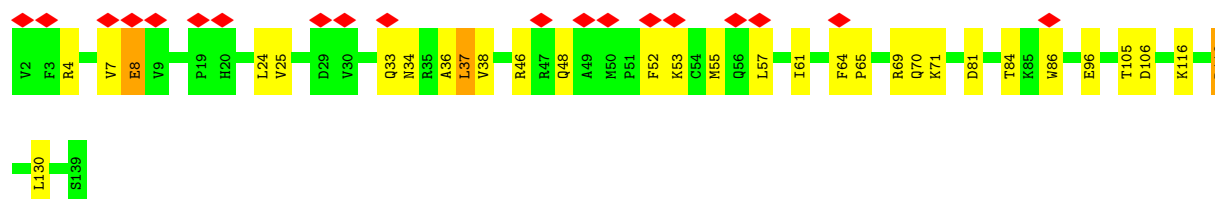
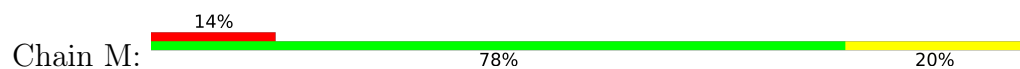
• Molecule 10: Ribosomal protein L11



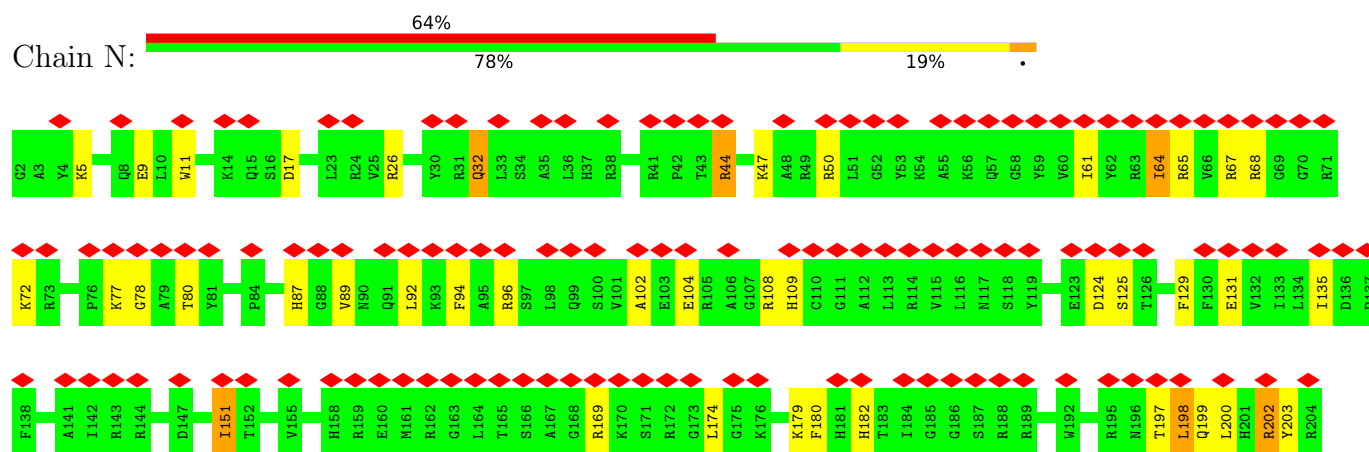
• Molecule 11: eL13



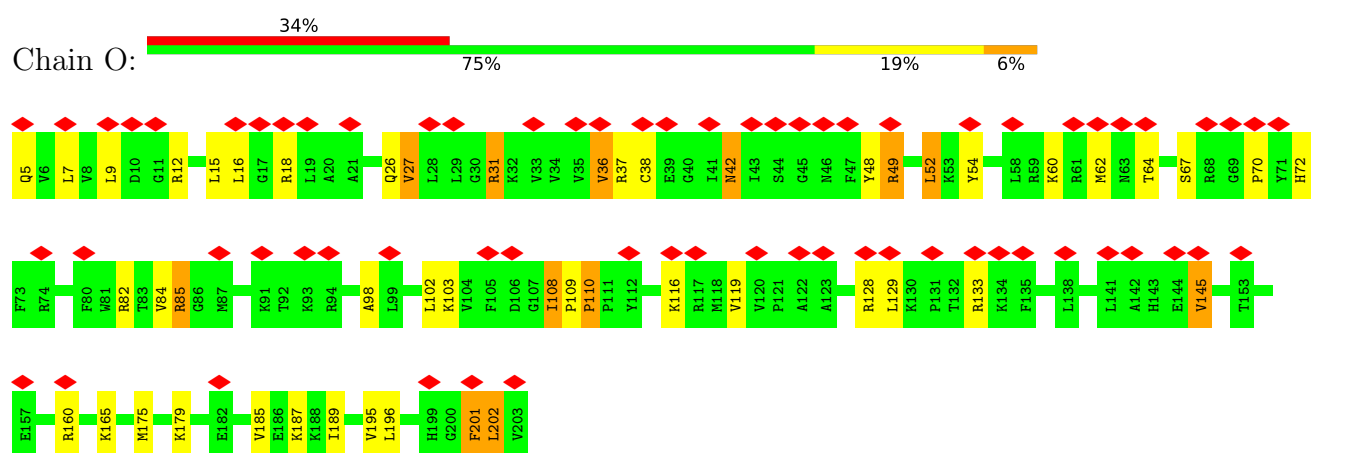
• Molecule 12: Ribosomal protein L14



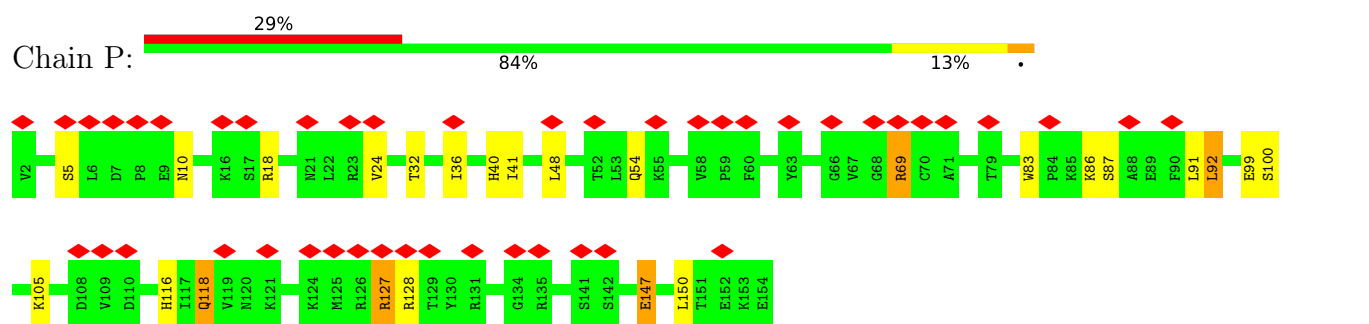
• Molecule 13: Ribosomal protein L15



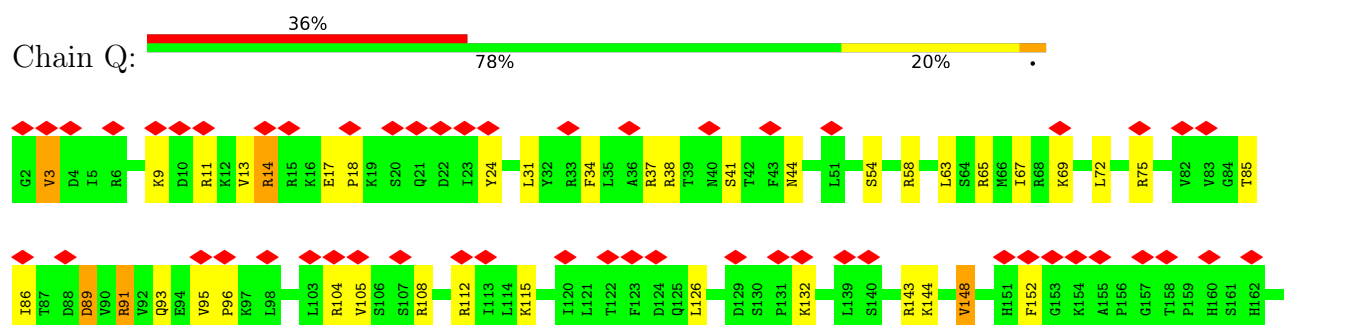
• Molecule 14: uL13

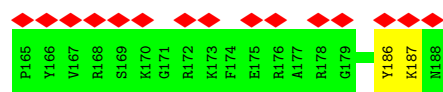


• Molecule 15: uL22

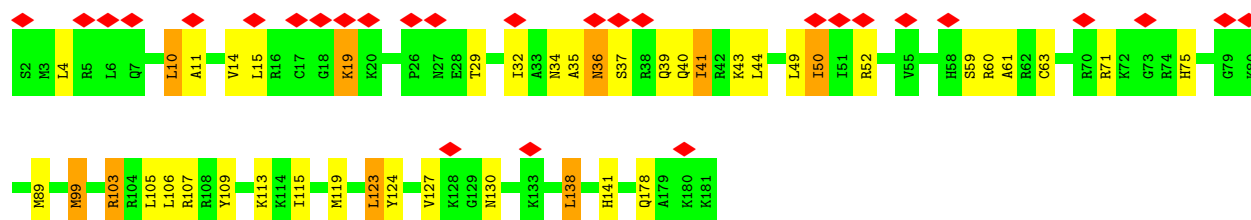
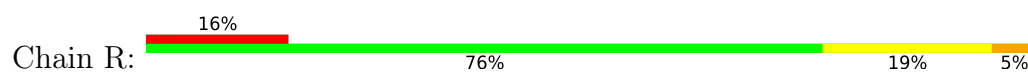


• Molecule 16: uL14

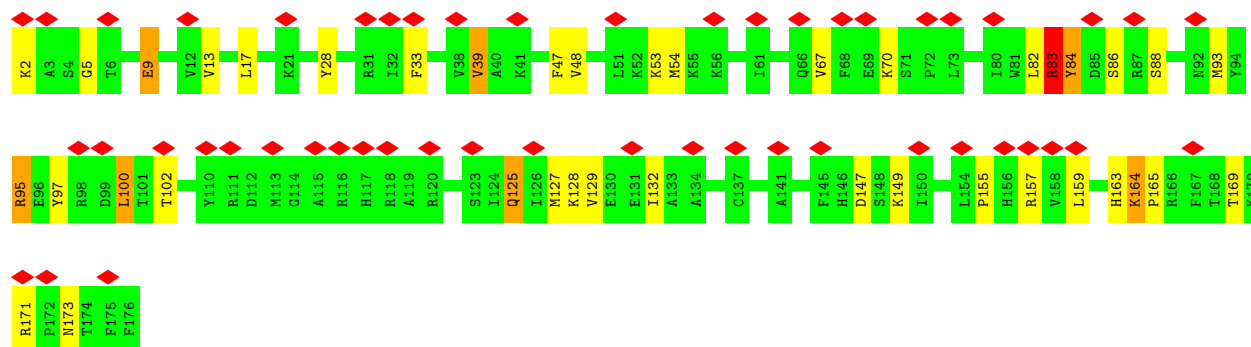
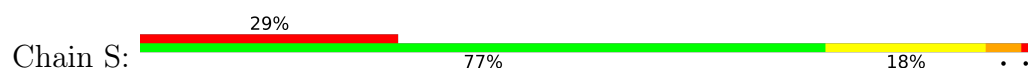




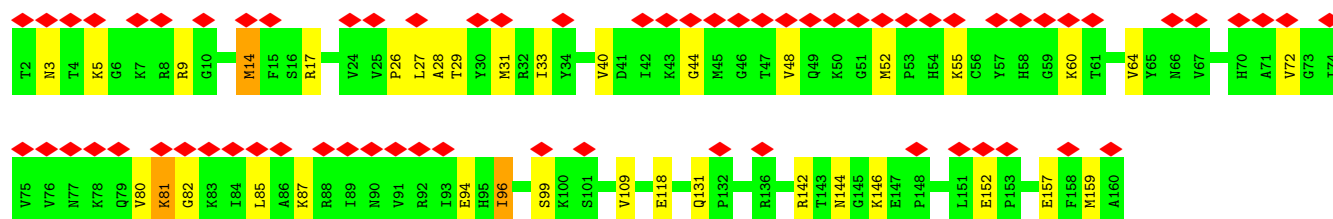
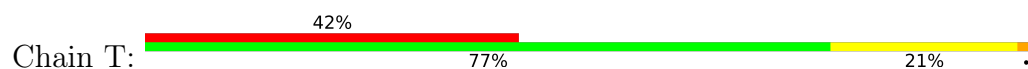
• Molecule 17: eL19



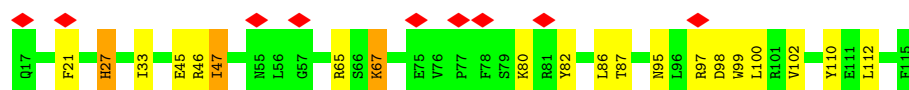
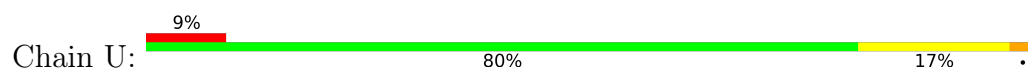
• Molecule 18: eL20



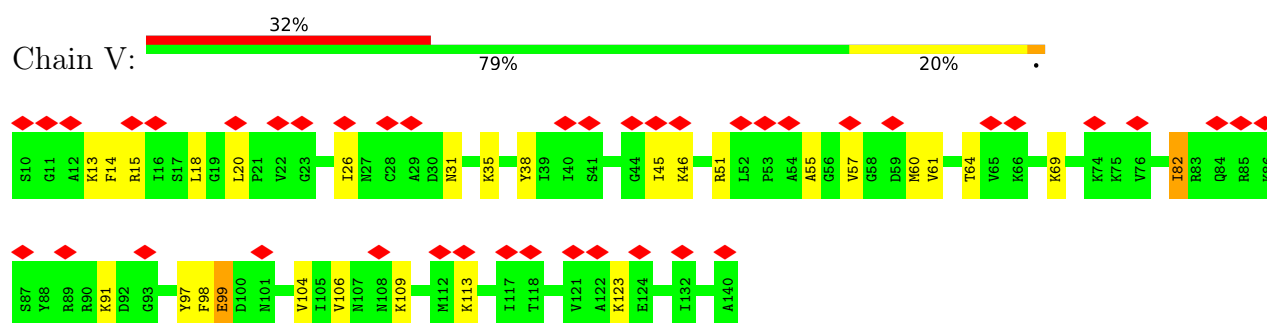
• Molecule 19: eL21



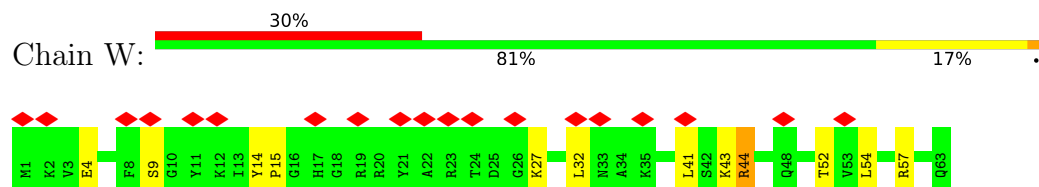
• Molecule 20: eL22



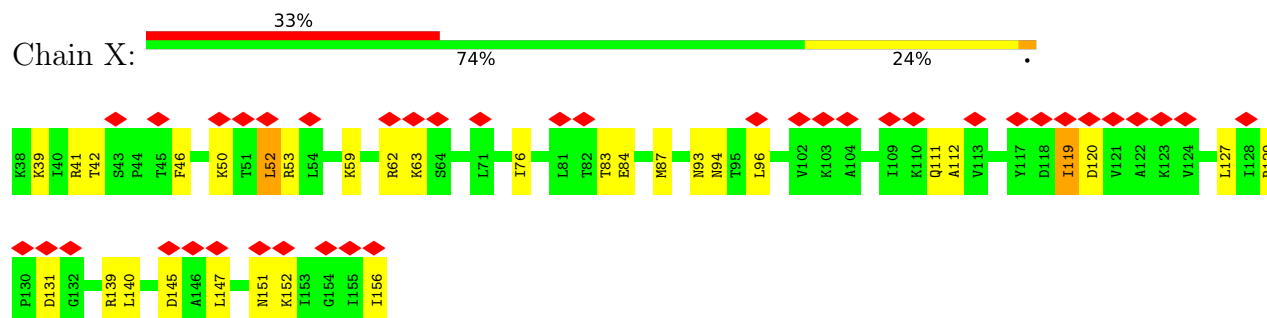
• Molecule 21: uL14



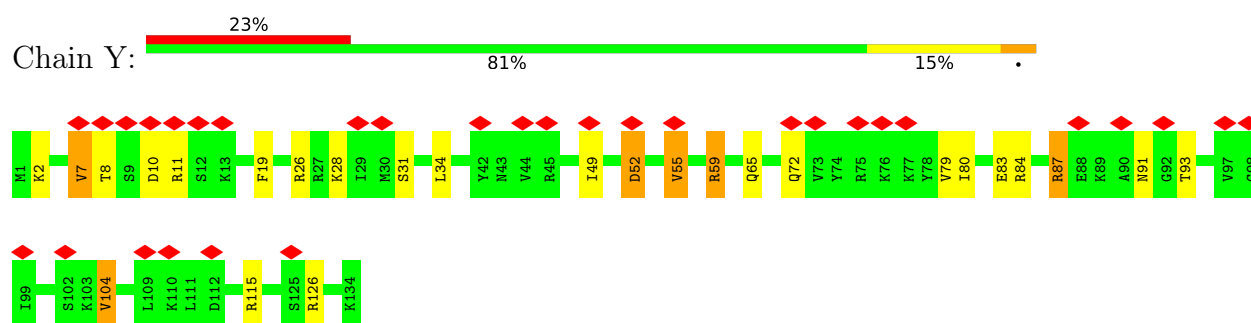
• Molecule 22: Ribosomal protein L24



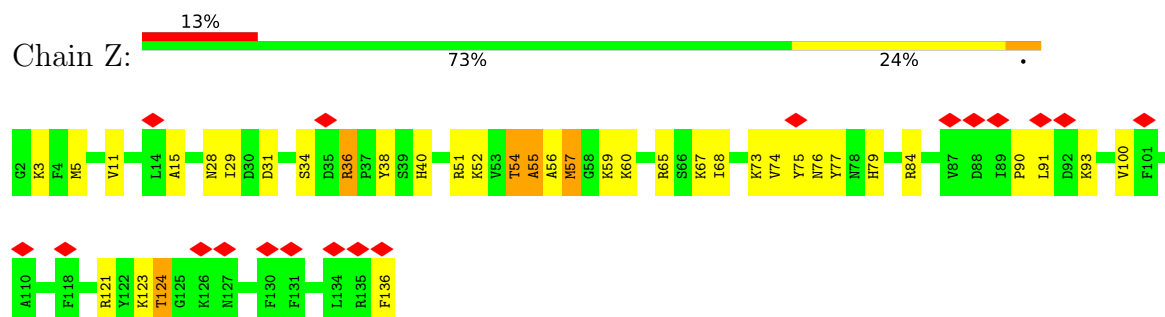
• Molecule 23: uL23



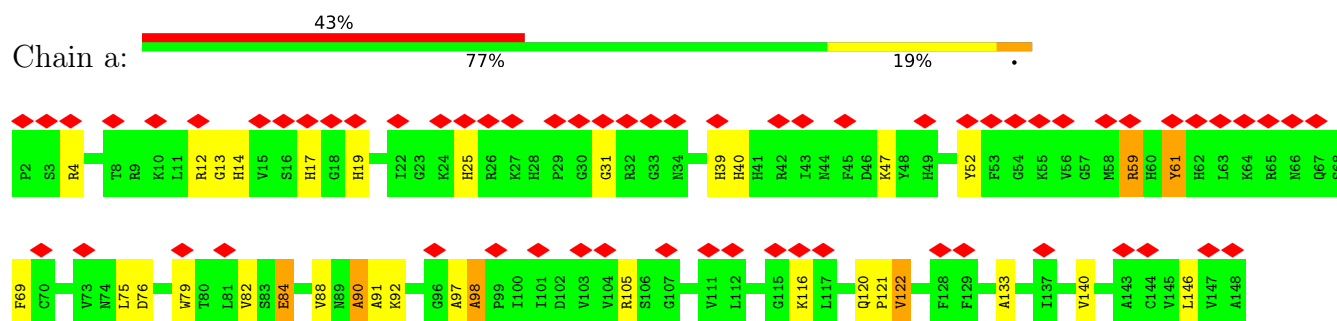
• Molecule 24: Ribosomal protein L26



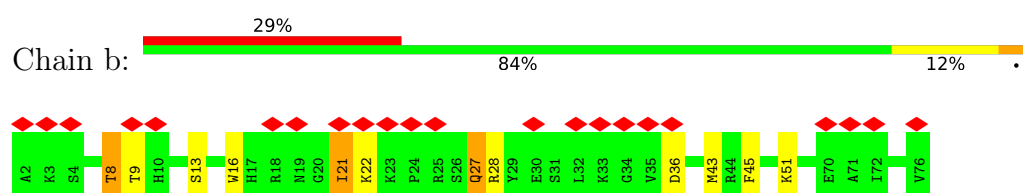
• Molecule 25: 60S ribosomal protein L27



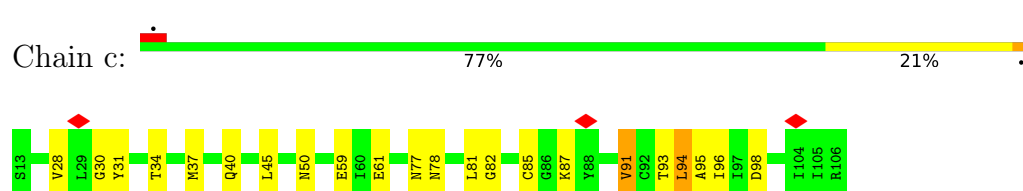
- Molecule 26: uL15



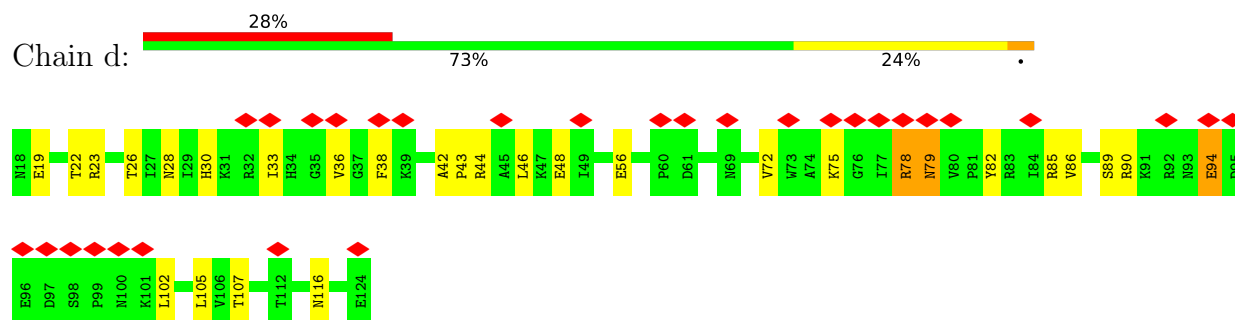
- Molecule 27: 60S ribosomal protein L29



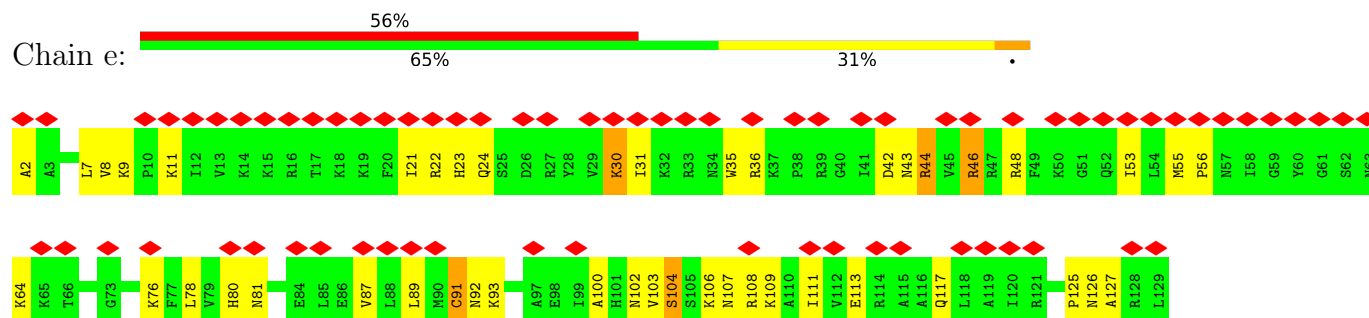
- Molecule 28: eL30



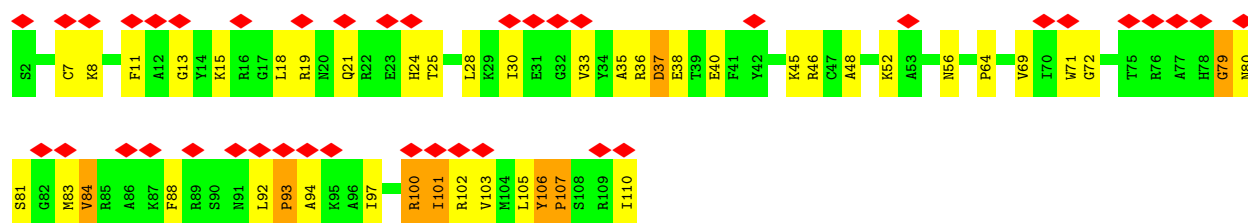
- Molecule 29: eL31



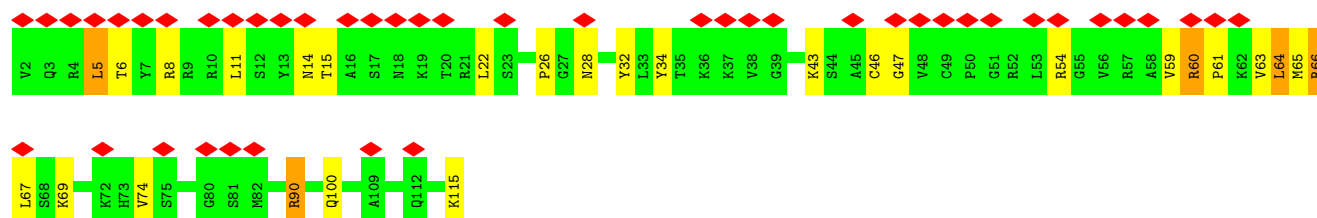
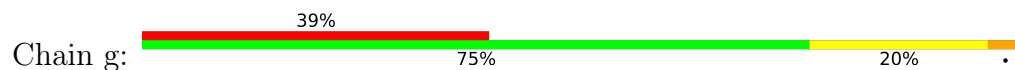
- Molecule 30: eL32



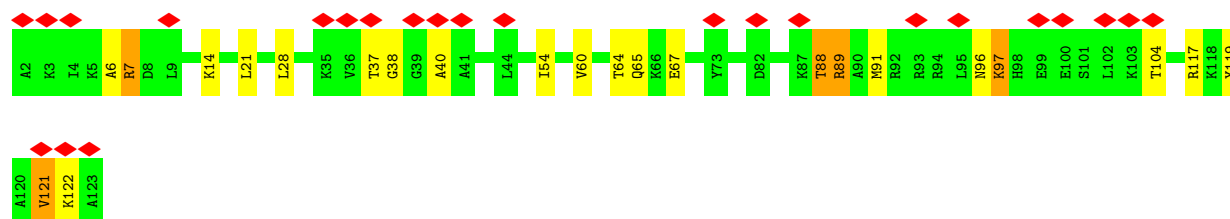
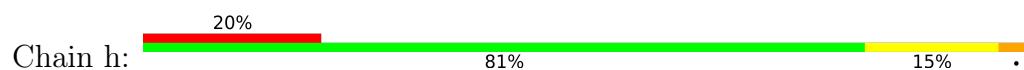
- Molecule 31: eL33



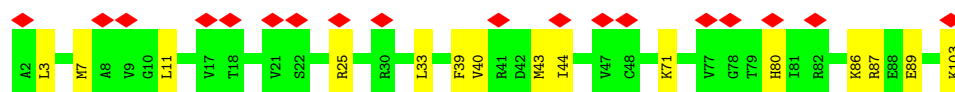
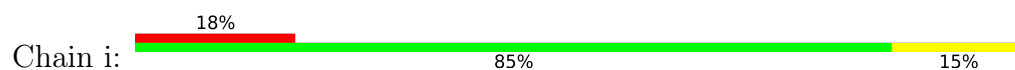
• Molecule 32: eL34



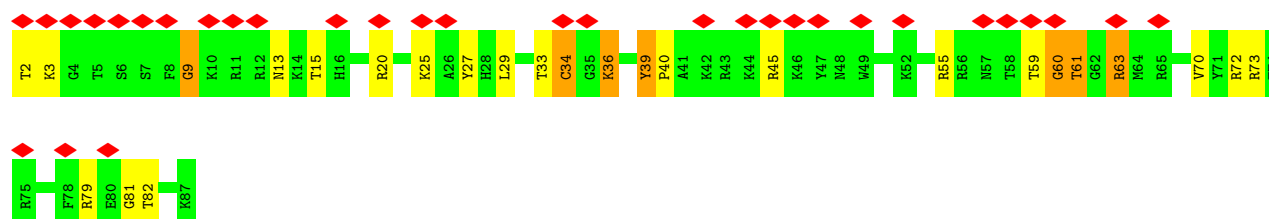
• Molecule 33: eL29



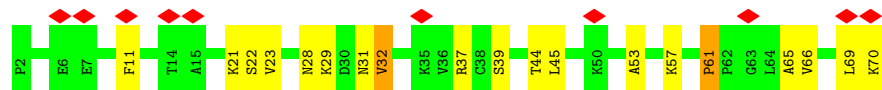
• Molecule 34: 60S ribosomal protein L36



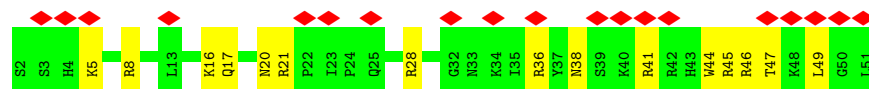
• Molecule 35: Ribosomal protein L37



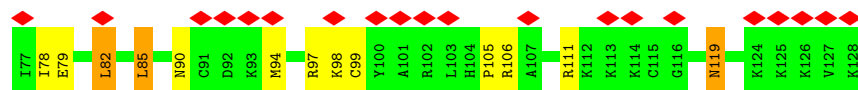
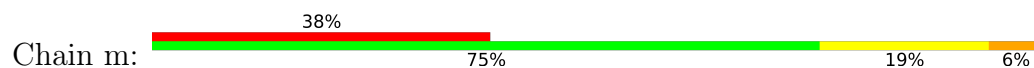
- Molecule 36: eL38



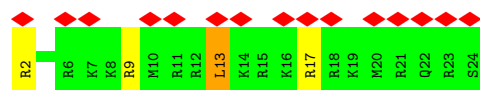
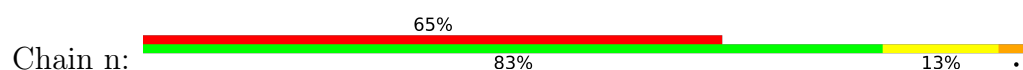
- Molecule 37: eL39



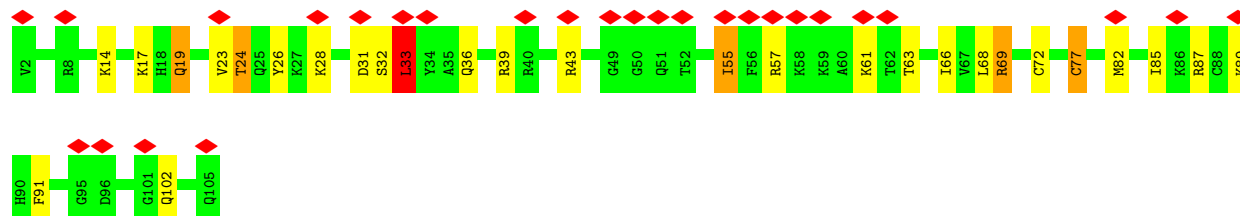
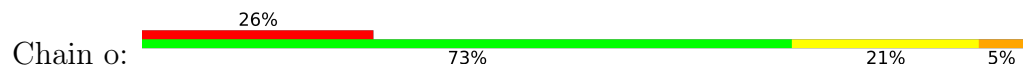
- Molecule 38: eL40



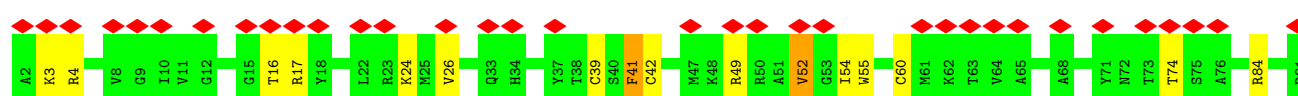
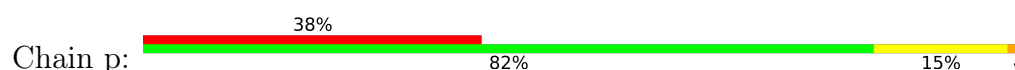
- Molecule 39: 60s ribosomal protein l41



- Molecule 40: eL42

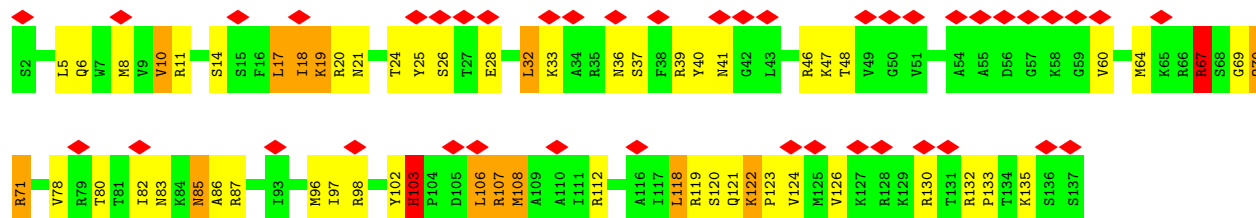


- Molecule 41: Ribosomal protein L37a

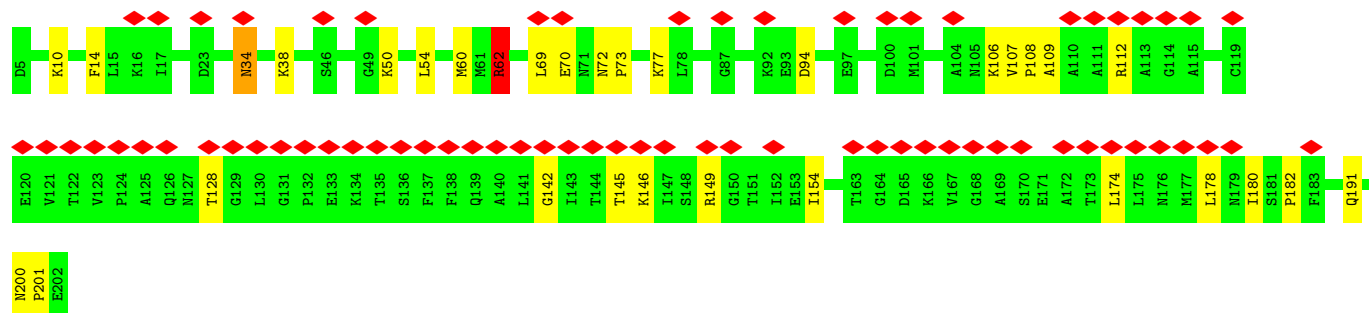
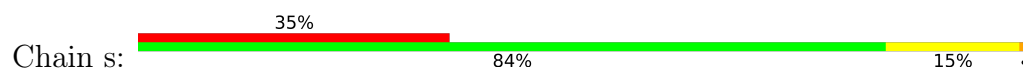




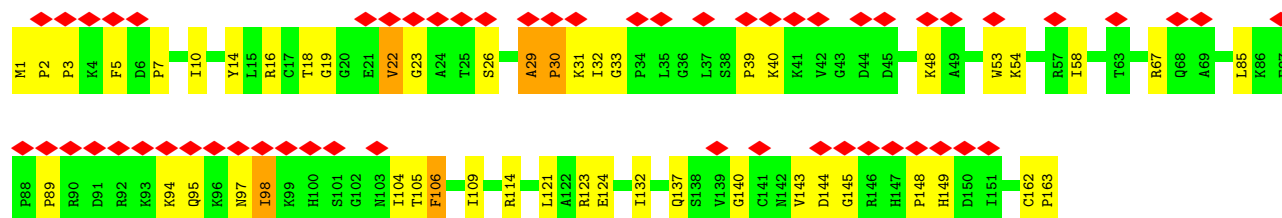
• Molecule 42: eL28



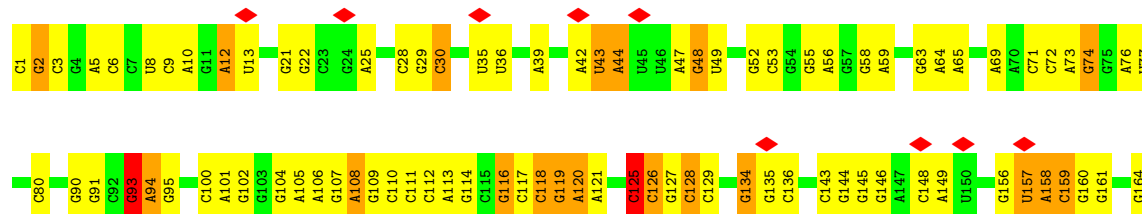
• Molecule 43: 60S acidic ribosomal protein P0

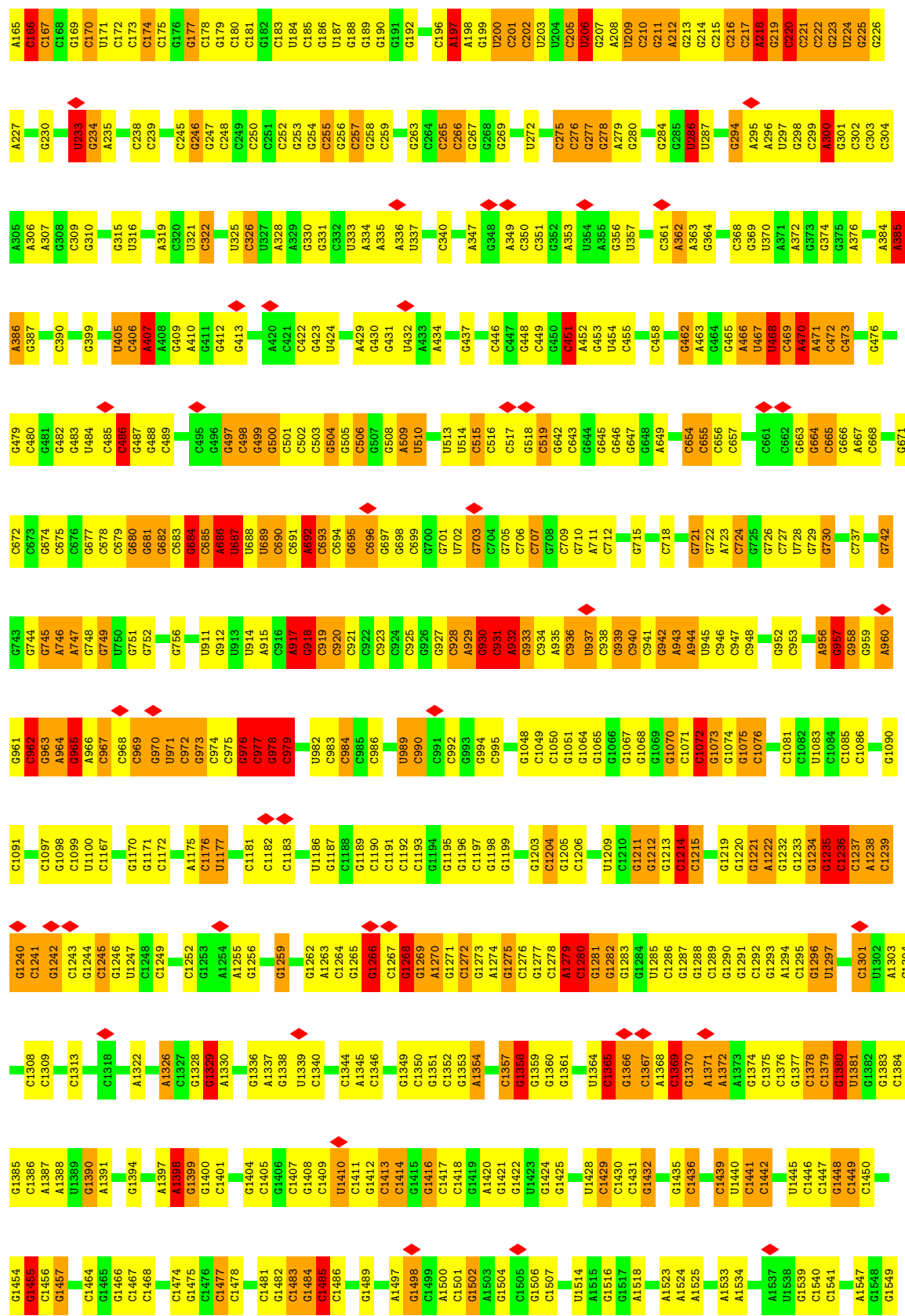


• Molecule 44: Ribosomal protein L12



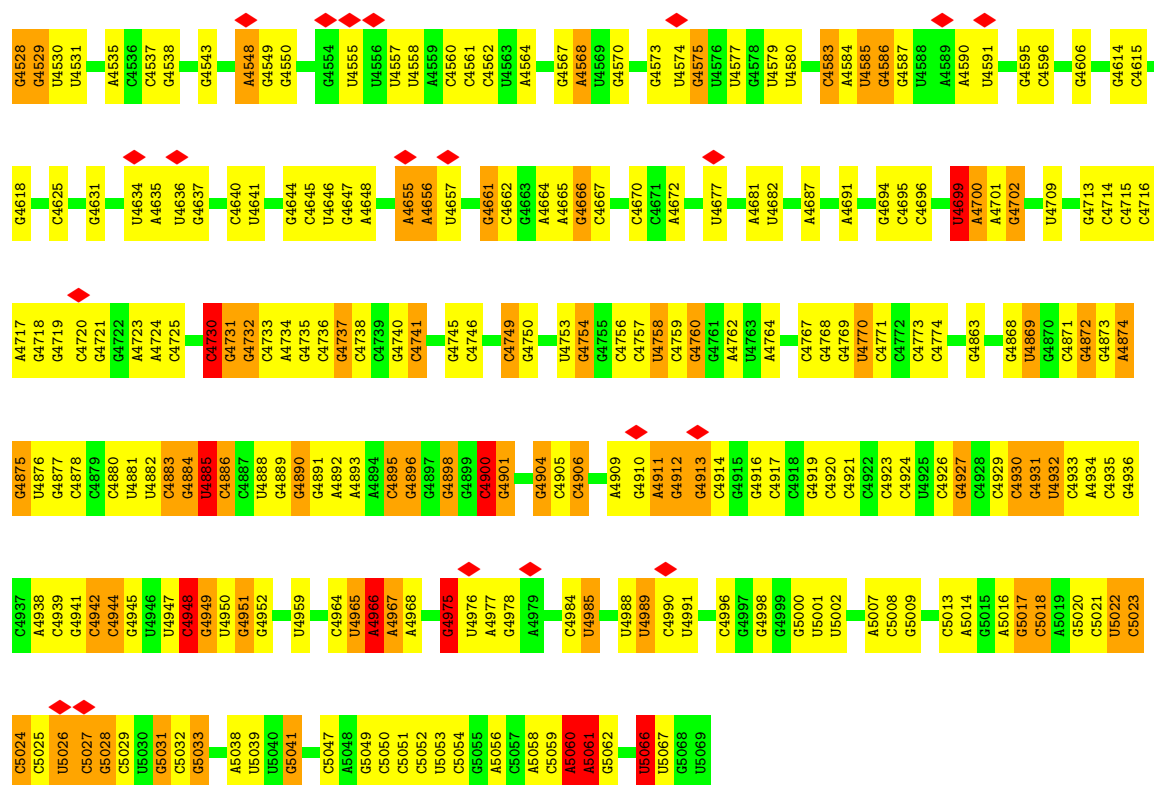
• Molecule 45: 28S ribosomal RNA



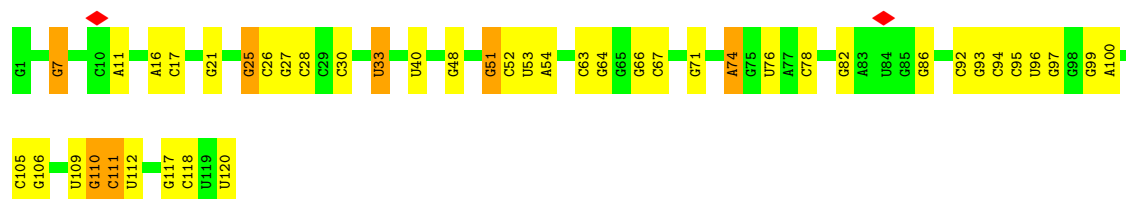




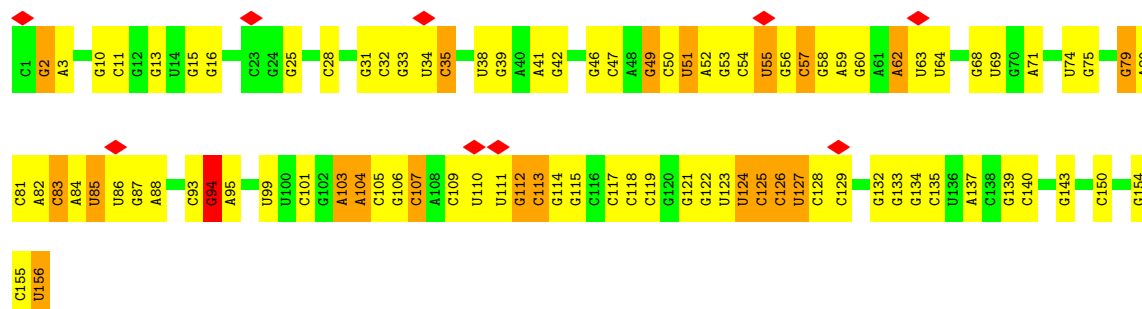
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A4376	A4377	A4378	A4380	A4387	A4388	A4389	A4390	A4391	A4394	A4395	A4396	A4397	A4398	A4399	G4400	G4405	G4408	G4409	G4410	G4411	G4412	G4416	G4417	G4418	G4419	G4420	G4421	G4422	G4423	G4424	G4425	G4426	G4430	G4431	G4432	G4433	G4434	G4435	G4436	G4437	G4438	G4439	G4440	G4441	G4444	G4445	G4446	G4447	G4448	G4449	G4450																
G4451	G4452	G4453	G4454	G4457	G4458	G4459	G4460	G4461	G4462	G4463	G4464	G4471	G4472	G4473	G4474	G4475	G4476	G4481	G4482	G4483	G4484	G4485	G4486	G4487	G4488	G4489	G4490	G4491	G4492	G4495	G4500	G4506	G4507	G4508	G4509	G4510	G4511	G4512	G4513	G4514	G4515	G4516	G4517	G4518	G4519	G4520	G4521	G4522	G4523	G4524	G4525	G4526	G4527														



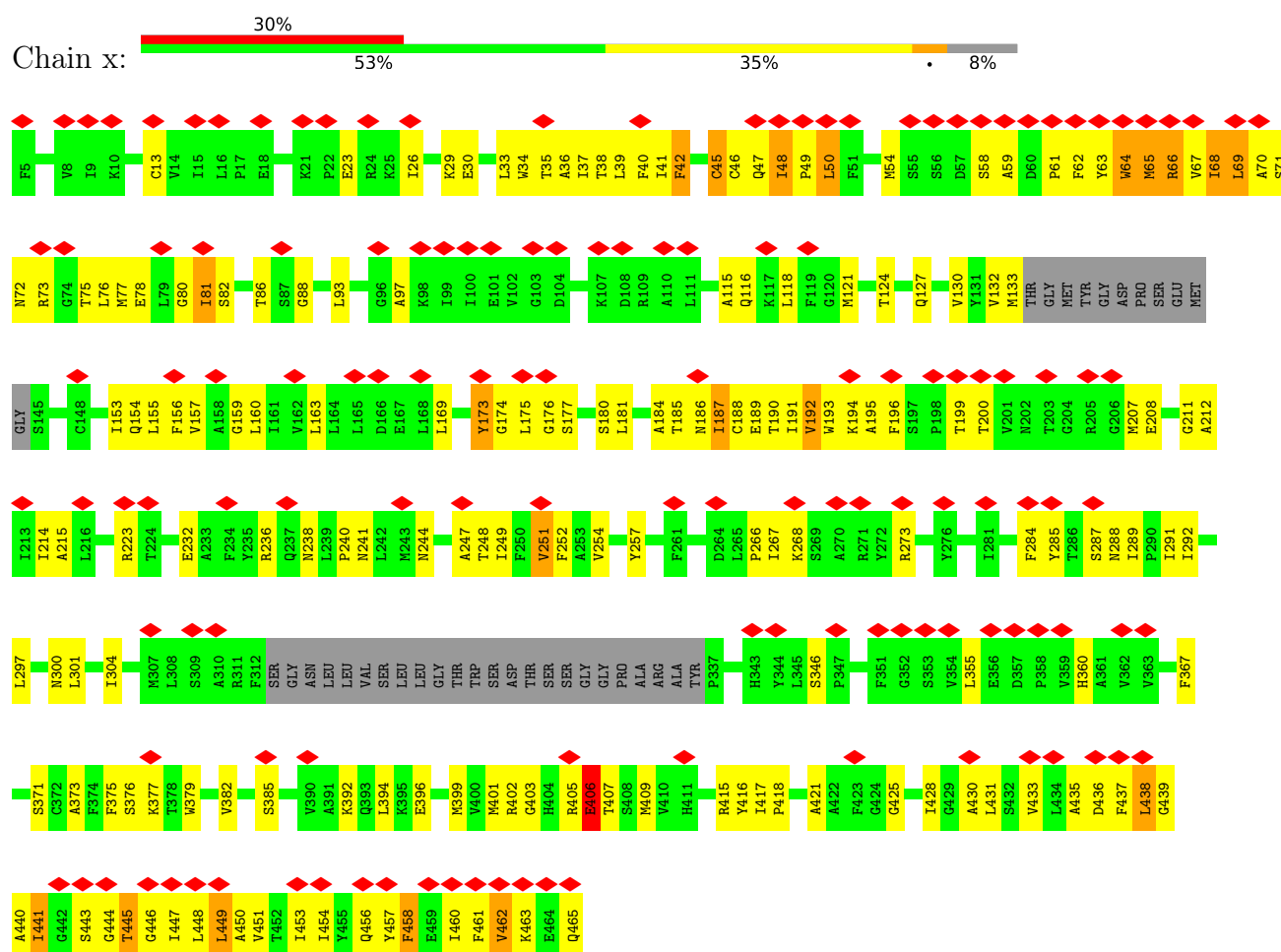
• Molecule 46: 5S ribosomal RNA



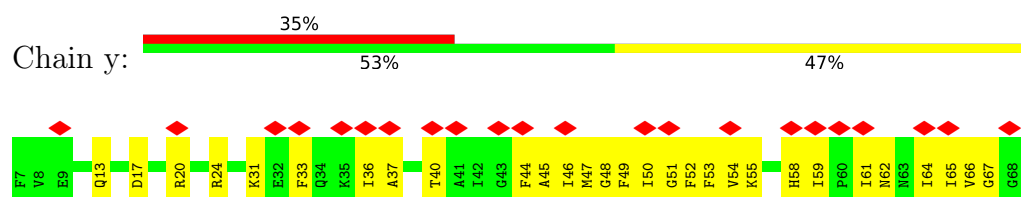
• Molecule 47: 5.8S ribosomal RNA



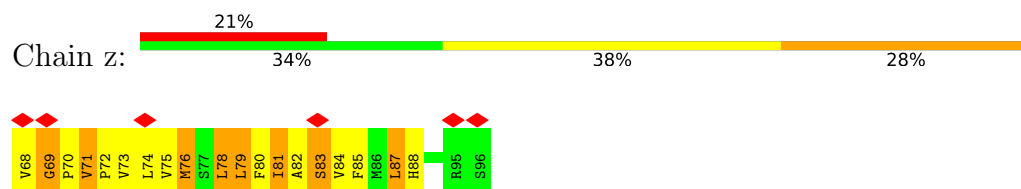
• Molecule 48: Protein transport protein Sec61 subunit alpha isoform 1



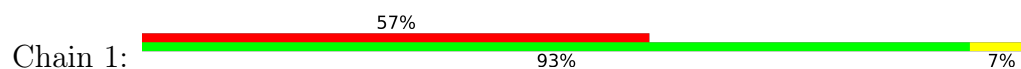
• Molecule 49: Protein transport protein Sec61 subunit gamma

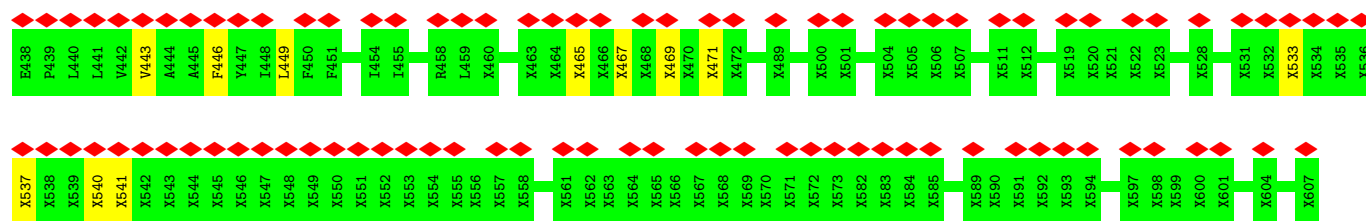


• Molecule 50: Protein transport protein Sec61 subunit beta

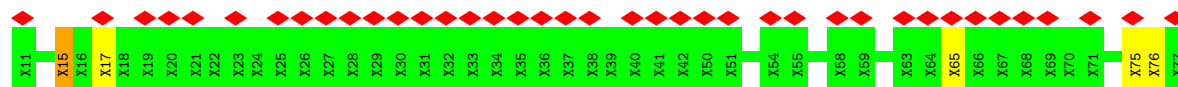


• Molecule 51: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1, RPN1

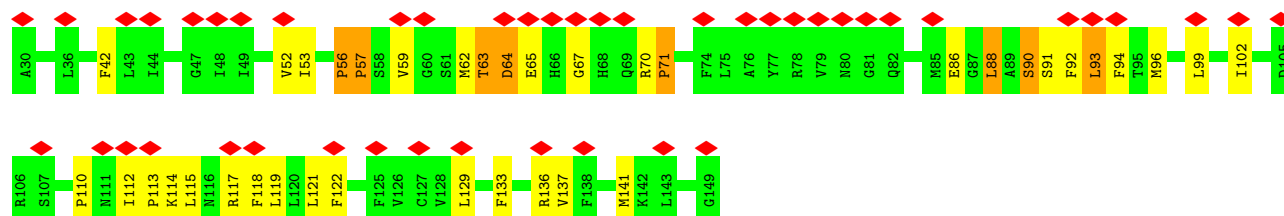
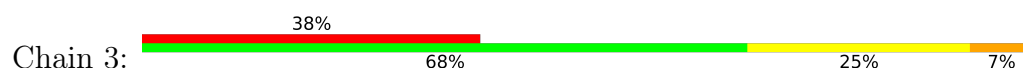




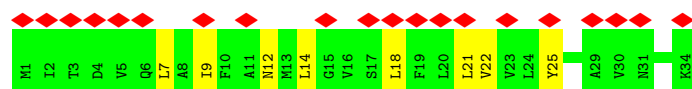
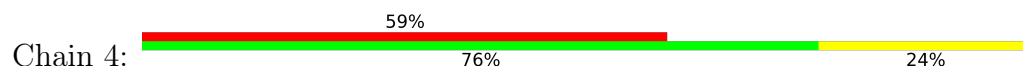
• Molecule 52: TMEM258



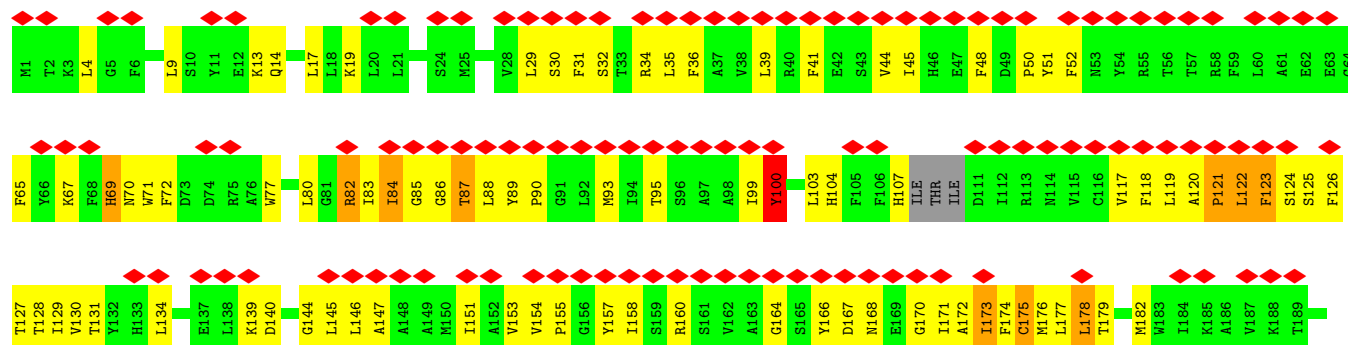
• Molecule 53: Oligosaccharyltransferase complex subunit OSTC

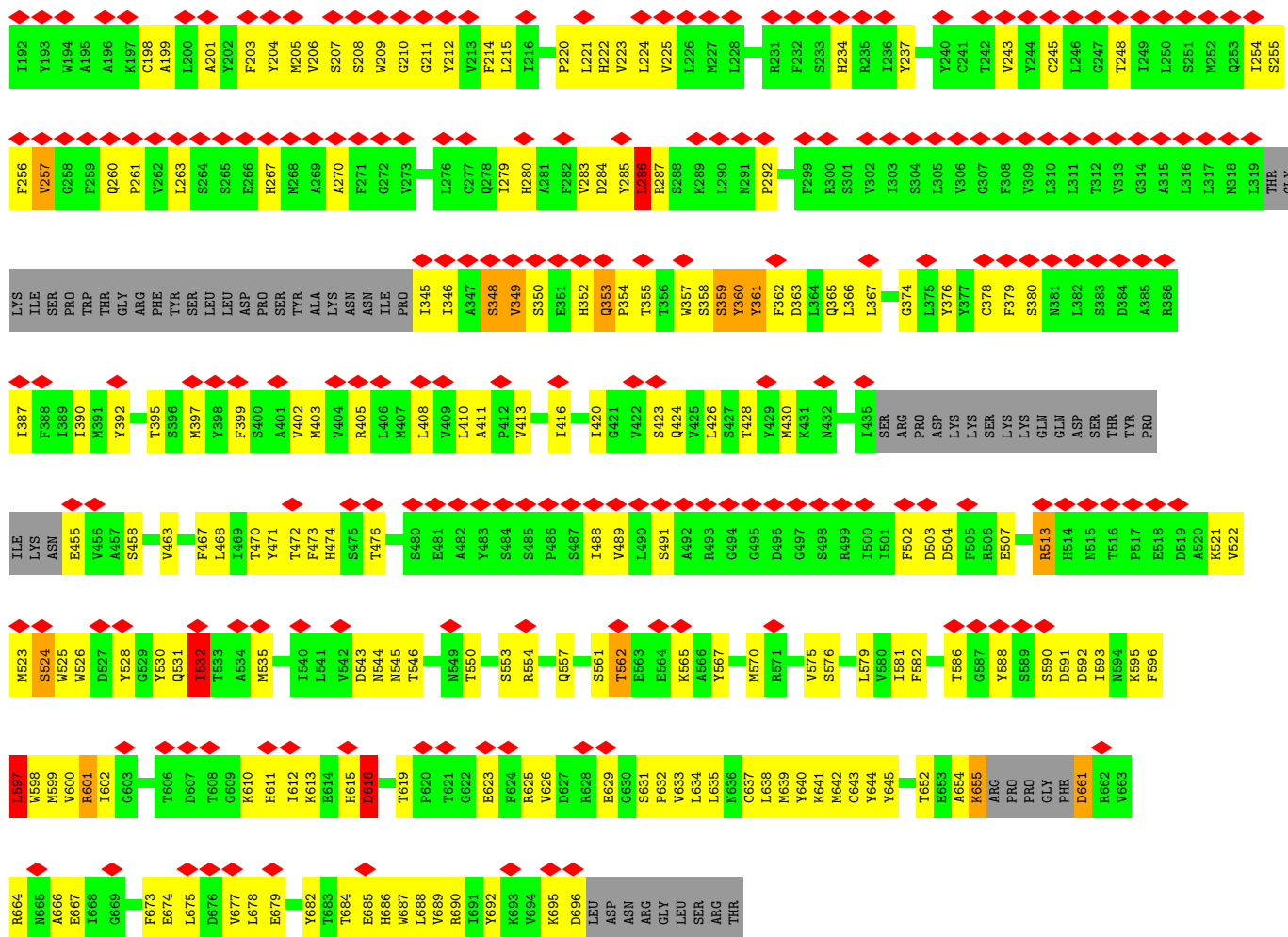


• Molecule 54: OST4

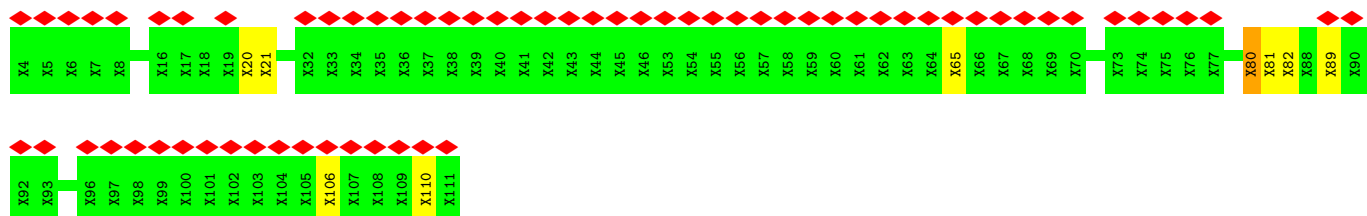
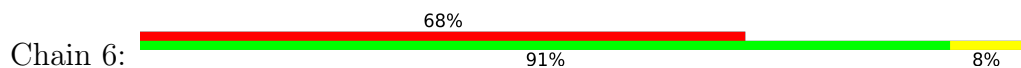


• Molecule 55: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A

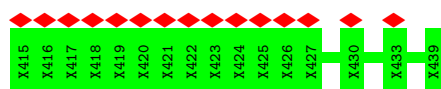




- Molecule 56: DAD1

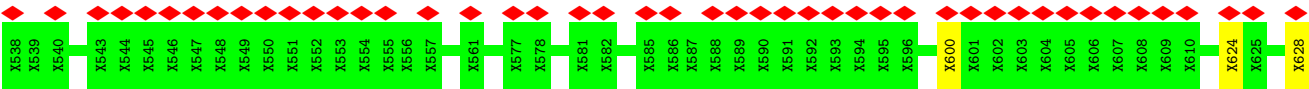


- Molecule 57: OST48

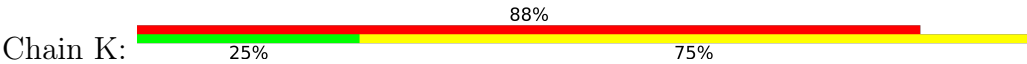


- Molecule 58: RPN2





● Molecule 59: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	17600	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; On each individual tilt image	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	23.787	Depositor
Minimum map value	-20.681	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.3	Depositor
Map size ($\text{\AA}$)	597.36, 597.36, 597.36	wwPDB
Map dimensions	228, 228, 228	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.62, 2.62, 2.62	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, ZN, NAG, MG, 9UB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	3/1906 (0.2%)	0.92	2/2556 (0.1%)
2	B	0.53	0/3216	0.93	13/4311 (0.3%)
3	C	0.56	2/2938 (0.1%)	0.96	3/3946 (0.1%)
4	D	0.48	0/2432	0.86	0/3257
5	E	0.65	3/1936 (0.2%)	1.00	7/2600 (0.3%)
6	F	0.51	0/1905	0.87	0/2539
7	G	0.54	0/1967	0.94	2/2647 (0.1%)
8	H	0.52	1/1535 (0.1%)	0.82	2/2063 (0.1%)
9	I	0.56	1/1693 (0.1%)	0.87	3/2260 (0.1%)
10	J	0.48	0/1376	0.85	0/1841
11	L	0.55	1/1734 (0.1%)	0.92	1/2317 (0.0%)
12	M	0.49	0/1158	0.94	1/1547 (0.1%)
13	N	0.58	1/1746 (0.1%)	0.96	3/2338 (0.1%)
14	O	0.54	0/1671	0.95	3/2234 (0.1%)
15	P	0.59	3/1268 (0.2%)	0.91	4/1701 (0.2%)
16	Q	0.54	0/1530	0.89	0/2041
17	R	0.58	2/1524 (0.1%)	0.95	2/2013 (0.1%)
18	S	0.52	0/1493	0.95	2/2002 (0.1%)
19	T	0.55	1/1326 (0.1%)	0.84	1/1770 (0.1%)
20	U	0.52	1/822 (0.1%)	0.77	0/1103
21	V	0.55	0/993	0.88	1/1332 (0.1%)
22	W	0.58	0/541	0.94	2/720 (0.3%)
23	X	0.55	1/993 (0.1%)	0.90	0/1334
24	Y	0.48	0/1132	0.91	1/1504 (0.1%)
25	Z	0.51	0/1130	0.90	3/1507 (0.2%)
26	a	0.52	0/1191	0.97	4/1590 (0.3%)
27	b	0.57	1/619 (0.2%)	0.96	1/818 (0.1%)
28	c	0.49	0/742	0.93	0/996
29	d	0.51	0/903	0.87	0/1216
30	e	0.62	1/1071 (0.1%)	0.98	1/1429 (0.1%)
31	f	0.70	3/895 (0.3%)	1.02	7/1198 (0.6%)
32	g	0.55	1/916 (0.1%)	0.89	1/1220 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.49	0/1021	0.93	1/1348 (0.1%)
34	i	0.57	1/841 (0.1%)	0.94	2/1112 (0.2%)
35	j	0.61	0/720	1.03	1/952 (0.1%)
36	k	0.55	0/575	0.90	1/761 (0.1%)
37	l	0.67	0/454	0.92	0/599
38	m	0.51	0/435	0.90	0/575
39	n	0.55	0/223	0.88	0/284
40	o	0.52	0/864	0.86	0/1140
41	p	0.57	0/718	0.94	1/953 (0.1%)
42	r	0.62	2/1110 (0.2%)	0.98	2/1484 (0.1%)
43	s	0.59	0/1547	0.81	3/2088 (0.1%)
44	t	0.64	0/1257	0.97	3/1697 (0.2%)
45	u	0.44	7/87790 (0.0%)	0.90	299/136937 (0.2%)
46	v	0.38	0/2858	0.77	1/4455 (0.0%)
47	w	0.40	0/3701	0.82	3/5766 (0.1%)
48	x	0.52	0/3382	0.97	10/4581 (0.2%)
49	y	0.47	0/504	0.93	0/673
50	z	0.53	0/236	1.50	5/321 (1.6%)
51	1	0.28	0/190	0.67	0/260
53	3	0.53	0/815	1.16	10/1107 (0.9%)
54	4	0.43	0/273	0.68	0/371
55	5	0.80	4/5224 (0.1%)	1.11	28/7093 (0.4%)
All	All	0.50	40/161040 (0.0%)	0.91	440/236507 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	4
3	C	0	2
4	D	0	1
5	E	0	1
7	G	0	1
9	I	0	2
11	L	0	3
17	R	0	1
18	S	0	2
19	T	0	1
20	U	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	Y	0	1
31	f	0	1
42	r	0	2
45	u	0	1
48	x	0	2
52	2	0	1
53	3	0	3
55	5	0	6
56	6	0	5
All	All	0	42

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	5	545	ASN	C-N	-29.88	0.91	1.33
55	5	550	THR	C-N	-28.92	0.96	1.33
45	u	680	G	O3'-P	-26.91	1.20	1.61
45	u	692	A	O3'-P	26.39	2.00	1.61
45	u	1965	G	O3'-P	-18.43	1.33	1.61
55	5	513	ARG	C-N	15.88	1.58	1.33
45	u	472	C	O3'-P	-15.71	1.37	1.61
45	u	197	A	O3'-P	10.55	1.76	1.61
45	u	462	G	O3'-P	-7.39	1.50	1.61
55	5	532	ILE	C-N	6.60	1.43	1.33
19	T	3	ASN	CG-OD1	5.77	1.34	1.23
42	r	6	GLN	CD-OE1	5.50	1.33	1.23
5	E	187	GLN	CD-OE1	5.47	1.33	1.23
32	g	28	ASN	CG-OD1	5.38	1.33	1.23
31	f	24	HIS	ND1-CE1	5.34	1.37	1.32
23	X	93	ASN	CG-OD1	5.33	1.33	1.23
3	C	212	ASN	CG-OD1	5.32	1.33	1.23
3	C	119	GLN	CD-OE1	5.30	1.33	1.23
17	R	34	ASN	CG-OD1	5.29	1.33	1.23
27	b	27	GLN	CD-OE1	5.28	1.33	1.23
15	P	116	HIS	ND1-CE1	5.26	1.37	1.32
17	R	141	HIS	ND1-CE1	5.24	1.37	1.32
45	u	223	G	O3'-P	-5.24	1.53	1.61
34	i	80	HIS	ND1-CE1	5.22	1.37	1.32
30	e	102	ASN	CG-OD1	5.17	1.33	1.23
42	r	83	ASN	CG-OD1	5.17	1.33	1.23
15	P	40	HIS	CD2-NE2	-5.15	1.32	1.37
31	f	21	GLN	CD-OE1	5.15	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	109	HIS	ND1-CE1	5.15	1.37	1.32
15	P	40	HIS	ND1-CE1	5.13	1.37	1.32
20	U	95	ASN	CG-OD1	5.12	1.33	1.23
1	A	216	HIS	ND1-CE1	5.10	1.37	1.32
8	H	76	HIS	ND1-CE1	5.09	1.37	1.32
1	A	216	HIS	CD2-NE2	-5.09	1.32	1.37
31	f	21	GLN	CD-NE2	-5.06	1.22	1.33
5	E	39	HIS	ND1-CE1	5.05	1.37	1.32
5	E	163	GLN	CD-OE1	5.05	1.33	1.23
9	I	95	HIS	ND1-CE1	5.04	1.37	1.32
1	A	162	ASN	CG-OD1	5.04	1.33	1.23
11	L	188	ASN	CG-OD1	5.03	1.33	1.23

All (440) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	5	545	ASN	CA-C-N	-22.02	79.48	121.54
55	5	545	ASN	C-N-CA	-22.02	79.48	121.54
55	5	545	ASN	O-C-N	20.77	146.47	122.79
45	u	680	G	O3'-P-O5'	18.20	131.31	104.00
55	5	550	THR	O-C-N	-14.62	106.30	122.09
55	5	550	THR	CA-C-N	13.82	139.31	120.38
55	5	550	THR	C-N-CA	13.82	139.31	120.38
3	C	98	GLY	N-CA-C	-13.76	99.01	111.67
45	u	1358	G	C4'-C3'-O3'	13.60	133.39	113.00
45	u	462	G	P-O3'-C3'	-13.35	100.18	120.20
45	u	4975	G	C2'-C3'-O3'	13.14	129.20	109.50
45	u	1357	C	C4'-C3'-O3'	12.92	132.38	113.00
53	3	56	PRO	N-CA-CB	12.86	109.91	103.22
55	5	359	SER	N-CA-C	-12.29	97.89	111.28
45	u	47	A	C4'-C3'-O3'	11.98	127.38	109.40
50	z	69	GLY	CA-C-N	11.51	134.22	119.84
50	z	69	GLY	C-N-CA	11.51	134.22	119.84
55	5	349	VAL	N-CA-C	-11.23	94.59	109.30
55	5	532	ILE	O-C-N	-10.98	110.78	121.87
14	O	110	PRO	N-CA-C	10.95	124.06	110.70
55	5	292	PRO	N-CA-CB	10.63	109.69	102.25
45	u	5061	A	C2'-C3'-O3'	10.56	125.34	109.50
45	u	2695	A	C2'-C3'-O3'	10.48	125.22	109.50
55	5	513	ARG	O-C-N	-10.39	108.12	122.46
55	5	257	VAL	N-CA-C	-10.29	92.97	107.99
55	5	350	SER	CA-C-N	-10.26	104.17	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	5	350	SER	C-N-CA	-10.26	104.17	121.92
45	u	1485	C	C2'-C3'-O3'	10.19	124.78	109.50
45	u	2858	A	C4'-C3'-O3'	10.16	128.24	113.00
48	x	48	ILE	CA-C-N	10.15	130.08	120.03
48	x	48	ILE	C-N-CA	10.15	130.08	120.03
45	u	1279	A	C2'-C3'-O3'	10.04	124.57	109.50
45	u	2046	G	C2'-C3'-O3'	10.03	124.54	109.50
45	u	3718	A	C4'-C3'-O3'	9.99	127.99	113.00
45	u	215	C	C4'-C3'-O3'	-9.90	98.14	113.00
53	3	94	PHE	N-CA-C	9.79	122.03	111.36
45	u	1365	C	C4'-C3'-O3'	9.58	123.77	109.40
45	u	90	G	C2'-C3'-O3'	9.50	127.95	113.70
45	u	1398	A	C2'-C3'-O3'	9.49	123.74	109.50
45	u	4528	G	C2'-C3'-O3'	9.45	127.88	113.70
55	5	513	ARG	CA-C-N	9.45	134.84	121.71
55	5	513	ARG	C-N-CA	9.45	134.84	121.71
45	u	2123	C	C2'-C3'-O3'	9.45	123.67	109.50
45	u	1239	C	C2'-C3'-O3'	9.41	123.61	109.50
45	u	3888	G	C2'-C3'-O3'	9.39	127.78	113.70
45	u	1847	C	C4'-C3'-O3'	-9.27	99.09	113.00
45	u	218	A	C3'-C2'-O2'	9.26	124.58	110.70
48	x	48	ILE	N-CA-C	9.25	119.13	108.96
45	u	118	C	C4'-C3'-O3'	-9.18	99.23	113.00
45	u	1696	C	C2'-C3'-O3'	9.09	123.13	109.50
45	u	4948	C	C2'-C3'-O3'	9.01	127.22	113.70
45	u	3753	G	N9-C1'-C2'	-9.01	98.49	112.00
50	z	69	GLY	N-CA-C	-8.99	103.80	115.22
45	u	4951	G	C2'-C3'-O3'	8.97	122.95	109.50
45	u	4872	G	C2'-C3'-O3'	8.96	122.94	109.50
45	u	385	A	C4'-C3'-O3'	8.95	122.82	109.40
45	u	220	C	C2'-C3'-O3'	8.92	127.08	113.70
45	u	276	C	C4'-C3'-O3'	-8.90	99.65	113.00
45	u	197	A	P-O3'-C3'	8.87	133.51	120.20
45	u	1211	G	C2'-C3'-O3'	8.87	127.00	113.70
45	u	93	G	C4'-C3'-O3'	8.87	126.30	113.00
45	u	3697	U	C2'-C3'-O3'	8.81	126.91	113.70
45	u	1455	G	C2'-C3'-O3'	8.59	126.59	113.70
45	u	209	U	C4'-C3'-O3'	8.59	125.89	113.00
45	u	2083	C	C4'-C3'-O3'	8.56	125.85	113.00
45	u	930	G	C4'-C3'-O3'	8.35	121.92	109.40
45	u	1969	G	C4'-C3'-O3'	8.32	125.48	113.00
45	u	220	C	N1-C1'-C2'	-8.28	99.58	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	67	TRP	N-CA-C	-8.28	97.42	109.59
45	u	2661	U	C2'-C3'-O3'	8.27	121.91	109.50
45	u	1292	C	C2'-C3'-O3'	8.24	126.06	113.70
45	u	1292	C	C4'-C3'-O3'	-8.20	100.69	113.00
45	u	1755	C	C2'-C3'-O3'	8.19	121.79	109.50
45	u	2068	C	C4'-C3'-O3'	8.06	121.49	109.40
45	u	1410	U	C2'-C3'-O3'	8.04	121.56	109.50
45	u	4975	G	C4'-C3'-O3'	-8.03	97.36	109.40
45	u	275	C	C2'-C3'-O3'	7.97	125.66	113.70
45	u	5060	A	C2'-C3'-O3'	7.95	125.62	113.70
45	u	125	C	C2'-C3'-O3'	7.94	125.61	113.70
45	u	5027	C	C2'-C3'-O3'	7.90	121.35	109.50
45	u	1477	C	C2'-C3'-O3'	7.88	125.52	113.70
45	u	4170	A	C2'-C3'-O3'	7.85	121.27	109.50
53	3	71	PRO	N-CA-CB	7.73	110.53	103.34
45	u	686	A	C4'-C3'-O3'	7.73	120.99	109.40
45	u	5059	C	C2'-C3'-O3'	7.68	125.22	113.70
45	u	2028	C	C2'-C3'-O3'	-7.68	102.18	113.70
45	u	406	C	C2'-C3'-O3'	7.67	125.20	113.70
45	u	48	G	C2'-C3'-O3'	7.64	120.97	109.50
45	u	2116	C	C2'-C3'-O3'	7.58	120.87	109.50
45	u	3718	A	N9-C1'-C2'	-7.58	100.64	112.00
45	u	462	G	O3'-P-O5'	7.54	115.31	104.00
45	u	4699	U	C4'-C3'-O3'	7.54	120.72	109.40
26	a	31	GLY	N-CA-C	-7.52	104.80	111.95
2	B	17	LEU	N-CA-C	7.49	122.86	108.12
45	u	1724	G	C4'-C3'-O3'	7.47	120.61	109.40
48	x	81	ILE	N-CA-C	-7.44	105.30	112.29
45	u	3718	A	C2'-C3'-O3'	-7.43	102.55	113.70
45	u	4075	U	C4'-C3'-O3'	7.40	120.50	109.40
3	C	232	VAL	CB-CA-C	-7.39	102.02	112.22
45	u	3619	G	C4'-C3'-O3'	-7.36	101.96	113.00
45	u	1500	A	C4'-C3'-O3'	-7.33	102.01	113.00
45	u	4965	U	C4'-C3'-O3'	-7.30	102.04	113.00
45	u	1357	C	C2'-C3'-O3'	-7.30	102.75	113.70
2	B	258	HIS	CA-C-N	-7.27	110.75	119.84
2	B	258	HIS	C-N-CA	-7.27	110.75	119.84
45	u	956	A	C4'-C3'-O3'	7.27	120.31	109.40
47	w	94	G	C2'-C3'-O3'	7.27	120.40	109.50
45	u	4730	C	C4'-C3'-O3'	7.26	120.29	109.40
45	u	4666	G	C4'-C3'-O3'	-7.25	102.12	113.00
45	u	2349	A	C4'-C3'-O3'	-7.21	102.19	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	u	917	A	C4'-C3'-O3'	7.21	120.21	109.40
36	k	61	PRO	N-CA-C	7.17	119.44	110.70
45	u	1236	C	C2'-C3'-O3'	7.15	124.43	113.70
45	u	977	C	C2'-C3'-O3'	7.13	124.39	113.70
55	5	286	LEU	CA-C-N	-7.13	107.92	121.54
55	5	286	LEU	C-N-CA	-7.13	107.92	121.54
45	u	1268	G	C4'-C3'-O3'	7.12	120.08	109.40
45	u	3858	C	C4'-C3'-O3'	-7.11	102.34	113.00
45	u	4885	U	C2'-C3'-O3'	7.11	124.36	113.70
45	u	2256	C	C2'-C3'-O3'	7.09	120.13	109.50
15	P	40	HIS	CB-CG-CD2	-7.08	121.99	131.20
45	u	928	C	C2'-C3'-O3'	-7.06	103.11	113.70
48	x	69	LEU	CA-C-N	-7.03	112.10	122.86
48	x	69	LEU	C-N-CA	-7.03	112.10	122.86
21	V	13	LYS	N-CA-C	7.00	118.99	111.36
45	u	3876	A	C2'-C3'-O3'	7.00	120.00	109.50
45	u	2769	U	C4'-C3'-O3'	6.99	119.89	109.40
45	u	1818	G	C2'-C3'-O3'	6.97	124.16	113.70
45	u	2107	C	C2'-C3'-O3'	6.92	119.88	109.50
45	u	1974	U	C4'-C3'-O3'	6.90	119.75	109.40
45	u	223	G	P-O3'-C3'	6.90	130.55	120.20
45	u	1380	G	C1'-C2'-O2'	-6.88	101.47	111.80
45	u	965	G	C2'-C3'-O3'	6.87	119.81	109.50
5	E	39	HIS	CB-CG-CD2	-6.86	122.29	131.20
45	u	692	A	P-O3'-C3'	6.85	130.48	120.20
30	e	42	ASP	N-CA-C	-6.85	98.07	109.24
1	A	216	HIS	CB-CG-CD2	-6.83	122.32	131.20
45	u	4378	A	C2'-C3'-O3'	6.82	119.72	109.50
45	u	3657	U	C2'-C3'-O3'	6.80	123.90	113.70
47	w	124	U	C4'-C3'-O3'	6.76	119.53	109.40
45	u	1474	C	C2'-C3'-O3'	6.73	123.80	113.70
45	u	4115	G	C4'-C3'-O3'	6.73	119.50	109.40
45	u	1969	G	C2'-C3'-O3'	-6.72	103.62	113.70
45	u	2093	A	C2'-C3'-O3'	6.70	119.56	109.50
45	u	2588	C	C2'-C3'-O3'	-6.69	103.67	113.70
15	P	116	HIS	CB-CG-CD2	-6.68	122.51	131.20
45	u	1500	A	C2'-C3'-O3'	6.68	123.72	113.70
45	u	2632	U	N1-C1'-C2'	6.68	122.02	112.00
45	u	2797	C	N1-C1'-C2'	-6.67	103.99	114.00
45	u	957	G	C2'-C3'-O3'	6.67	119.51	109.50
45	u	4449	A	C4'-C3'-O3'	6.67	119.41	109.40
45	u	1835	G	C2'-C3'-O3'	6.67	119.50	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	u	3670	C	C4'-C3'-O3'	6.65	122.97	113.00
45	u	4548	A	C4'-C3'-O3'	6.64	119.35	109.40
45	u	1	C	C4'-C3'-O3'	6.63	119.35	109.40
55	5	255	SER	N-CA-C	6.63	118.58	111.36
17	R	141	HIS	CB-CG-CD2	-6.61	122.60	131.20
45	u	1380	G	C4'-C3'-O3'	6.61	119.31	109.40
5	E	72	PRO	N-CA-CB	6.60	110.26	103.00
45	u	90	G	C4'-C3'-O3'	-6.59	103.11	113.00
45	u	1388	A	C4'-C3'-O3'	-6.59	103.11	113.00
31	f	24	HIS	CB-CG-CD2	-6.59	122.64	131.20
45	u	1672	U	N1-C1'-C2'	6.57	121.85	112.00
7	G	77	PRO	CA-C-N	6.55	126.18	119.56
7	G	77	PRO	C-N-CA	6.55	126.18	119.56
2	B	261	ARG	N-CA-C	-6.55	98.77	108.79
34	i	80	HIS	CB-CG-CD2	-6.55	122.69	131.20
45	u	1282	G	C1'-C2'-O2'	6.54	118.21	108.40
45	u	1369	C	C2'-C3'-O3'	-6.49	103.97	113.70
45	u	2714	G	C4'-C3'-O3'	-6.49	103.27	113.00
45	u	207	G	C2'-C3'-O3'	-6.48	103.98	113.70
2	B	258	HIS	N-CA-C	6.48	124.12	109.81
45	u	4400	G	C4'-C3'-O3'	-6.47	103.29	113.00
45	u	4888	U	C2'-C3'-O3'	6.47	119.21	109.50
45	u	3715	U	C4'-C3'-O3'	6.47	122.71	113.00
44	t	140	GLY	N-CA-C	6.46	120.72	112.83
45	u	4213	A	C4'-C3'-O3'	-6.46	103.31	113.00
45	u	4543	G	C4'-C3'-O3'	-6.45	103.33	113.00
45	u	1975	G	C4'-C3'-O3'	6.44	119.06	109.40
45	u	407	A	C4'-C3'-O3'	-6.40	103.40	113.00
45	u	1848	C	C2'-C3'-O3'	6.40	123.30	113.70
45	u	2395	A	C2'-C3'-O3'	6.40	119.10	109.50
13	N	109	HIS	CB-CG-CD2	-6.40	122.88	131.20
13	N	78	GLY	N-CA-C	-6.39	104.39	110.21
45	u	932	A	C2'-C3'-O3'	6.39	119.09	109.50
45	u	1329	G	C4'-C3'-O3'	6.36	122.55	113.00
45	u	4517	A	C4'-C3'-O3'	-6.36	103.46	113.00
45	u	1697	G	C4'-C3'-O3'	6.36	118.93	109.40
45	u	944	A	C4'-C3'-O3'	-6.35	103.48	113.00
45	u	936	C	C2'-C3'-O3'	6.33	119.00	109.50
8	H	76	HIS	CB-CG-CD2	-6.33	122.97	131.20
45	u	1390	G	C2'-C3'-O3'	6.33	123.19	113.70
45	u	2506	G	C4'-C3'-O3'	6.30	118.85	109.40
24	Y	87	ARG	NE-CZ-NH2	6.29	124.86	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	u	4211	C	C4'-C3'-O3'	-6.28	103.58	113.00
45	u	2858	A	C1'-C2'-O2'	-6.28	98.98	108.40
18	S	164	LYS	N-CA-C	-6.28	101.08	110.24
44	t	29	ALA	CA-C-N	6.27	127.68	119.84
44	t	29	ALA	C-N-CA	6.27	127.68	119.84
45	u	1613	A	C2'-C3'-O3'	6.27	118.91	109.50
45	u	2266	C	C2'-C3'-O3'	6.27	118.91	109.50
53	3	113	PRO	N-CA-CB	6.27	109.83	103.25
55	5	348	SER	N-CA-C	6.26	118.10	111.28
45	u	2429	A	C4'-C3'-O3'	-6.25	103.62	113.00
45	u	1280	C	C4'-C3'-O3'	-6.25	103.63	113.00
45	u	964	A	O4'-C1'-C2'	-6.24	101.36	107.60
45	u	4473	A	C4'-C3'-O3'	-6.24	103.64	113.00
45	u	218	A	C4'-C3'-O3'	-6.23	103.66	113.00
45	u	5024	C	C2'-C3'-O3'	6.22	118.83	109.50
45	u	684	G	C3'-C2'-O2'	6.21	120.02	110.70
45	u	1232	G	C2'-C3'-O3'	6.20	118.80	109.50
45	u	223	G	C1'-C2'-O2'	6.19	117.69	108.40
48	x	449	LEU	CA-CB-CG	-6.18	94.65	116.30
45	u	978	G	C2'-C3'-O3'	6.18	122.97	113.70
45	u	3593	C	C4'-C3'-O3'	6.18	118.67	109.40
45	u	4084	G	C2'-C3'-O3'	6.17	118.76	109.50
45	u	1891	A	C2'-C3'-O3'	6.16	118.75	109.50
45	u	3657	U	C4'-C3'-O3'	-6.16	103.75	113.00
45	u	1329	G	C2'-C3'-O3'	6.15	122.92	113.70
55	5	597	LEU	N-CA-C	-6.14	104.58	111.28
45	u	4144	C	C4'-C3'-O3'	6.11	118.57	109.40
31	f	92	LEU	CA-C-N	6.09	125.98	119.28
31	f	92	LEU	C-N-CA	6.09	125.98	119.28
31	f	93	PRO	N-CA-C	6.08	121.86	113.65
5	E	90	LYS	CA-C-N	6.07	127.43	119.84
5	E	90	LYS	C-N-CA	6.07	127.43	119.84
45	u	4473	A	N9-C1'-C2'	6.07	121.10	112.00
45	u	1969	G	N9-C1'-C2'	-6.06	102.91	112.00
5	E	39	HIS	CB-CG-ND1	6.03	131.75	122.70
22	W	14	TYR	CA-C-N	6.03	127.38	119.84
22	W	14	TYR	C-N-CA	6.03	127.38	119.84
45	u	2474	G	C3'-C2'-O2'	6.03	119.74	110.70
45	u	1965	G	O3'-P-O5'	-6.02	94.97	104.00
45	u	4900	C	C2'-C3'-O3'	6.00	118.50	109.50
45	u	2088	A	C2'-C3'-O3'	5.99	118.48	109.50
45	u	3672	G	C2'-C3'-O3'	-5.99	104.72	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	121	LYS	N-CA-C	-5.99	102.34	110.36
45	u	497	G	C2'-C3'-O3'	-5.97	104.74	113.70
45	u	212	A	N9-C1'-C2'	5.97	120.95	112.00
46	v	96	U	C2'-C3'-O3'	-5.95	104.77	113.70
45	u	3859	G	C4'-C3'-O3'	-5.95	104.07	113.00
45	u	4318	C	C4'-C3'-O3'	-5.95	104.07	113.00
15	P	40	HIS	CB-CG-ND1	5.95	131.62	122.70
45	u	1214	C	C4'-C3'-O3'	5.93	118.30	109.40
2	B	254	ILE	N-CA-C	-5.93	104.55	110.30
45	u	462	G	OP1-P-O3'	-5.92	90.23	108.00
45	u	5049	G	C4'-C3'-O3'	5.92	118.28	109.40
55	5	348	SER	O-C-N	5.88	128.35	122.12
45	u	1357	C	C3'-C2'-O2'	5.86	119.49	110.70
45	u	1457	G	C4'-C3'-O3'	-5.86	104.21	113.00
9	I	95	HIS	CB-CG-CD2	-5.86	123.59	131.20
45	u	1553	A	C4'-C3'-O3'	-5.85	104.22	113.00
45	u	4083	U	C4'-C3'-O3'	-5.85	104.23	113.00
45	u	3753	G	C4'-C3'-O3'	5.84	121.76	113.00
45	u	294	G	C4'-C3'-O3'	-5.83	104.26	113.00
25	Z	36	ARG	CA-C-N	5.82	125.50	119.56
25	Z	36	ARG	C-N-CA	5.82	125.50	119.56
45	u	979	C	C2'-C3'-O3'	5.82	122.43	113.70
45	u	4116	C	C2'-C3'-O3'	5.81	118.22	109.50
50	z	69	GLY	O-C-N	5.81	123.16	121.07
45	u	451	C	C2'-C3'-O3'	5.80	118.19	109.50
45	u	918	G	C2'-C3'-O3'	-5.78	105.03	113.70
45	u	1429	C	C4'-C3'-O3'	-5.77	104.34	113.00
1	A	216	HIS	CB-CG-ND1	5.77	131.36	122.70
45	u	2468	U	C4'-C3'-O3'	5.77	118.05	109.40
55	5	353	GLN	CA-C-N	5.76	125.67	119.85
55	5	353	GLN	C-N-CA	5.76	125.67	119.85
45	u	4435	U	C4'-C3'-O3'	-5.75	104.37	113.00
45	u	1633	G	C4'-C3'-O3'	5.75	121.63	113.00
45	u	1636	U	C4'-C3'-O3'	-5.75	104.38	113.00
45	u	497	G	C4'-C3'-O3'	5.74	121.61	113.00
45	u	2427	G	C4'-C3'-O3'	-5.74	104.39	113.00
45	u	4568	A	C4'-C3'-O3'	-5.74	104.39	113.00
45	u	2827	G	C2'-C3'-O3'	-5.73	100.91	109.50
45	u	3864	C	C2'-C3'-O3'	-5.72	105.12	113.70
43	s	200	ASN	CA-C-N	5.71	126.98	119.84
43	s	200	ASN	C-N-CA	5.71	126.98	119.84
45	u	4228	G	C4'-C3'-O3'	-5.69	100.86	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	u	265	C	C4'-C3'-O3'	5.68	117.92	109.40
45	u	2554	U	C4'-C3'-O3'	5.68	121.52	113.00
31	f	24	HIS	CB-CG-ND1	5.68	131.22	122.70
45	u	286	U	N1-C1'-C2'	5.67	120.50	112.00
18	S	83	ARG	NE-CZ-NH2	5.66	124.30	119.20
15	P	116	HIS	CB-CG-ND1	5.66	131.19	122.70
17	R	141	HIS	CB-CG-ND1	5.65	131.18	122.70
45	u	486	C	C2'-C3'-O3'	5.65	122.18	113.70
45	u	1266	G	C2'-C3'-O3'	5.65	122.17	113.70
43	s	72	ASN	N-CA-C	5.64	116.76	109.65
45	u	1912	G	C4'-C3'-O3'	-5.63	104.56	113.00
50	z	83	SER	N-CA-C	-5.62	105.15	111.28
55	5	121	PRO	N-CA-C	-5.62	105.72	113.53
45	u	664	G	C4'-C3'-O3'	5.62	117.83	109.40
45	u	468	U	N1-C1'-C2'	5.61	120.42	112.00
45	u	4656	A	C2'-C3'-O3'	5.61	117.91	109.50
45	u	2251	G	C4'-C3'-O3'	5.60	117.80	109.40
45	u	2858	A	N9-C1'-C2'	-5.60	103.60	112.00
45	u	220	C	C4'-C3'-O3'	-5.59	104.61	113.00
45	u	209	U	C1'-C2'-O2'	5.59	116.79	108.40
45	u	2053	C	C4'-C3'-O3'	-5.59	104.61	113.00
45	u	3717	A	C2'-C3'-O3'	-5.59	105.32	113.70
45	u	4521	U	C4'-C3'-O3'	-5.58	104.63	113.00
45	u	680	G	OP2-P-O3'	-5.57	91.28	108.00
35	j	9	GLY	N-CA-C	5.57	119.62	112.83
45	u	5041	G	C2'-C3'-O3'	-5.55	105.37	113.70
45	u	4655	A	C4'-C3'-O3'	-5.55	104.68	113.00
2	B	16	PHE	CA-C-N	-5.53	116.18	122.26
2	B	16	PHE	C-N-CA	-5.53	116.18	122.26
45	u	1633	G	C2'-C3'-O3'	-5.53	105.41	113.70
45	u	4882	U	C2'-C3'-O3'	5.53	117.79	109.50
53	3	62	MET	CA-C-N	5.53	132.09	121.54
53	3	62	MET	C-N-CA	5.53	132.09	121.54
45	u	222	C	C1'-C2'-O2'	5.51	116.67	108.40
34	i	80	HIS	CB-CG-ND1	5.51	130.96	122.70
45	u	977	C	C4'-C3'-O3'	-5.50	104.75	113.00
45	u	1477	C	C4'-C3'-O3'	-5.50	104.75	113.00
45	u	1280	C	N1-C1'-C2'	5.49	120.24	112.00
55	5	172	ALA	N-CA-C	-5.49	105.29	111.28
45	u	3673	C	C2'-C3'-O3'	5.49	117.74	109.50
25	Z	54	THR	N-CA-C	5.49	119.28	112.47
45	u	1968	G	C2'-C3'-O3'	-5.49	105.47	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	u	2700	G	C4'-C3'-O3'	-5.47	104.79	113.00
13	N	109	HIS	CB-CG-ND1	5.47	130.90	122.70
45	u	3807	A	C4'-C3'-O3'	-5.47	104.80	113.00
45	u	277	G	C4'-C3'-O3'	5.46	117.58	109.40
45	u	2119	C	C2'-C3'-O3'	5.45	117.68	109.50
33	h	96	ASN	N-CA-C	5.44	119.39	112.87
45	u	2027	U	C4'-C3'-O3'	5.43	121.15	113.00
27	b	8	THR	N-CA-C	5.43	115.71	108.38
45	u	4375	C	C2'-C3'-O3'	-5.43	105.56	113.70
48	x	63	TYR	N-CA-C	5.42	117.00	111.14
8	H	76	HIS	CB-CG-ND1	5.42	130.83	122.70
45	u	470	A	O4'-C1'-C2'	-5.42	102.18	107.60
45	u	4331	G	C2'-C3'-O3'	5.41	117.62	109.50
2	B	18	PRO	N-CA-C	-5.41	101.33	112.47
45	u	4965	U	C2'-C3'-O3'	5.41	121.81	113.70
2	B	36	ASP	CA-C-N	-5.40	113.09	119.84
2	B	36	ASP	C-N-CA	-5.40	113.09	119.84
45	u	4998	G	C4'-C3'-O3'	-5.40	104.90	113.00
45	u	1380	G	N9-C1'-C2'	5.38	122.06	114.00
41	p	52	VAL	CB-CA-C	-5.37	103.22	111.71
53	3	63	THR	CA-C-N	5.36	131.78	121.54
53	3	63	THR	C-N-CA	5.36	131.78	121.54
45	u	1235	G	C2'-C3'-O3'	-5.36	105.66	113.70
5	E	217	GLN	N-CA-C	5.35	117.74	110.35
45	u	1214	C	C2'-C3'-O3'	5.35	117.53	109.50
2	B	36	ASP	N-CA-C	-5.35	102.85	109.64
45	u	2083	C	C2'-C3'-O3'	-5.35	105.68	113.70
31	f	106	TYR	N-CA-C	5.34	121.62	109.81
45	u	1236	C	C3'-C2'-O2'	5.34	118.71	110.70
53	3	57	PRO	N-CA-C	5.34	123.47	112.47
45	u	2246	C	C2'-C3'-O3'	5.34	121.71	113.70
45	u	2864	A	C4'-C3'-O3'	-5.33	105.00	113.00
45	u	2546	G	C3'-C2'-O2'	5.33	118.69	110.70
45	u	4938	A	C2'-C3'-O3'	-5.33	105.71	113.70
45	u	1847	C	C2'-C3'-O3'	5.32	121.68	113.70
45	u	2474	G	C2'-C3'-O3'	5.32	121.68	113.70
45	u	2068	C	C2'-C3'-O3'	5.31	117.46	109.50
48	x	406	GLU	N-CA-C	5.30	116.75	111.07
45	u	5066	U	N1-C1'-C2'	5.30	119.95	112.00
45	u	430	G	C4'-C3'-O3'	-5.30	105.05	113.00
45	u	1921	C	C4'-C3'-O3'	5.28	117.32	109.40
45	u	4558	U	C4'-C3'-O3'	-5.28	105.08	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	u	134	G	C4'-C3'-O3'	5.28	117.32	109.40
45	u	3594	C	N1-C1'-C2'	5.27	119.90	112.00
45	u	4087	G	C2'-C3'-O3'	-5.27	105.80	113.70
45	u	1990	A	C2'-C3'-O3'	5.27	121.60	113.70
45	u	1072	C	N1-C1'-C2'	5.27	121.90	114.00
45	u	1725	U	C1'-C2'-O2'	5.27	116.30	108.40
45	u	4966	A	C4'-C3'-O3'	-5.27	105.10	113.00
11	L	99	ASP	N-CA-C	-5.26	102.51	110.50
45	u	2027	U	N1-C1'-C2'	-5.25	104.12	112.00
45	u	4625	C	C4'-C3'-O3'	-5.25	105.13	113.00
45	u	4364	G	C4'-C3'-O3'	-5.24	105.14	113.00
45	u	4966	A	N9-C1'-C2'	5.24	119.86	112.00
26	a	120	GLN	CA-C-N	5.23	125.22	119.89
26	a	120	GLN	C-N-CA	5.23	125.22	119.89
45	u	2257	C	C4'-C3'-O3'	5.23	117.24	109.40
45	u	1358	G	O4'-C1'-C2'	-5.22	102.38	107.60
45	u	989	U	C3'-C2'-O2'	5.21	118.52	110.70
45	u	1648	C	C4'-C3'-O3'	-5.21	105.19	113.00
45	u	4696	C	C4'-C3'-O3'	-5.20	105.19	113.00
32	g	67	LEU	N-CA-C	5.20	117.00	110.24
45	u	2313	A	C3'-C2'-O2'	5.20	118.50	110.70
45	u	976	G	C3'-C2'-O2'	5.20	118.50	110.70
45	u	2260	C	C3'-C2'-O2'	5.20	118.49	110.70
14	O	108	ILE	CA-C-N	5.19	125.73	120.38
14	O	108	ILE	C-N-CA	5.19	125.73	120.38
45	u	300	A	N9-C1'-C2'	5.19	119.79	112.00
45	u	2064	G	C2'-C3'-O3'	5.19	121.49	113.70
45	u	3903	A	C4'-C3'-O3'	-5.19	105.22	113.00
45	u	5022	U	C3'-C2'-O2'	5.18	118.47	110.70
45	u	1428	U	C4'-C3'-O3'	-5.17	105.24	113.00
45	u	1677	U	C4'-C3'-O3'	-5.16	105.25	113.00
19	T	27	LEU	N-CA-C	5.16	119.29	112.89
45	u	206	U	C2'-C3'-O3'	5.16	121.44	113.70
45	u	4307	A	C4'-C3'-O3'	-5.16	105.26	113.00
45	u	4266	G	C2'-C3'-O3'	-5.16	105.97	113.70
42	r	103	HIS	CA-C-N	-5.15	114.31	119.56
42	r	103	HIS	C-N-CA	-5.15	114.31	119.56
47	w	93	C	C4'-C3'-O3'	-5.15	105.28	113.00
5	E	123	SER	N-CA-C	5.14	118.82	112.24
45	u	931	C	C3'-C2'-O2'	5.13	118.40	110.70
45	u	4228	G	C2'-C3'-O3'	5.13	117.19	109.50
26	a	61	TYR	N-CA-C	5.12	116.72	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	u	2422	C	C3'-C2'-O2'	5.12	118.38	110.70
45	u	93	G	C1'-C2'-O2'	-5.11	100.73	108.40
55	5	87	THR	CA-CB-CG2	5.11	119.19	110.50
9	I	49	CYS	N-CA-C	5.11	118.67	111.52
45	u	166	C	C4'-C3'-O3'	5.11	120.66	113.00
45	u	2084	C	C4'-C3'-O3'	5.10	117.05	109.40
45	u	4312	U	C4'-C3'-O3'	-5.09	105.36	113.00
45	u	962	C	C2'-C3'-O3'	5.09	117.13	109.50
53	3	110	PRO	N-CA-CB	5.09	110.14	103.42
55	5	100	TYR	CA-CB-CG	5.09	123.06	113.90
12	M	8	GLU	N-CA-C	-5.08	102.27	110.14
45	u	687	U	C1'-C2'-O2'	5.07	116.00	108.40
45	u	2262	G	C3'-C2'-O2'	5.07	118.30	110.70
45	u	3697	U	C3'-C2'-O2'	5.07	118.30	110.70
45	u	4640	C	C4'-C3'-O3'	-5.07	105.40	113.00
45	u	1804	A	C2'-C3'-O3'	5.06	117.09	109.50
45	u	1848	C	C4'-C3'-O3'	-5.06	105.40	113.00
45	u	1358	G	C2'-C3'-O3'	-5.06	106.11	113.70
31	f	83	MET	N-CA-C	-5.06	103.72	110.55
48	x	50	LEU	N-CA-C	5.06	119.14	112.92
45	u	4069	U	C3'-C2'-O2'	5.05	118.27	110.70
2	B	101	THR	N-CA-CB	5.05	117.39	109.97
45	u	1898	C	C2'-C3'-O3'	5.04	117.07	109.50
45	u	4888	U	C4'-C3'-O3'	5.04	116.96	109.40
45	u	5026	U	N1-C1'-C2'	5.04	119.56	112.00
45	u	48	G	C4'-C3'-O3'	5.04	116.95	109.40
45	u	4585	U	C4'-C3'-O3'	-5.04	105.45	113.00
45	u	693	C	C2'-C3'-O3'	5.03	121.25	113.70
45	u	486	C	C3'-C2'-O2'	5.03	118.25	110.70
45	u	266	C	C2'-C3'-O3'	-5.03	106.16	113.70
45	u	233	U	C2'-C3'-O3'	5.02	117.04	109.50
45	u	2264	C	C4'-C3'-O3'	-5.02	105.47	113.00
45	u	3752	C	C2'-C3'-O3'	-5.02	106.17	113.70
45	u	2505	C	C4'-C3'-O3'	5.01	116.92	109.40
45	u	1336	G	C2'-C3'-O3'	-5.01	106.18	113.70
45	u	1612	G	C2'-C3'-O3'	5.00	117.01	109.50

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	2	15	UNK	Peptide

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Mol	Chain	Res	Type	Group
53	3	56	PRO	Peptide
53	3	64	ASP	Peptide
53	3	67	GLY	Peptide
55	5	100	TYR	Peptide
55	5	263	LEU	Peptide
55	5	532	ILE	Mainchain
55	5	616	ASP	Peptide
55	5	655	LYS	Peptide
55	5	69	HIS	Peptide
56	6	20	UNK	Peptide
56	6	21	UNK	Peptide
56	6	80	UNK	Peptide
56	6	81	UNK	Peptide
56	6	89	UNK	Peptide
1	A	196	TRP	Peptide
2	B	17	LEU	Peptide
2	B	257	TRP	Peptide
2	B	258	HIS	Peptide
2	B	351	LEU	Peptide
3	C	245	HIS	Peptide
3	C	339	THR	Peptide
4	D	36	LEU	Peptide
5	E	123	SER	Peptide
7	G	238	GLY	Peptide
9	I	188	LYS	Peptide
9	I	202	ASN	Peptide
11	L	27	ASN	Peptide
11	L	46	ILE	Peptide
11	L	66	TYR	Peptide
17	R	19	LYS	Peptide
18	S	163	HIS	Peptide
18	S	164	LYS	Peptide
19	T	26	PRO	Peptide
20	U	27	HIS	Peptide
24	Y	7	VAL	Peptide
31	f	105	LEU	Peptide
42	r	106	LEU	Peptide
42	r	70	GLN	Peptide
45	u	2793	G	Sidechain
48	x	173	TYR	Peptide
48	x	42	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1868	0	1959	31	0
2	B	3148	0	3267	63	0
3	C	2884	0	3062	46	0
4	D	2386	0	2419	34	0
5	E	1898	0	2035	93	0
6	F	1870	0	1994	27	0
7	G	1934	0	2087	31	0
8	H	1516	0	1597	18	0
9	I	1655	0	1704	42	0
10	J	1353	0	1386	11	0
11	L	1703	0	1820	27	0
12	M	1137	0	1211	18	0
13	N	1701	0	1749	20	0
14	O	1638	0	1777	31	0
15	P	1242	0	1269	13	0
16	Q	1506	0	1623	17	0
17	R	1508	0	1664	23	0
18	S	1454	0	1496	15	0
19	T	1298	0	1366	11	0
20	U	808	0	831	7	0
21	V	979	0	1039	5	0
22	W	528	0	541	5	0
23	X	976	0	1052	37	0
24	Y	1115	0	1205	22	0
25	Z	1107	0	1182	16	0
26	a	1162	0	1209	19	0
27	b	609	0	650	5	0
28	c	732	0	769	7	0
29	d	888	0	930	9	0
30	e	1053	0	1147	29	0
31	f	876	0	912	19	0
32	g	906	0	999	12	0
33	h	1013	0	1147	18	0
34	i	830	0	916	4	0
35	j	705	0	738	16	0
36	k	569	0	637	6	0
37	l	444	0	483	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	429	0	466	9	0
39	n	222	0	264	1	0
40	o	851	0	921	12	0
41	p	708	0	756	7	0
42	r	1094	0	1168	125	0
43	s	1523	0	1577	27	0
44	t	1238	0	1295	10	0
45	u	78486	0	39663	1524	0
46	v	2558	0	1296	27	0
47	w	3314	0	1683	55	0
48	x	3313	0	3425	507	0
49	y	494	0	521	131	0
50	z	229	0	245	65	0
51	1	885	0	344	8	0
52	2	300	0	64	5	0
53	3	802	0	705	83	0
54	4	268	0	285	6	0
55	5	5090	0	4915	426	0
56	6	485	0	104	3	0
57	7	125	0	27	0	0
58	8	400	0	86	2	0
59	K	94	0	79	0	0
60	B	1	0	0	0	0
60	C	1	0	0	0	0
60	I	1	0	0	0	0
60	P	1	0	0	0	0
60	V	1	0	0	0	0
60	g	1	0	0	0	0
60	u	146	0	0	0	0
60	v	5	0	0	0	0
60	w	2	0	0	0	0
61	g	1	0	0	0	0
61	j	1	0	0	0	0
61	m	1	0	0	1	0
61	o	1	0	0	2	0
61	p	1	0	0	0	0
62	5	43	0	0	24	0
All	All	152114	0	111761	3313	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 13.

All (3313) 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)
53:3:92:PHE:CE1	53:3:96:MET:CE	1.78	1.63
48:x:66:ARG:HH22	48:x:70:ALA:CA	1.06	1.63
48:x:157:VAL:HB	50:z:80:PHE:CZ	1.28	1.62
48:x:157:VAL:CG1	50:z:80:PHE:CD2	1.76	1.61
53:3:92:PHE:CZ	53:3:96:MET:CE	1.84	1.61
24:Y:93:THR:HG22	48:x:26:ILE:CD1	1.30	1.61
48:x:157:VAL:CB	50:z:80:PHE:CE2	1.75	1.57
53:3:92:PHE:CE1	53:3:96:MET:HE2	1.33	1.55
48:x:185:THR:CB	49:y:50:ILE:HD12	1.38	1.53
55:5:86:GLY:C	55:5:256:PHE:CZ	1.86	1.50
30:e:2:ALA:CB	42:r:130:ARG:NH1	1.75	1.50
49:y:67:GLY:CA	53:3:70:ARG:CB	1.86	1.50
55:5:504:ASP:CB	55:5:688:LEU:HG	1.40	1.49
55:5:86:GLY:C	55:5:256:PHE:HZ	1.11	1.49
48:x:157:VAL:HG12	50:z:80:PHE:CD2	1.33	1.48
24:Y:93:THR:CG2	48:x:26:ILE:HD13	1.40	1.47
48:x:46:CYS:C	49:y:58:HIS:HE1	1.21	1.46
37:l:21:ARG:NH1	48:x:273:ARG:CZ	1.79	1.44
48:x:157:VAL:CG1	50:z:80:PHE:CZ	1.94	1.44
48:x:175:LEU:CG	48:x:461:PHE:O	1.65	1.43
53:3:92:PHE:CE1	53:3:96:MET:SD	2.09	1.43
48:x:186:ASN:OD1	49:y:50:ILE:CG2	1.64	1.43
48:x:66:ARG:HD2	48:x:72:ASN:ND2	1.19	1.42
55:5:348:SER:HB3	55:5:598:TRP:CZ2	1.53	1.42
48:x:48:ILE:CB	49:y:61:ILE:HD12	0.95	1.41
55:5:521:LYS:CE	55:5:523:MET:HE2	1.47	1.41
48:x:61:PRO:O	48:x:65:MET:CB	1.69	1.41
48:x:157:VAL:CB	50:z:80:PHE:CZ	1.87	1.40
53:3:92:PHE:CD1	53:3:96:MET:HE2	1.57	1.40
37:l:21:ARG:CZ	48:x:273:ARG:NH1	1.85	1.39
37:l:21:ARG:CZ	48:x:273:ARG:HH12	1.36	1.39
55:5:127:THR:CG2	55:5:174:PHE:HD2	1.33	1.39
48:x:48:ILE:HB	49:y:61:ILE:CD1	0.92	1.38
53:3:92:PHE:CZ	53:3:96:MET:HE1	1.48	1.38
55:5:359:SER:O	55:5:363:ASP:CB	1.70	1.37
5:E:279:PRO:HG2	31:f:7:CYS:SG	1.65	1.37
48:x:184:ALA:HB3	49:y:47:MET:CG	1.16	1.37
45:u:976:G:H2'	45:u:977:C:O4'	1.25	1.36
48:x:184:ALA:CB	49:y:47:MET:HG3	1.31	1.35
55:5:214:PHE:HD1	62:5:801:9UB:C05	1.36	1.35
48:x:46:CYS:C	49:y:58:HIS:CE1	2.04	1.35
55:5:214:PHE:CD1	62:5:801:9UB:C05	2.09	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:52:PHE:HB2	55:5:530:TYR:CG	1.65	1.32
55:5:359:SER:O	55:5:363:ASP:HB2	1.14	1.32
55:5:590:SER:OG	55:5:591:ASP:N	1.58	1.31
48:x:199:THR:HG22	53:3:57:PRO:CB	1.59	1.31
48:x:66:ARG:CD	48:x:72:ASN:ND2	1.94	1.30
23:X:156:ILE:HD11	48:x:415:ARG:NH1	1.45	1.29
48:x:61:PRO:C	48:x:65:MET:CE	1.98	1.29
55:5:87:THR:N	55:5:256:PHE:HZ	1.27	1.29
48:x:199:THR:CG2	53:3:57:PRO:CB	2.10	1.29
55:5:157:TYR:CE1	55:5:173:ILE:HD13	1.67	1.29
55:5:209:TRP:CZ2	62:5:801:9UB:C19	2.02	1.29
55:5:127:THR:HG23	55:5:174:PHE:CD2	1.68	1.28
49:y:67:GLY:HA3	53:3:70:ARG:CB	1.56	1.28
55:5:168:ASN:ND2	62:5:801:9UB:C29	1.95	1.28
30:e:2:ALA:HB3	42:r:130:ARG:NH1	0.97	1.27
48:x:175:LEU:HG	48:x:461:PHE:C	1.25	1.27
55:5:30:SER:OG	55:5:124:SER:HB3	1.33	1.27
55:5:209:TRP:HZ2	62:5:801:9UB:C19	1.29	1.27
48:x:188:CYS:SG	49:y:45:ALA:HA	1.73	1.26
48:x:185:THR:HB	49:y:50:ILE:CD1	1.65	1.26
42:r:47:LYS:CG	42:r:102:TYR:HE2	1.49	1.25
45:u:2367:A:N1	45:u:2788:U:O4	1.66	1.25
23:X:156:ILE:CG2	48:x:416:TYR:OH	1.84	1.25
48:x:180:SER:OG	48:x:457:TYR:CD1	1.90	1.25
48:x:435:ALA:O	48:x:441:ILE:CD1	1.85	1.25
55:5:348:SER:HB3	55:5:598:TRP:CE2	1.71	1.24
45:u:469:C:O2	45:u:688:U:H1'	1.36	1.24
50:z:74:LEU:O	50:z:78:LEU:CD1	1.85	1.24
5:E:126:ARG:NH1	45:u:712:C:H1'	1.50	1.24
48:x:180:SER:OG	48:x:457:TYR:CG	1.78	1.23
48:x:185:THR:CB	49:y:50:ILE:CD1	2.13	1.23
48:x:66:ARG:NH2	48:x:70:ALA:HA	0.91	1.23
45:u:4213:A:N1	45:u:4218:U:O4	1.72	1.22
55:5:127:THR:CG2	55:5:174:PHE:CD2	2.20	1.22
55:5:175:CYS:SG	55:5:204:TYR:HD2	1.60	1.22
55:5:214:PHE:HD1	62:5:801:9UB:C06	1.51	1.22
48:x:46:CYS:O	49:y:58:HIS:HE1	1.13	1.22
48:x:188:CYS:SG	49:y:48:GLY:N	2.01	1.21
5:E:202:VAL:HG13	5:E:256:LYS:NZ	1.55	1.21
48:x:62:PHE:HA	48:x:65:MET:SD	1.79	1.21
55:5:357:TRP:O	55:5:360:TYR:C	1.80	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:93:THR:CG2	48:x:26:ILE:HG21	1.71	1.21
50:z:68:VAL:CG1	50:z:70:PRO:O	1.89	1.21
45:u:2468:U:O4	45:u:2473:A:N1	1.73	1.20
12:M:116:LYS:CG	14:O:196:LEU:HD21	1.72	1.20
48:x:435:ALA:O	48:x:441:ILE:HD13	1.04	1.19
55:5:52:PHE:CG	55:5:530:TYR:CZ	2.31	1.19
45:u:1929:A:N1	45:u:2054:U:O4	1.75	1.19
48:x:46:CYS:SG	48:x:77:MET:HG3	1.82	1.19
48:x:153:ILE:O	48:x:157:VAL:HG23	1.35	1.19
45:u:1958:A:H5''	45:u:1962:A:O2'	1.03	1.19
48:x:244:ASN:ND2	48:x:439:GLY:O	1.74	1.19
23:X:156:ILE:HG21	48:x:416:TYR:OH	1.35	1.18
45:u:692:A:O3'	45:u:693:C:P	2.00	1.18
33:h:38:GLY:N	48:x:266:PRO:HG3	1.58	1.18
55:5:590:SER:O	55:5:591:ASP:CB	1.90	1.18
9:I:191:ILE:CD1	9:I:200:ILE:HD12	1.74	1.17
48:x:176:GLY:HA2	48:x:457:TYR:O	1.43	1.17
48:x:437:PHE:HD2	48:x:438:LEU:CD2	1.58	1.17
55:5:357:TRP:CA	55:5:360:TYR:HB2	1.73	1.17
43:s:14:PHE:CE2	43:s:62:ARG:CD	2.28	1.16
55:5:71:TRP:O	55:5:83:ILE:HG12	1.45	1.16
55:5:346:ILE:O	55:5:349:VAL:HG12	1.44	1.16
48:x:124:THR:OG1	48:x:156:PHE:HE1	1.26	1.16
50:z:68:VAL:HG12	50:z:70:PRO:O	1.43	1.16
48:x:186:ASN:OD1	49:y:50:ILE:HG21	1.18	1.16
48:x:184:ALA:CB	49:y:47:MET:CG	1.96	1.15
55:5:71:TRP:O	55:5:83:ILE:CG1	1.95	1.15
5:E:254:LEU:HD23	5:E:257:ILE:HD11	1.24	1.15
11:L:163:LYS:HE2	45:u:509:A:H4'	1.16	1.15
43:s:14:PHE:CD2	43:s:62:ARG:CD	2.29	1.15
48:x:185:THR:OG1	49:y:50:ILE:CD1	1.94	1.15
48:x:66:ARG:NH2	48:x:70:ALA:CA	1.76	1.15
55:5:399:PHE:CG	62:5:801:9UB:C03	2.19	1.15
48:x:180:SER:OG	48:x:457:TYR:CD2	1.99	1.14
55:5:522:VAL:HG11	55:5:532:ILE:HG21	1.18	1.14
5:E:202:VAL:HG13	5:E:256:LYS:HZ2	1.05	1.14
48:x:124:THR:OG1	48:x:156:PHE:CE1	1.97	1.14
55:5:513:ARG:HD2	55:5:535:MET:O	1.46	1.14
23:X:156:ILE:CD1	48:x:415:ARG:NH1	2.11	1.14
48:x:61:PRO:C	48:x:65:MET:SD	2.30	1.14
48:x:180:SER:CB	48:x:457:TYR:CD1	2.30	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:86:GLY:HA2	55:5:256:PHE:CE1	1.82	1.13
45:u:1958:A:C5'	45:u:1962:A:O2'	1.96	1.13
48:x:184:ALA:HB3	49:y:47:MET:HG2	1.30	1.13
48:x:443:SER:HB3	48:x:447:ILE:CD1	1.78	1.13
55:5:245:CYS:SG	56:6:65:UNK:CB	2.36	1.13
55:5:504:ASP:HB2	55:5:688:LEU:HG	1.26	1.13
42:r:97:ILE:HG21	42:r:107:ARG:HB2	1.19	1.13
45:u:472:C:N3	45:u:473:C:C4	2.16	1.13
5:E:59:TYR:CD2	5:E:64:LEU:HD12	1.83	1.12
7:G:156:VAL:HG11	7:G:184:LEU:HD12	1.29	1.12
42:r:47:LYS:CG	42:r:102:TYR:CE2	2.33	1.12
42:r:47:LYS:HG2	42:r:102:TYR:HE2	1.07	1.11
51:1:443:VAL:CG2	52:2:65:UNK:CB	2.27	1.11
43:s:14:PHE:CD2	43:s:62:ARG:HD3	1.85	1.11
48:x:50:LEU:CD1	50:z:88:HIS:HA	1.80	1.11
48:x:50:LEU:HD12	50:z:88:HIS:HA	1.11	1.11
55:5:399:PHE:CD1	62:5:801:9UB:C03	2.34	1.11
55:5:51:TYR:CD2	55:5:531:GLN:HG2	1.86	1.11
48:x:173:TYR:CE1	48:x:461:PHE:CE1	2.19	1.10
55:5:52:PHE:CD1	55:5:530:TYR:CE1	2.39	1.10
49:y:67:GLY:HA2	53:3:70:ARG:CB	1.65	1.10
55:5:521:LYS:HE2	55:5:523:MET:HE2	1.33	1.10
5:E:226:GLY:N	42:r:135:LYS:HD3	1.65	1.09
48:x:47:GLN:N	49:y:58:HIS:CE1	2.21	1.09
55:5:348:SER:CB	55:5:598:TRP:CZ2	2.35	1.09
55:5:601:ARG:HB2	55:5:613:LYS:NZ	1.67	1.09
48:x:66:ARG:NH1	48:x:69:LEU:O	1.84	1.09
55:5:52:PHE:CB	55:5:530:TYR:CD2	2.35	1.09
55:5:357:TRP:HA	55:5:360:TYR:CB	1.82	1.09
53:3:92:PHE:CZ	53:3:96:MET:SD	2.41	1.09
5:E:126:ARG:HH11	45:u:712:C:C1'	1.67	1.08
9:I:191:ILE:HD11	9:I:200:ILE:HD12	1.29	1.08
48:x:121:MET:CE	48:x:156:PHE:CD1	2.36	1.08
55:5:504:ASP:HB3	55:5:688:LEU:HG	1.09	1.08
5:E:279:PRO:CG	31:f:7:CYS:SG	2.40	1.08
48:x:33:LEU:HD12	53:3:118:PHE:CD1	1.88	1.08
5:E:126:ARG:NH1	45:u:712:C:C1'	2.15	1.08
5:E:202:VAL:CG1	5:E:256:LYS:NZ	2.17	1.08
48:x:47:GLN:CA	49:y:58:HIS:NE2	2.16	1.08
30:e:2:ALA:CB	42:r:130:ARG:HH11	1.48	1.07
9:I:191:ILE:HD12	9:I:200:ILE:CD1	1.84	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:37:ILE:HD11	53:3:121:LEU:HD21	1.11	1.07
48:x:185:THR:HB	49:y:50:ILE:HD12	1.08	1.07
55:5:399:PHE:CE1	62:5:801:9UB:C03	2.24	1.07
12:M:116:LYS:HG3	14:O:196:LEU:HD21	1.33	1.07
48:x:33:LEU:CD1	53:3:118:PHE:CD1	2.37	1.07
48:x:121:MET:HE1	48:x:156:PHE:CD1	1.88	1.07
9:I:191:ILE:CD1	9:I:200:ILE:CD1	2.33	1.07
5:E:202:VAL:CG1	5:E:256:LYS:HZ2	1.68	1.07
11:L:42:ARG:NH1	11:L:51:ALA:O	1.88	1.06
23:X:156:ILE:OXT	48:x:415:ARG:NH2	1.87	1.06
48:x:46:CYS:O	49:y:58:HIS:CE1	2.01	1.06
53:3:115:LEU:HA	53:3:119:LEU:HD11	1.36	1.06
48:x:46:CYS:HB3	49:y:54:VAL:HG12	1.21	1.06
48:x:157:VAL:HG13	50:z:80:PHE:HE2	0.91	1.06
55:5:87:THR:N	55:5:256:PHE:CZ	2.11	1.06
42:r:118:LEU:HA	42:r:121:GLN:HE21	1.19	1.06
42:r:120:SER:N	42:r:122:LYS:HZ2	1.52	1.06
55:5:590:SER:C	55:5:591:ASP:CG	2.22	1.06
53:3:88:LEU:HD22	53:3:88:LEU:H	1.21	1.06
55:5:214:PHE:CD1	62:5:801:9UB:C06	2.35	1.06
43:s:14:PHE:CD2	43:s:62:ARG:HD2	1.91	1.06
55:5:86:GLY:HA2	55:5:256:PHE:HE1	0.99	1.06
48:x:61:PRO:C	48:x:65:MET:HB3	1.81	1.05
55:5:175:CYS:SG	55:5:204:TYR:CD2	2.48	1.05
48:x:66:ARG:HD2	48:x:72:ASN:CG	1.82	1.05
5:E:62:LYS:HE3	45:u:978:G:OP1	1.57	1.05
23:X:156:ILE:CD1	48:x:415:ARG:HH12	1.68	1.05
55:5:358:SER:O	55:5:362:PHE:HB3	1.54	1.05
50:z:74:LEU:O	50:z:78:LEU:HD13	1.51	1.05
51:1:443:VAL:HG23	52:2:65:UNK:CB	1.85	1.05
55:5:596:PHE:O	55:5:600:VAL:HG23	1.54	1.05
24:Y:93:THR:HG23	48:x:26:ILE:HG21	1.06	1.04
48:x:437:PHE:HD2	48:x:438:LEU:HD23	1.18	1.04
55:5:168:ASN:HD21	62:5:801:9UB:C29	1.62	1.04
55:5:130:VAL:HG23	55:5:177:LEU:HD12	1.30	1.04
45:u:2409:U:C4	45:u:2783:A:N1	2.25	1.04
53:3:92:PHE:CE2	53:3:96:MET:HE1	1.93	1.04
5:E:126:ARG:HH11	45:u:712:C:H1'	0.94	1.04
45:u:471:A:C6	45:u:472:C:C6	2.46	1.04
48:x:47:GLN:C	49:y:58:HIS:NE2	2.15	1.04
55:5:52:PHE:CD2	55:5:530:TYR:CZ	2.46	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:37:ILE:HD11	53:3:121:LEU:CD2	1.88	1.03
48:x:47:GLN:H	48:x:75:THR:HB	1.19	1.03
48:x:62:PHE:CA	48:x:65:MET:SD	2.47	1.03
48:x:200:THR:OG1	48:x:208:GLU:OE1	1.54	1.03
43:s:14:PHE:CE1	45:u:1960:A:C2	2.46	1.03
55:5:526:TRP:CE3	55:5:544:ASN:HA	1.92	1.03
55:5:590:SER:O	55:5:591:ASP:HB3	1.59	1.03
43:s:14:PHE:HE2	43:s:62:ARG:CG	1.72	1.03
48:x:188:CYS:SG	49:y:45:ALA:CA	2.46	1.03
5:E:62:LYS:NZ	45:u:978:G:OP2	1.91	1.02
48:x:437:PHE:C	48:x:438:LEU:HD23	1.84	1.02
55:5:590:SER:C	55:5:591:ASP:OD1	2.02	1.02
42:r:97:ILE:CG2	42:r:107:ARG:HB2	1.88	1.02
55:5:30:SER:HG	55:5:124:SER:HB3	0.97	1.02
9:I:184:MET:HE2	9:I:190:LEU:HG	1.40	1.02
48:x:61:PRO:C	48:x:65:MET:HE3	1.46	1.02
45:u:3751:G:C2'	45:u:3752:C:H5'	1.90	1.01
48:x:157:VAL:CB	50:z:80:PHE:HE2	1.34	1.01
48:x:157:VAL:HG11	50:z:80:PHE:CD2	1.61	1.01
53:3:42:PHE:HB2	53:3:91:SER:HB2	1.05	1.01
45:u:470:A:C5	45:u:471:A:C8	2.47	1.01
45:u:472:C:C2	45:u:473:C:C5	2.48	1.01
48:x:42:PHE:HD1	48:x:45:CYS:HB2	1.26	1.01
55:5:504:ASP:CB	55:5:688:LEU:CG	2.37	1.01
48:x:175:LEU:HG	48:x:461:PHE:O	0.84	1.01
55:5:123:PHE:CG	55:5:171:ILE:HG22	1.96	1.01
5:E:62:LYS:CE	45:u:978:G:P	2.49	1.01
42:r:47:LYS:HD2	42:r:102:TYR:CD2	1.94	1.01
42:r:119:ARG:C	42:r:122:LYS:HZ2	1.68	1.01
48:x:443:SER:HB3	48:x:447:ILE:CG1	1.90	1.01
55:5:31:PHE:CE2	55:5:121:PRO:HB2	1.96	1.01
55:5:359:SER:O	55:5:363:ASP:HB3	1.60	1.01
55:5:590:SER:CB	55:5:591:ASP:N	2.23	1.01
5:E:225:GLU:C	42:r:135:LYS:HD3	1.85	1.00
45:u:205:C:O2'	45:u:2305:U:H5	1.44	1.00
48:x:443:SER:HB3	48:x:447:ILE:HG13	1.42	1.00
23:X:156:ILE:HG21	48:x:416:TYR:HH	1.23	1.00
48:x:47:GLN:CA	49:y:58:HIS:CE1	2.45	1.00
48:x:437:PHE:CD2	48:x:438:LEU:CD2	2.44	1.00
51:1:443:VAL:HG22	52:2:65:UNK:CB	1.91	1.00
55:5:51:TYR:HD2	55:5:531:GLN:HG2	1.26	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:s:14:PHE:HE2	43:s:62:ARG:HG3	1.22	1.00
55:5:504:ASP:HB3	55:5:688:LEU:CG	1.89	1.00
9:I:184:MET:HE2	9:I:190:LEU:CD1	1.91	1.00
55:5:279:ILE:O	55:5:283:VAL:HG23	1.62	0.99
55:5:590:SER:O	55:5:591:ASP:CG	2.04	0.99
9:I:202:ASN:O	46:v:63:C:C5	2.15	0.99
55:5:83:ILE:O	55:5:85:GLY:N	1.96	0.99
5:E:126:ARG:NH1	45:u:712:C:C2'	2.26	0.99
48:x:175:LEU:CG	48:x:461:PHE:C	2.01	0.99
55:5:521:LYS:CE	55:5:523:MET:CE	2.41	0.99
55:5:526:TRP:HE3	55:5:544:ASN:HA	1.20	0.99
50:z:69:GLY:N	50:z:70:PRO:CD	2.25	0.98
55:5:123:PHE:CD1	55:5:171:ILE:HG22	1.95	0.98
48:x:185:THR:OG1	49:y:50:ILE:HD12	1.59	0.98
55:5:86:GLY:CA	55:5:256:PHE:CE1	2.46	0.98
42:r:47:LYS:CD	42:r:102:TYR:CE2	2.47	0.97
48:x:189:GLU:OE1	49:y:50:ILE:CG2	2.02	0.97
48:x:180:SER:O	48:x:454:ILE:HD11	1.64	0.97
53:3:92:PHE:HE1	53:3:96:MET:SD	1.60	0.97
55:5:130:VAL:CG2	55:5:177:LEU:HD12	1.93	0.97
45:u:470:A:C6	45:u:471:A:C8	2.52	0.97
48:x:66:ARG:CZ	48:x:66:ARG:HA	1.94	0.97
48:x:186:ASN:CG	49:y:50:ILE:HG21	1.88	0.97
55:5:52:PHE:HB2	55:5:530:TYR:CD1	2.00	0.97
55:5:123:PHE:CD2	55:5:171:ILE:HG22	1.96	0.97
55:5:348:SER:CB	55:5:598:TRP:CE2	2.48	0.97
5:E:62:LYS:CE	45:u:978:G:OP2	2.13	0.97
55:5:52:PHE:HB2	55:5:530:TYR:CD2	1.94	0.97
10:J:80:GLU:OE2	10:J:170:TYR:OH	1.82	0.96
45:u:77:U:O4	45:u:335:A:N1	1.98	0.96
43:s:14:PHE:CE1	45:u:1960:A:N3	2.33	0.96
48:x:437:PHE:CD2	48:x:438:LEU:HD21	2.00	0.96
45:u:1968:G:H1	45:u:2018:C:H42	1.12	0.96
23:X:84:GLU:N	48:x:403:GLY:O	1.97	0.96
55:5:127:THR:HG22	55:5:174:PHE:CD2	1.97	0.96
48:x:48:ILE:CG2	49:y:61:ILE:HD12	1.96	0.96
48:x:180:SER:HB3	48:x:457:TYR:CD1	2.01	0.96
2:B:163:LEU:HD21	2:B:182:GLU:CG	1.95	0.95
48:x:42:PHE:CD1	48:x:45:CYS:HB2	2.00	0.95
45:u:1278:C:H3'	45:u:1279:A:H4'	1.48	0.95
55:5:214:PHE:HA	62:5:801:9UB:C06	1.94	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:2:ALA:O	42:r:130:ARG:NH2	1.98	0.95
45:u:1983:A:N1	45:u:2008:U:O4	2.00	0.95
9:I:184:MET:HE2	9:I:190:LEU:CG	1.95	0.95
33:h:38:GLY:HA3	48:x:266:PRO:HB3	1.49	0.95
45:u:471:A:C5	45:u:472:C:C6	2.55	0.95
45:u:4278:C:HO2'	45:u:4281:A:H8	1.06	0.95
48:x:61:PRO:O	48:x:65:MET:HB3	0.78	0.95
12:M:116:LYS:HG2	14:O:196:LEU:HD21	1.49	0.95
45:u:1983:A:N1	45:u:2008:U:C4	2.35	0.95
48:x:47:GLN:O	48:x:75:THR:CB	2.15	0.95
55:5:31:PHE:CZ	55:5:121:PRO:HB2	1.55	0.95
55:5:521:LYS:HE3	55:5:523:MET:HE2	1.46	0.95
45:u:3751:G:O2'	45:u:3752:C:H5'	1.65	0.95
45:u:2409:U:O4	45:u:2783:A:N1	1.99	0.95
2:B:163:LEU:CD2	2:B:182:GLU:HG2	1.96	0.94
5:E:126:ARG:NH1	45:u:712:C:O2'	2.00	0.94
45:u:957:G:H1'	45:u:958:G:OP2	1.67	0.94
55:5:127:THR:HG23	55:5:174:PHE:HD2	0.78	0.94
48:x:47:GLN:HA	49:y:58:HIS:CE1	2.02	0.94
55:5:601:ARG:HB2	55:5:613:LYS:HZ2	1.24	0.94
38:m:99:CYS:HG	61:m:201:ZN:ZN	0.71	0.94
48:x:50:LEU:HD12	50:z:88:HIS:CA	1.97	0.94
53:3:42:PHE:HB2	53:3:91:SER:CB	1.95	0.94
55:5:52:PHE:HB3	55:5:530:TYR:CD2	2.01	0.94
42:r:32:LEU:HD11	42:r:106:LEU:HD12	1.48	0.94
45:u:472:C:N4	45:u:473:C:N4	2.16	0.94
55:5:86:GLY:O	55:5:256:PHE:CZ	2.19	0.94
55:5:30:SER:OG	55:5:124:SER:CB	2.13	0.94
48:x:66:ARG:CD	48:x:72:ASN:CG	2.38	0.94
42:r:98:ARG:HH22	42:r:107:ARG:HH12	1.12	0.94
45:u:1958:A:H5''	45:u:1962:A:HO2'	1.21	0.94
45:u:1929:A:H61	45:u:2054:U:H3	1.10	0.93
5:E:126:ARG:HH12	45:u:712:C:C2'	1.80	0.93
48:x:66:ARG:NE	48:x:72:ASN:HB3	1.83	0.93
48:x:186:ASN:OD1	49:y:50:ILE:HG22	1.66	0.93
48:x:180:SER:OG	48:x:457:TYR:CE1	2.21	0.93
48:x:33:LEU:HD11	53:3:122:PHE:CE1	2.04	0.93
33:h:37:THR:C	48:x:266:PRO:HG3	1.93	0.93
48:x:62:PHE:N	48:x:65:MET:SD	2.41	0.93
55:5:601:ARG:CB	55:5:613:LYS:NZ	2.32	0.93
55:5:590:SER:O	55:5:591:ASP:N	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:156:ILE:HD11	48:x:415:ARG:HH12	1.14	0.92
48:x:46:CYS:HA	48:x:75:THR:OG1	1.69	0.92
48:x:66:ARG:NH2	48:x:70:ALA:C	2.26	0.92
55:5:524:SER:OG	55:5:579:LEU:O	1.88	0.92
40:o:77:CYS:HG	61:o:201:ZN:ZN	0.62	0.92
5:E:279:PRO:HG2	31:f:7:CYS:HG	1.28	0.92
55:5:178:LEU:HD23	55:5:179:THR:N	1.84	0.92
23:X:156:ILE:HG23	48:x:416:TYR:OH	1.67	0.92
45:u:469:C:O2	45:u:688:U:C1'	2.17	0.92
48:x:37:ILE:CD1	53:3:121:LEU:HD21	1.99	0.92
45:u:2468:U:N3	45:u:2473:A:N6	2.17	0.92
55:5:86:GLY:C	55:5:256:PHE:CE1	2.47	0.92
4:D:200:MET:HE2	4:D:241:LYS:HE3	1.50	0.92
42:r:47:LYS:HG2	42:r:102:TYR:CE2	1.98	0.92
2:B:163:LEU:CD2	2:B:182:GLU:CG	2.48	0.91
45:u:472:C:C2	45:u:473:C:C6	2.58	0.91
45:u:472:C:C4	45:u:473:C:N4	2.38	0.91
53:3:42:PHE:CB	53:3:91:SER:HB2	1.98	0.91
9:I:48:LEU:HD21	9:I:145:LYS:HG2	1.48	0.91
42:r:98:ARG:NH2	42:r:107:ARG:NH1	2.17	0.91
48:x:48:ILE:HB	49:y:61:ILE:HD11	1.50	0.91
55:5:175:CYS:HG	55:5:204:TYR:HD2	1.08	0.91
30:e:2:ALA:HB3	42:r:130:ARG:CZ	2.01	0.91
45:u:466:A:C2	45:u:467:U:C5	2.58	0.91
45:u:976:G:C2'	45:u:977:C:O4'	2.17	0.91
55:5:280:HIS:O	55:5:284:ASP:OD2	1.88	0.91
42:r:98:ARG:NH2	42:r:107:ARG:HH12	1.66	0.91
48:x:157:VAL:HG13	50:z:80:PHE:CE2	1.66	0.91
55:5:52:PHE:CG	55:5:530:TYR:CE1	2.56	0.91
55:5:357:TRP:HA	55:5:360:TYR:HB2	0.92	0.91
48:x:42:PHE:HE1	48:x:45:CYS:HG	1.11	0.90
42:r:47:LYS:CD	42:r:102:TYR:CD2	2.54	0.90
42:r:118:LEU:HA	42:r:121:GLN:NE2	1.87	0.90
43:s:14:PHE:CE2	43:s:62:ARG:HG3	2.06	0.90
45:u:1958:A:O2'	45:u:1959:U:H5''	1.71	0.90
55:5:52:PHE:CB	55:5:530:TYR:CG	2.51	0.90
55:5:521:LYS:NZ	55:5:523:MET:HE2	1.86	0.90
9:I:191:ILE:HD12	9:I:200:ILE:HD11	1.52	0.90
55:5:157:TYR:HE1	55:5:173:ILE:HD13	1.05	0.90
24:Y:93:THR:HG23	48:x:26:ILE:CG2	1.98	0.90
55:5:345:ILE:HD11	55:5:595:LYS:HD3	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:66:ARG:HH21	48:x:70:ALA:HA	1.34	0.90
55:5:130:VAL:HG23	55:5:177:LEU:CD1	2.02	0.90
2:B:174:ARG:NH1	45:u:4985:U:O2	2.04	0.90
43:s:14:PHE:CE2	43:s:62:ARG:HD3	2.01	0.90
48:x:175:LEU:CD1	48:x:461:PHE:O	2.18	0.90
50:z:74:LEU:O	50:z:78:LEU:HD12	1.70	0.90
43:s:14:PHE:HE1	45:u:1960:A:N3	1.70	0.90
45:u:102:G:O2'	45:u:1381:U:O2'	1.90	0.90
42:r:119:ARG:HG3	42:r:122:LYS:HE3	1.54	0.89
43:s:14:PHE:HD2	43:s:62:ARG:CD	1.84	0.89
55:5:168:ASN:HD22	62:5:801:9UB:C29	1.78	0.89
55:5:214:PHE:CE1	62:5:801:9UB:C05	2.55	0.89
48:x:46:CYS:SG	48:x:77:MET:CG	2.60	0.89
2:B:156:TYR:CD1	45:u:4909:A:H2'	2.08	0.89
42:r:47:LYS:HB3	42:r:102:TYR:CE2	2.07	0.89
45:u:390:C:H4'	48:x:23:GLU:CD	1.97	0.89
48:x:189:GLU:OE1	49:y:50:ILE:HG22	1.69	0.89
42:r:107:ARG:HD2	42:r:108:MET:N	1.87	0.89
45:u:211:G:C2	45:u:212:A:C8	2.60	0.89
5:E:251:SER:O	5:E:255:PRO:CD	2.20	0.89
53:3:93:LEU:HD23	53:3:137:VAL:HG22	1.52	0.89
50:z:68:VAL:HG13	50:z:70:PRO:O	1.71	0.89
55:5:52:PHE:CG	55:5:530:TYR:CE2	2.60	0.89
55:5:157:TYR:CE1	55:5:173:ILE:CD1	2.55	0.89
55:5:31:PHE:CZ	55:5:121:PRO:CB	2.38	0.88
43:s:14:PHE:HE2	43:s:62:ARG:CD	1.82	0.88
5:E:62:LYS:CE	45:u:978:G:OP1	2.21	0.88
55:5:597:LEU:H	55:5:597:LEU:HD12	1.39	0.88
45:u:689:U:N3	45:u:690:C:C5	2.42	0.88
53:3:115:LEU:HA	53:3:119:LEU:CD1	2.02	0.88
48:x:46:CYS:HB3	49:y:54:VAL:CG1	2.04	0.88
55:5:346:ILE:O	55:5:349:VAL:CG1	2.22	0.88
48:x:48:ILE:HD11	49:y:65:ILE:HG12	1.53	0.88
48:x:191:ILE:CD1	49:y:44:PHE:HZ	1.86	0.88
48:x:47:GLN:O	48:x:75:THR:HB	1.74	0.88
48:x:48:ILE:HB	49:y:61:ILE:CG1	2.01	0.88
48:x:157:VAL:HG11	50:z:80:PHE:CZ	1.84	0.88
55:5:521:LYS:HE3	55:5:523:MET:HB3	1.56	0.88
33:h:38:GLY:CA	48:x:266:PRO:HB3	2.04	0.88
45:u:205:C:O2'	45:u:2305:U:C5	2.26	0.88
48:x:47:GLN:C	48:x:75:THR:HG22	1.99	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:521:LYS:HE2	55:5:523:MET:CE	2.03	0.87
42:r:47:LYS:CB	42:r:102:TYR:CE2	2.58	0.87
55:5:52:PHE:CZ	55:5:82:ARG:NH1	2.42	0.87
42:r:103:HIS:ND1	42:r:106:LEU:HD23	1.89	0.87
48:x:48:ILE:CG1	49:y:61:ILE:HD12	2.04	0.87
55:5:590:SER:C	55:5:591:ASP:N	2.33	0.87
7:G:156:VAL:HG11	7:G:184:LEU:CD1	2.05	0.87
5:E:238:ILE:O	5:E:239:THR:OG1	1.93	0.86
43:s:14:PHE:CE2	43:s:62:ARG:HD2	2.06	0.86
11:L:163:LYS:CE	45:u:509:A:H4'	2.05	0.86
48:x:153:ILE:O	48:x:157:VAL:CG2	2.23	0.86
45:u:2027:U:O2'	45:u:2028:C:H5'	1.76	0.86
48:x:443:SER:CB	48:x:447:ILE:CD1	2.54	0.86
55:5:52:PHE:CD2	55:5:530:TYR:CE2	2.63	0.86
45:u:1279:A:H3'	45:u:1280:C:H5''	1.57	0.86
5:E:254:LEU:CD2	5:E:257:ILE:HD11	2.05	0.86
48:x:180:SER:OG	48:x:457:TYR:CE2	2.28	0.86
45:u:470:A:N6	45:u:471:A:C5	2.44	0.86
42:r:135:LYS:NZ	45:u:451:C:H2'	1.90	0.85
45:u:472:C:C4	45:u:473:C:C4	2.64	0.85
55:5:52:PHE:CB	55:5:530:TYR:CE2	2.58	0.85
9:I:49:CYS:SG	9:I:51:HIS:NE2	2.48	0.85
42:r:47:LYS:O	42:r:103:HIS:CD2	2.28	0.85
48:x:66:ARG:CZ	48:x:69:LEU:O	2.24	0.85
30:e:2:ALA:O	42:r:130:ARG:NH1	2.10	0.85
55:5:86:GLY:CA	55:5:256:PHE:HE1	1.82	0.85
55:5:118:PHE:O	55:5:121:PRO:HD2	1.76	0.85
48:x:47:GLN:N	48:x:75:THR:HB	1.91	0.85
4:D:200:MET:HE1	4:D:241:LYS:HG3	1.57	0.85
45:u:2526:C:O4'	48:x:405:ARG:NH2	2.10	0.85
5:E:225:GLU:OE2	42:r:135:LYS:N	2.10	0.85
45:u:1279:A:C3'	45:u:1280:C:H5''	2.07	0.85
45:u:1956:A:O2'	45:u:1957:U:H5'	1.77	0.85
53:3:53:ILE:HD11	55:5:354:PRO:CG	2.07	0.85
33:h:38:GLY:CA	48:x:266:PRO:HG3	2.07	0.85
30:e:2:ALA:CA	42:r:130:ARG:NH1	2.40	0.84
37:l:21:ARG:CZ	48:x:273:ARG:CZ	2.43	0.84
45:u:1957:U:O2'	45:u:1958:A:C8	2.29	0.84
48:x:33:LEU:HD11	53:3:118:PHE:CD1	2.12	0.84
48:x:47:GLN:N	49:y:58:HIS:NE2	2.22	0.84
55:5:395:THR:HG23	62:5:801:9UB:C01	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:180:SER:CB	48:x:457:TYR:CE1	2.60	0.84
53:3:92:PHE:CE2	53:3:96:MET:CE	2.57	0.84
48:x:42:PHE:HE1	48:x:45:CYS:SG	2.00	0.84
48:x:33:LEU:HD11	53:3:122:PHE:CZ	2.12	0.83
47:w:79:G:OP1	49:y:31:LYS:NZ	2.11	0.83
42:r:135:LYS:NZ	45:u:451:C:C2'	2.42	0.83
43:s:14:PHE:HD2	43:s:62:ARG:HD3	1.37	0.83
49:y:67:GLY:N	53:3:70:ARG:CB	2.41	0.83
50:z:71:VAL:HG13	50:z:74:LEU:HD12	1.61	0.83
30:e:2:ALA:O	42:r:130:ARG:CZ	2.27	0.82
48:x:46:CYS:CB	49:y:54:VAL:HG12	2.08	0.82
55:5:157:TYR:OH	55:5:173:ILE:HD12	1.78	0.82
5:E:62:LYS:HE2	45:u:978:G:P	2.17	0.82
48:x:121:MET:HE3	48:x:156:PHE:CD1	2.13	0.82
55:5:254:ILE:O	55:5:257:VAL:O	1.97	0.82
5:E:94:GLY:HA3	45:u:686:A:N7	1.95	0.82
55:5:601:ARG:HB3	55:5:613:LYS:HG3	1.61	0.82
4:D:33:ARG:NH2	46:v:7:G:O3'	2.13	0.82
45:u:472:C:N3	45:u:473:C:C5	2.48	0.82
42:r:119:ARG:O	42:r:122:LYS:HE3	1.80	0.82
24:Y:93:THR:CG2	48:x:26:ILE:CD1	2.20	0.81
45:u:470:A:C5	45:u:471:A:N7	2.48	0.81
45:u:1367:C:C2	45:u:1370:G:H2'	2.15	0.81
5:E:62:LYS:HE2	45:u:978:G:OP2	1.79	0.81
48:x:48:ILE:HD12	49:y:61:ILE:CG1	2.10	0.81
53:3:53:ILE:CD1	55:5:354:PRO:CG	2.58	0.81
4:D:200:MET:HE1	4:D:241:LYS:CG	2.10	0.81
7:G:87:LEU:HD23	7:G:184:LEU:CD2	2.10	0.81
23:X:84:GLU:H	48:x:403:GLY:C	1.88	0.81
45:u:690:C:N3	45:u:691:C:C5	2.48	0.81
53:3:53:ILE:HD11	55:5:354:PRO:HG3	1.62	0.81
5:E:157:ARG:O	5:E:178:ASN:ND2	2.13	0.81
48:x:47:GLN:H	48:x:75:THR:CB	1.92	0.81
12:M:81:ASP:OD1	12:M:84:THR:HG23	1.80	0.81
42:r:135:LYS:HD2	42:r:135:LYS:O	1.80	0.81
55:5:544:ASN:O	55:5:546:THR:HG22	1.79	0.81
45:u:390:C:H4'	48:x:23:GLU:OE1	1.80	0.81
48:x:180:SER:HB3	48:x:457:TYR:CE1	2.16	0.81
55:5:52:PHE:CE2	55:5:530:TYR:OH	2.33	0.81
7:G:86:VAL:HG21	7:G:185:LYS:HE3	1.62	0.80
42:r:122:LYS:HB2	42:r:123:PRO:CD	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:690:C:C2	45:u:691:C:C6	2.69	0.80
48:x:199:THR:HG23	53:3:57:PRO:CB	2.10	0.80
48:x:443:SER:HB3	48:x:447:ILE:HD11	1.62	0.80
48:x:121:MET:HE1	48:x:156:PHE:HD1	1.46	0.80
55:5:52:PHE:HZ	55:5:82:ARG:HH11	1.29	0.80
55:5:212:TYR:HE2	55:5:257:VAL:HG21	1.45	0.80
2:B:163:LEU:HD21	2:B:182:GLU:HG3	1.61	0.80
7:G:86:VAL:HG12	7:G:87:LEU:N	1.96	0.80
5:E:251:SER:O	5:E:255:PRO:HD2	1.81	0.80
42:r:135:LYS:HZ1	45:u:451:C:H2'	1.45	0.80
45:u:463:A:N1	45:u:692:A:C2	2.49	0.80
55:5:212:TYR:CE2	55:5:257:VAL:HG21	2.16	0.80
55:5:525:TRP:CE3	55:5:599:MET:HE2	2.17	0.80
2:B:156:TYR:CE1	45:u:4909:A:H2'	2.16	0.80
45:u:1379:C:H4'	45:u:1380:G:O4'	1.81	0.80
55:5:211:GLY:O	55:5:214:PHE:HB3	1.82	0.80
45:u:2395:A:O2'	45:u:2806:A:H1'	1.82	0.80
55:5:30:SER:OG	55:5:34:ARG:NH2	2.15	0.80
45:u:1929:A:N6	45:u:2054:U:H3	1.80	0.79
7:G:87:LEU:HD23	7:G:184:LEU:HD21	1.64	0.79
30:e:2:ALA:C	42:r:130:ARG:HH12	1.90	0.79
45:u:957:G:N2	45:u:959:G:O6	2.15	0.79
48:x:66:ARG:HH22	48:x:70:ALA:C	1.86	0.79
48:x:47:GLN:N	48:x:75:THR:CB	2.45	0.79
48:x:48:ILE:HD12	49:y:61:ILE:CB	2.13	0.79
48:x:48:ILE:HD12	49:y:61:ILE:HG13	1.62	0.79
48:x:173:TYR:CD1	48:x:461:PHE:CE1	2.60	0.79
53:3:141:MET:SD	55:5:357:TRP:HZ3	2.06	0.79
55:5:513:ARG:CD	55:5:535:MET:O	2.29	0.79
9:I:202:ASN:O	46:v:63:C:C4	2.34	0.79
47:w:55:U:O4	47:w:62:A:N1	2.16	0.79
45:u:919:C:N4	45:u:920:C:C4	2.51	0.79
2:B:163:LEU:HD23	2:B:182:GLU:HG2	1.64	0.79
45:u:4723:A:H2'	45:u:4724:A:C8	2.18	0.79
53:3:53:ILE:CD1	55:5:354:PRO:HG2	2.13	0.79
45:u:212:A:H2'	45:u:213:G:H8	1.47	0.79
45:u:688:U:N3	45:u:689:U:C6	2.50	0.79
48:x:33:LEU:HD11	53:3:118:PHE:HD1	1.46	0.78
55:5:88:LEU:HD12	55:5:256:PHE:HB3	1.63	0.78
5:E:279:PRO:CD	31:f:7:CYS:SG	2.71	0.78
45:u:2026:A:C2'	45:u:2027:U:H5'	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:3751:G:H2'	45:u:3752:C:H5'	1.65	0.78
48:x:157:VAL:CG1	50:z:80:PHE:CE2	0.73	0.78
45:u:1213:G:C6	45:u:1215:C:C2	2.72	0.78
48:x:437:PHE:CD2	48:x:438:LEU:HD23	2.10	0.78
55:5:122:LEU:HD12	55:5:122:LEU:O	1.83	0.78
45:u:216:C:H5	45:u:217:C:O2	1.65	0.78
55:5:126:PHE:C	55:5:174:PHE:HE2	1.92	0.78
2:B:163:LEU:HD21	2:B:182:GLU:HG2	1.59	0.78
43:s:14:PHE:CE1	45:u:1960:A:H2	2.02	0.78
33:h:38:GLY:HA3	48:x:266:PRO:CB	2.13	0.78
2:B:36:ASP:OD2	2:B:39:LYS:HE2	1.83	0.78
45:u:2769:U:C2	45:u:2770:C:C5	2.72	0.78
48:x:33:LEU:CD1	53:3:122:PHE:CE1	2.67	0.78
24:Y:59:ARG:NH2	45:u:200:U:O2'	2.17	0.77
42:r:119:ARG:O	42:r:122:LYS:CE	2.32	0.77
45:u:745:G:H2'	45:u:746:A:O4'	1.83	0.77
45:u:77:U:N3	45:u:335:A:N6	2.32	0.77
48:x:42:PHE:CD1	48:x:45:CYS:CB	2.67	0.77
50:z:69:GLY:N	50:z:70:PRO:HD2	1.97	0.77
53:3:86:GLU:OE1	55:5:357:TRP:NE1	2.15	0.77
55:5:52:PHE:HZ	55:5:82:ARG:NH1	1.81	0.77
15:P:127:ARG:NH2	45:u:2422:C:OP1	2.17	0.77
45:u:504:G:N1	45:u:654:C:C2	2.52	0.77
48:x:185:THR:CA	49:y:50:ILE:HD12	2.14	0.77
55:5:178:LEU:HD21	55:5:201:ALA:HB1	1.65	0.77
4:D:35:ARG:HB2	45:u:4325:A:C2	2.20	0.77
55:5:357:TRP:O	55:5:361:TYR:N	2.18	0.77
55:5:601:ARG:CB	55:5:613:LYS:HZ3	1.95	0.77
42:r:122:LYS:HB2	42:r:123:PRO:HD2	1.66	0.77
45:u:3723:A:H2'	45:u:3724:A:C8	2.20	0.77
48:x:180:SER:OG	48:x:457:TYR:CZ	2.38	0.77
53:3:114:LYS:O	53:3:119:LEU:HG	1.85	0.77
9:I:191:ILE:HD11	9:I:200:ILE:CD1	2.08	0.76
55:5:504:ASP:HB2	55:5:688:LEU:CG	2.10	0.76
45:u:466:A:C2	45:u:467:U:C6	2.73	0.76
48:x:48:ILE:CA	49:y:61:ILE:CD1	2.62	0.76
42:r:119:ARG:C	42:r:122:LYS:NZ	2.43	0.76
48:x:48:ILE:CA	49:y:61:ILE:HD12	2.10	0.76
53:3:93:LEU:O	53:3:133:PHE:CE1	2.38	0.76
5:E:226:GLY:N	42:r:135:LYS:CD	2.46	0.76
42:r:119:ARG:HG3	42:r:122:LYS:CE	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:173:TYR:CE1	48:x:461:PHE:HE1	2.00	0.76
55:5:522:VAL:CG1	55:5:532:ILE:HG21	2.09	0.76
9:I:184:MET:CE	9:I:190:LEU:CD1	2.64	0.76
55:5:168:ASN:HD21	62:5:801:9UB:P26	2.07	0.76
45:u:209:U:C4	45:u:211:G:C8	2.74	0.76
45:u:2793:G:C6	45:u:2797:C:C4	2.73	0.76
43:s:14:PHE:CE2	43:s:62:ARG:CG	2.57	0.76
48:x:184:ALA:HB2	48:x:454:ILE:CD1	2.16	0.75
51:1:540:UNK:O	51:1:541:UNK:CB	2.34	0.75
52:2:75:UNK:O	52:2:76:UNK:CB	2.33	0.75
55:5:86:GLY:CA	55:5:256:PHE:CZ	2.69	0.75
45:u:470:A:N6	45:u:471:A:C4	2.55	0.75
45:u:504:G:C2	45:u:654:C:O2	2.39	0.75
55:5:357:TRP:O	55:5:360:TYR:CA	2.34	0.75
48:x:443:SER:CB	48:x:447:ILE:HD11	2.16	0.75
45:u:2468:U:C4	45:u:2473:A:N1	2.54	0.75
55:5:87:THR:HA	62:5:801:9UB:O38	1.87	0.75
55:5:345:ILE:CD1	55:5:595:LYS:HD3	2.16	0.75
3:C:159:GLU:OE1	3:C:159:GLU:N	2.20	0.75
42:r:118:LEU:CA	42:r:121:GLN:HE21	1.98	0.75
45:u:211:G:C2	45:u:212:A:N7	2.55	0.75
5:E:202:VAL:CG1	5:E:256:LYS:HZ1	1.97	0.75
48:x:176:GLY:H	48:x:461:PHE:HD2	1.31	0.75
48:x:443:SER:N	48:x:447:ILE:HD12	2.02	0.74
55:5:157:TYR:HE1	55:5:173:ILE:CD1	1.93	0.74
42:r:97:ILE:HG21	42:r:107:ARG:CB	2.11	0.74
55:5:31:PHE:CD2	55:5:121:PRO:HB2	2.23	0.74
48:x:47:GLN:C	48:x:75:THR:CG2	2.59	0.74
48:x:176:GLY:N	48:x:461:PHE:CD2	2.45	0.74
45:u:208:A:N1	45:u:233:U:C2	2.55	0.74
55:5:348:SER:HB3	55:5:598:TRP:HZ2	1.44	0.74
48:x:66:ARG:HD2	48:x:72:ASN:HD22	0.92	0.74
55:5:525:TRP:HB2	55:5:592:ASP:OD2	1.88	0.74
50:z:71:VAL:N	50:z:72:PRO:HD2	2.02	0.74
55:5:34:ARG:CZ	55:5:124:SER:OG	2.36	0.74
55:5:357:TRP:C	55:5:360:TYR:HB2	2.12	0.74
3:C:158:VAL:HA	3:C:161:TYR:CE2	2.22	0.74
45:u:688:U:C4	45:u:689:U:C5	2.75	0.74
55:5:52:PHE:CD1	55:5:530:TYR:CZ	2.73	0.74
55:5:72:PHE:HA	55:5:83:ILE:HG12	1.69	0.74
7:G:86:VAL:HG11	7:G:185:LYS:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:120:SER:HA	42:r:122:LYS:NZ	2.02	0.74
45:u:1279:A:H3'	45:u:1280:C:C5'	2.18	0.74
9:I:184:MET:CE	9:I:190:LEU:HG	2.16	0.74
23:X:156:ILE:HG13	48:x:415:ARG:CZ	2.16	0.74
48:x:66:ARG:NH2	48:x:69:LEU:O	2.20	0.74
48:x:157:VAL:CB	50:z:80:PHE:HZ	1.59	0.74
11:L:116:ARG:NH1	11:L:155:MET:O	2.21	0.73
48:x:29:LYS:O	53:3:118:PHE:HE1	1.68	0.73
42:r:47:LYS:HD2	42:r:102:TYR:HD2	1.50	0.73
48:x:444:GLY:O	48:x:446:GLY:N	2.21	0.73
50:z:74:LEU:C	50:z:78:LEU:HD13	2.12	0.73
55:5:525:TRP:CD1	55:5:595:LYS:HD2	2.24	0.73
55:5:590:SER:O	55:5:591:ASP:CA	2.37	0.73
55:5:597:LEU:HD12	55:5:597:LEU:N	2.04	0.73
43:s:10:LYS:NZ	45:u:1960:A:O2'	2.20	0.73
24:Y:93:THR:CG2	48:x:26:ILE:CG2	2.62	0.73
30:e:2:ALA:CB	42:r:130:ARG:CZ	2.64	0.73
48:x:185:THR:HG23	49:y:47:MET:SD	2.27	0.73
55:5:468:LEU:O	55:5:471:TYR:HB3	1.89	0.73
55:5:521:LYS:HD2	55:5:575:VAL:HA	1.68	0.73
45:u:22:G:N2	47:w:35:C:C2	2.56	0.73
45:u:467:U:N3	45:u:468:U:C5	2.56	0.73
45:u:3914:U:H3	45:u:4378:A:N6	1.86	0.73
45:u:2779:C:O2'	47:w:112:G:OP1	2.05	0.73
30:e:117:GLN:O	42:r:122:LYS:HD3	1.88	0.73
53:3:92:PHE:CG	53:3:96:MET:HE2	2.21	0.72
33:h:38:GLY:CA	48:x:266:PRO:CB	2.68	0.72
42:r:135:LYS:HZ3	45:u:451:C:C2'	2.02	0.72
45:u:212:A:H2'	45:u:213:G:C8	2.24	0.72
55:5:123:PHE:CD2	55:5:170:GLY:O	2.43	0.72
55:5:524:SER:OG	55:5:579:LEU:C	2.33	0.72
55:5:544:ASN:O	55:5:546:THR:CG2	2.36	0.72
11:L:161:PHE:CE1	26:a:105:ARG:HG3	2.24	0.72
45:u:1280:C:C4	45:u:1282:G:C6	2.77	0.72
55:5:157:TYR:OH	55:5:173:ILE:CD1	2.37	0.72
55:5:177:LEU:C	55:5:177:LEU:HD13	2.15	0.72
53:3:90:SER:OG	55:5:357:TRP:NE1	2.22	0.72
55:5:593:ILE:HD13	55:5:639:MET:HG3	1.70	0.72
48:x:48:ILE:HD11	49:y:65:ILE:CG1	2.20	0.72
48:x:185:THR:O	49:y:50:ILE:HB	1.88	0.72
45:u:690:C:C4	45:u:691:C:C5	2.77	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:48:ILE:HD12	49:y:61:ILE:HB	1.72	0.72
45:u:1278:C:C3'	45:u:1279:A:H4'	2.18	0.71
45:u:1724:G:H4'	45:u:1725:U:OP2	1.89	0.71
45:u:3914:U:H3	45:u:4378:A:H61	1.37	0.71
2:B:261:ARG:HE	45:u:3870:C:H4'	1.55	0.71
5:E:254:LEU:HD22	5:E:258:LYS:HE3	1.72	0.71
45:u:2632:U:H2'	45:u:2633:U:C6	2.25	0.71
2:B:163:LEU:CD2	2:B:182:GLU:HG3	2.17	0.71
45:u:166:C:O2	45:u:166:C:H2'	1.90	0.71
45:u:977:C:C2'	45:u:978:G:H5'	2.20	0.71
42:r:120:SER:HA	42:r:122:LYS:HZ3	1.56	0.71
45:u:2026:A:O2'	45:u:2027:U:H5'	1.90	0.71
7:G:86:VAL:CG1	7:G:87:LEU:H	2.04	0.71
30:e:2:ALA:CB	42:r:130:ARG:HH12	2.01	0.71
45:u:2367:A:N1	45:u:2788:U:C4	2.57	0.71
5:E:217:GLN:NE2	5:E:233:LYS:HD2	2.05	0.71
23:X:147:LEU:CD2	49:y:20:ARG:HH22	2.03	0.71
3:C:157:LYS:O	3:C:160:GLY:N	2.20	0.71
45:u:516:C:C2	45:u:646:G:N2	2.59	0.71
45:u:977:C:C2	45:u:978:G:C8	2.79	0.71
30:e:30:LYS:NZ	45:u:2347:A:N3	2.39	0.71
45:u:956:A:H4'	45:u:957:G:OP2	1.89	0.71
53:3:88:LEU:HD22	53:3:88:LEU:N	2.02	0.71
7:G:87:LEU:CD2	7:G:184:LEU:HD21	2.20	0.71
48:x:430:ALA:O	48:x:433:VAL:HB	1.91	0.71
7:G:156:VAL:CG1	7:G:184:LEU:HD12	2.14	0.70
9:I:191:ILE:CD1	9:I:200:ILE:HD11	2.14	0.70
43:s:34:ASN:OD1	45:u:1969:G:P	2.49	0.70
48:x:191:ILE:HD11	49:y:44:PHE:HZ	1.55	0.70
45:u:4075:U:O2'	45:u:4076:G:H2'	1.91	0.70
50:z:69:GLY:N	50:z:70:PRO:HD3	2.06	0.70
42:r:130:ARG:HD2	42:r:130:ARG:C	2.17	0.70
45:u:723:A:C2	45:u:943:A:N1	2.59	0.70
45:u:1958:A:H4'	45:u:1962:A:H1'	1.72	0.70
48:x:42:PHE:CE1	48:x:45:CYS:SG	2.84	0.70
48:x:66:ARG:NH2	48:x:66:ARG:HA	2.07	0.70
30:e:91:CYS:O	30:e:93:LYS:N	2.25	0.70
48:x:47:GLN:O	48:x:75:THR:CG2	2.39	0.70
55:5:257:VAL:HG12	55:5:261:PRO:HD3	1.72	0.70
5:E:62:LYS:HE3	45:u:978:G:P	2.23	0.70
45:u:1279:A:C2'	45:u:1280:C:H5''	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:4481:U:H2'	45:u:4482:U:C6	2.27	0.70
55:5:601:ARG:CB	55:5:613:LYS:HZ2	1.95	0.70
45:u:181:C:N3	45:u:256:G:C2	2.59	0.70
45:u:4371:G:O2'	45:u:4372:U:OP2	2.05	0.70
48:x:69:LEU:HB2	48:x:80:GLY:HA2	1.74	0.70
48:x:157:VAL:HG11	50:z:80:PHE:CE2	0.87	0.70
48:x:185:THR:CG2	49:y:46:ILE:HG22	2.22	0.70
55:5:52:PHE:CD2	55:5:530:TYR:OH	2.44	0.70
5:E:251:SER:O	5:E:255:PRO:HD3	1.91	0.70
45:u:499:G:N2	45:u:656:C:C2	2.60	0.70
45:u:2367:A:N6	45:u:2788:U:H3	1.88	0.70
48:x:185:THR:HB	49:y:50:ILE:HD11	1.70	0.70
35:j:59:THR:O	47:w:42:G:OP1	2.10	0.70
45:u:211:G:H4'	45:u:234:G:C8	2.27	0.70
48:x:64:TRP:CD1	48:x:64:TRP:H	2.06	0.70
48:x:66:ARG:HD3	48:x:72:ASN:ND2	2.00	0.69
45:u:1929:A:N1	45:u:2054:U:C4	2.59	0.69
45:u:2773:G:N2	45:u:2774:C:C2	2.60	0.69
48:x:438:LEU:HD23	48:x:438:LEU:N	2.03	0.69
53:3:88:LEU:H	53:3:88:LEU:CD2	2.00	0.69
5:E:225:GLU:C	42:r:135:LYS:CD	2.62	0.69
9:I:187:GLU:OE1	9:I:189:ARG:NE	2.25	0.69
45:u:1991:A:N6	45:u:2003:G:OP1	2.25	0.69
55:5:134:LEU:HD13	55:5:177:LEU:HD21	1.74	0.69
55:5:424:GLN:NE2	55:5:428:THR:OG1	2.26	0.69
55:5:521:LYS:HE3	55:5:523:MET:CB	2.23	0.69
45:u:4510:A:O2'	45:u:4511:A:O4'	2.11	0.69
45:u:4901:G:N2	45:u:4921:C:C2	2.60	0.69
55:5:52:PHE:HB3	55:5:530:TYR:CE2	2.24	0.69
55:5:601:ARG:HB3	55:5:613:LYS:CG	2.22	0.69
45:u:499:G:C2	45:u:656:C:C2	2.81	0.69
45:u:2367:A:N6	45:u:2788:U:N3	2.40	0.69
48:x:33:LEU:HD12	53:3:118:PHE:CE1	2.27	0.69
48:x:47:GLN:O	48:x:75:THR:HG22	1.93	0.69
50:z:78:LEU:HD12	50:z:78:LEU:N	2.07	0.69
53:3:129:LEU:O	53:3:133:PHE:HB3	1.92	0.69
33:h:38:GLY:CA	48:x:266:PRO:CG	2.71	0.69
45:u:208:A:H3'	45:u:209:U:H5''	1.73	0.69
48:x:30:GLU:CD	53:3:118:PHE:N	2.36	0.69
55:5:71:TRP:O	55:5:83:ILE:CD1	2.40	0.69
45:u:468:U:O2	45:u:469:C:O4'	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:21:ARG:CZ	48:x:273:ARG:NH2	2.56	0.69
45:u:482:G:H2'	45:u:483:G:C8	2.27	0.69
50:z:79:LEU:C	50:z:79:LEU:HD23	2.18	0.69
55:5:522:VAL:CG1	55:5:532:ILE:HD13	2.22	0.69
9:I:87:ILE:HG12	9:I:138:ILE:HG12	1.74	0.69
45:u:197:A:N1	45:u:225:G:O2'	2.24	0.69
55:5:157:TYR:CZ	55:5:173:ILE:HD13	2.26	0.69
55:5:597:LEU:H	55:5:597:LEU:CD1	2.06	0.69
37:l:21:ARG:HH12	48:x:273:ARG:NH1	0.52	0.69
45:u:469:C:H2'	45:u:470:A:O4'	1.93	0.69
45:u:1635:C:H2'	45:u:1636:U:H5'	1.75	0.69
48:x:185:THR:C	49:y:50:ILE:HD12	2.18	0.69
7:G:86:VAL:HG12	7:G:87:LEU:H	1.55	0.68
37:l:21:ARG:NH1	48:x:273:ARG:NH1	0.72	0.68
45:u:200:U:C4	45:u:238:C:O4'	2.46	0.68
48:x:47:GLN:N	48:x:75:THR:CG2	2.56	0.68
23:X:83:THR:HA	48:x:403:GLY:HA2	1.74	0.68
45:u:1367:C:N3	45:u:1369:C:OP2	2.26	0.68
48:x:157:VAL:HB	50:z:80:PHE:HZ	0.72	0.68
35:j:34:CYS:SG	35:j:36:LYS:HB3	2.33	0.68
48:x:248:THR:OG1	48:x:440:ALA:C	2.17	0.68
45:u:465:G:C2	45:u:466:A:C8	2.82	0.68
45:u:1968:G:H1	45:u:2018:C:N4	1.89	0.68
48:x:48:ILE:HG13	48:x:49:PRO:HD2	1.75	0.68
4:D:69:ILE:HD11	19:T:28:ALA:HB1	1.75	0.68
39:n:13:LEU:HD11	39:n:17:ARG:CZ	2.23	0.68
45:u:978:G:H2'	45:u:979:C:O4'	1.92	0.68
33:h:38:GLY:HA3	48:x:266:PRO:CG	2.24	0.68
42:r:118:LEU:HD12	42:r:121:GLN:NE2	2.08	0.68
48:x:48:ILE:CB	49:y:61:ILE:CD1	1.86	0.68
55:5:601:ARG:HH11	55:5:601:ARG:CG	2.07	0.68
3:C:271:ALA:O	3:C:272:SER:OG	2.11	0.68
45:u:680:G:C2	45:u:681:G:C8	2.82	0.68
55:5:395:THR:CG2	62:5:801:9UB:C02	2.71	0.68
42:r:122:LYS:HD2	42:r:122:LYS:N	2.09	0.68
45:u:1958:A:O2'	45:u:1959:U:C5'	2.41	0.68
30:e:2:ALA:CA	42:r:130:ARG:HH12	2.03	0.67
45:u:209:U:C5	45:u:211:G:C8	2.82	0.67
45:u:1358:G:H8	45:u:1358:G:H3'	1.58	0.67
48:x:47:GLN:N	48:x:75:THR:HG21	2.07	0.67
50:z:78:LEU:HD12	50:z:78:LEU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:53:ILE:HD12	55:5:354:PRO:HG2	1.74	0.67
4:D:23:ARG:NH2	45:u:4280:A:OP2	2.27	0.67
45:u:166:C:O2	45:u:167:C:H5	1.76	0.67
45:u:504:G:C6	45:u:654:C:N3	2.61	0.67
3:C:210:ILE:HG21	3:C:252:TRP:CZ3	2.30	0.67
48:x:78:GLU:HG2	48:x:155:LEU:HD22	1.75	0.67
55:5:521:LYS:NZ	55:5:523:MET:CE	2.55	0.67
3:C:313:VAL:HG11	6:F:172:THR:HG21	1.76	0.67
42:r:120:SER:N	42:r:122:LYS:NZ	2.37	0.67
45:u:497:G:N2	45:u:657:C:C2	2.62	0.67
45:u:642:G:N2	45:u:643:C:C2	2.62	0.67
55:5:402:VAL:HG23	55:5:403:MET:HG2	1.76	0.67
37:l:21:ARG:HH11	48:x:273:ARG:NH1	1.23	0.67
45:u:973:G:N2	45:u:1282:G:O2'	2.28	0.67
45:u:4453:C:C2	45:u:4529:G:C2	2.82	0.67
48:x:45:CYS:HB3	48:x:77:MET:SD	2.35	0.67
55:5:348:SER:HB3	55:5:598:TRP:NE1	2.08	0.67
24:Y:93:THR:HG22	48:x:26:ILE:CG1	2.21	0.67
45:u:2288:G:N2	45:u:2290:C:C2	2.63	0.67
48:x:191:ILE:CD1	49:y:44:PHE:CZ	2.75	0.67
55:5:395:THR:CG2	62:5:801:9UB:C01	2.72	0.67
30:e:2:ALA:C	42:r:130:ARG:NH1	2.52	0.67
48:x:78:GLU:HG2	48:x:155:LEU:CD2	2.25	0.67
48:x:406:GLU:OE1	48:x:407:THR:N	2.27	0.67
55:5:220:PRO:O	55:5:223:VAL:HB	1.94	0.67
42:r:123:PRO:HG2	42:r:126:VAL:HB	1.74	0.67
42:r:130:ARG:HD2	42:r:130:ARG:O	1.93	0.67
45:u:1264:C:H2'	45:u:1265:G:O4'	1.95	0.67
45:u:166:C:O2	45:u:167:C:C5	2.48	0.67
50:z:72:PRO:O	50:z:76:MET:N	2.27	0.67
55:5:51:TYR:CE2	55:5:531:GLN:HG2	2.30	0.67
45:u:217:C:H3'	45:u:218:A:H4'	1.77	0.66
55:5:31:PHE:HZ	55:5:118:PHE:O	1.78	0.66
42:r:107:ARG:HD2	42:r:107:ARG:C	2.19	0.66
45:u:2409:U:C4	45:u:2783:A:C2	2.83	0.66
5:E:161:LEU:HD21	5:E:253:ILE:HD11	1.76	0.66
6:F:245:LEU:HD23	6:F:249:MET:HG3	1.77	0.66
8:H:95:VAL:HG22	38:m:82:LEU:HD22	1.76	0.66
45:u:22:G:C2	47:w:35:C:N3	2.64	0.66
45:u:471:A:C6	45:u:472:C:C5	2.83	0.66
45:u:1268:G:H4'	45:u:1269:G:OP1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:2468:U:H3	45:u:2473:A:N6	1.91	0.66
55:5:65:PHE:H	55:5:69:HIS:HB3	1.59	0.66
55:5:525:TRP:HE1	55:5:595:LYS:HD3	1.58	0.66
5:E:225:GLU:HA	42:r:135:LYS:HE2	1.76	0.66
55:5:507:GLU:OE2	55:5:685:GLU:HG3	1.96	0.66
45:u:723:A:H2	45:u:943:A:N1	1.93	0.66
48:x:175:LEU:HG	48:x:462:VAL:N	2.04	0.66
45:u:691:C:C2	45:u:692:A:C8	2.84	0.66
45:u:3752:C:O2'	45:u:3753:G:OP2	2.09	0.66
55:5:157:TYR:CZ	55:5:173:ILE:CD1	2.78	0.66
10:J:83:LEU:HD12	10:J:170:TYR:CZ	2.31	0.66
45:u:2258:C:O2	45:u:2258:C:H2'	1.96	0.66
45:u:2826:U:H4'	45:u:2827:G:H5'	1.77	0.66
48:x:185:THR:CB	49:y:50:ILE:HD11	2.19	0.66
12:M:116:LYS:HG3	14:O:196:LEU:CD2	2.20	0.66
45:u:466:A:N1	45:u:467:U:C4	2.65	0.66
45:u:1957:U:C2'	45:u:1958:A:C8	2.79	0.66
48:x:66:ARG:HD2	48:x:72:ASN:CB	2.25	0.66
7:G:86:VAL:CG1	7:G:87:LEU:N	2.57	0.65
45:u:680:G:C4	45:u:681:G:C8	2.85	0.65
45:u:1958:A:H3'	45:u:1958:A:OP2	1.96	0.65
48:x:29:LYS:O	53:3:118:PHE:CE1	2.42	0.65
48:x:47:GLN:O	48:x:75:THR:HA	1.96	0.65
4:D:200:MET:CE	4:D:241:LYS:HE3	2.26	0.65
45:u:1378:C:H3'	45:u:1379:C:C5'	2.26	0.65
55:5:50:PRO:HB3	55:5:166:TYR:HB3	1.79	0.65
2:B:120:LYS:N	45:u:4968:A:OP1	2.28	0.65
5:E:59:TYR:CD2	5:E:64:LEU:CD1	2.73	0.65
45:u:1358:G:C6	45:u:1379:C:N3	2.64	0.65
45:u:1359:G:H2'	45:u:1360:G:C8	2.30	0.65
45:u:1635:C:C2'	45:u:1636:U:H5'	2.26	0.65
11:L:56:ARG:O	11:L:116:ARG:NH2	2.28	0.65
45:u:220:C:H3'	45:u:220:C:OP1	1.96	0.65
2:B:14:LEU:HD23	2:B:17:LEU:HD21	1.77	0.65
25:Z:52:LYS:O	25:Z:65:ARG:NH2	2.29	0.65
42:r:119:ARG:C	42:r:122:LYS:CE	2.70	0.65
45:u:1879:C:O2'	45:u:1891:A:N3	2.29	0.65
48:x:174:GLY:HA2	48:x:461:PHE:CE2	2.31	0.65
10:J:83:LEU:HD12	10:J:170:TYR:OH	1.96	0.65
55:5:214:PHE:CA	62:5:801:9UB:C06	2.71	0.65
42:r:47:LYS:HD2	42:r:102:TYR:CE2	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:v:30:C:C2	46:v:48:G:N2	2.65	0.65
48:x:47:GLN:HA	49:y:58:HIS:NE2	2.01	0.65
48:x:346:SER:O	48:x:360:HIS:NE2	2.29	0.65
55:5:528:TYR:CE2	55:5:581:ILE:HD12	2.32	0.65
2:B:254:ILE:HG23	2:B:266:VAL:HG11	1.78	0.65
42:r:32:LEU:CD1	42:r:106:LEU:HD12	2.24	0.65
45:u:1404:G:C2	45:u:1414:C:C2	2.85	0.65
48:x:48:ILE:CD1	49:y:61:ILE:HB	2.26	0.65
55:5:167:ASP:OD2	55:5:405:ARG:NH1	2.30	0.65
9:I:184:MET:CE	9:I:190:LEU:HD11	2.27	0.64
37:l:21:ARG:NH1	48:x:273:ARG:NH2	2.41	0.64
45:u:1969:G:O2'	45:u:1970:A:H5'	1.97	0.64
45:u:5066:U:H2'	45:u:5067:U:C6	2.32	0.64
55:5:178:LEU:HD23	55:5:178:LEU:C	2.21	0.64
2:B:45:ALA:HB3	2:B:183:ILE:HG23	1.79	0.64
9:I:184:MET:HG2	9:I:189:ARG:HD2	1.79	0.64
45:u:1682:A:C2	45:u:1683:U:C2	2.85	0.64
55:5:51:TYR:HD2	55:5:531:GLN:CG	2.05	0.64
45:u:200:U:O4	45:u:238:C:C1'	2.46	0.64
37:l:21:ARG:HH11	48:x:273:ARG:HH12	0.72	0.64
45:u:206:U:O2	45:u:208:A:C8	2.51	0.64
45:u:986:C:C2	45:u:1068:G:N2	2.65	0.64
45:u:1358:G:H3'	45:u:1358:G:C8	2.32	0.64
45:u:2084:C:H3'	45:u:2085:G:C5'	2.27	0.64
50:z:71:VAL:CG1	50:z:74:LEU:HD12	2.27	0.64
55:5:286:LEU:O	55:5:287:ARG:CB	2.42	0.64
45:u:976:G:H4'	45:u:976:G:OP1	1.98	0.64
45:u:1957:U:O2'	45:u:1958:A:H8	1.78	0.64
48:x:189:GLU:HA	49:y:52:PHE:H	1.61	0.64
5:E:225:GLU:CA	42:r:135:LYS:HE2	2.28	0.64
45:u:209:U:C5	45:u:211:G:N7	2.66	0.64
45:u:211:G:N3	45:u:212:A:C8	2.66	0.64
45:u:471:A:C2	45:u:472:C:C1'	2.80	0.64
45:u:690:C:N3	45:u:691:C:C6	2.66	0.64
48:x:47:GLN:O	48:x:75:THR:CA	2.46	0.64
3:C:158:VAL:HA	3:C:161:TYR:CD2	2.33	0.64
26:a:4:ARG:NH2	45:u:2341:A:OP2	2.31	0.64
42:r:135:LYS:HZ1	45:u:451:C:C2'	2.09	0.64
45:u:470:A:C6	45:u:471:A:N9	2.65	0.64
48:x:78:GLU:OE2	48:x:155:LEU:O	2.14	0.64
48:x:187:ILE:HG22	49:y:44:PHE:CE1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:471:A:C5	45:u:472:C:C5	2.85	0.64
45:u:1380:G:O2'	45:u:1381:U:O2	2.10	0.64
48:x:62:PHE:HB2	48:x:72:ASN:HD22	1.63	0.64
48:x:184:ALA:HB3	49:y:47:MET:HG3	0.64	0.64
7:G:86:VAL:HG13	7:G:183:ILE:O	1.98	0.64
17:R:36:ASN:ND2	48:x:407:THR:CG2	2.60	0.64
45:u:4213:A:N1	45:u:4218:U:C4	2.61	0.64
48:x:192:VAL:HG11	49:y:52:PHE:HB2	1.76	0.64
48:x:437:PHE:O	48:x:438:LEU:HD23	1.98	0.64
24:Y:59:ARG:NH1	45:u:200:U:C2	2.66	0.63
48:x:157:VAL:HG12	50:z:80:PHE:CE2	0.88	0.63
55:5:118:PHE:C	55:5:121:PRO:HD2	2.23	0.63
28:c:34:THR:OG1	28:c:95:ALA:HB2	1.97	0.63
45:u:1823:G:O3'	45:u:1825:A:P	2.56	0.63
45:u:4579:U:H2'	45:u:4580:U:C6	2.33	0.63
48:x:157:VAL:HG12	50:z:80:PHE:CZ	2.00	0.63
48:x:444:GLY:O	48:x:445:THR:C	2.40	0.63
49:y:13:GLN:O	49:y:17:ASP:HB2	1.98	0.63
55:5:349:VAL:HG11	55:5:352:HIS:HD2	1.62	0.63
55:5:488:ILE:HG22	55:5:531:GLN:HE22	1.64	0.63
13:N:202:ARG:NH2	45:u:1372:A:OP1	2.32	0.63
45:u:167:C:C2	45:u:269:G:N2	2.66	0.63
45:u:3668:C:C2	45:u:3675:G:C2	2.87	0.63
48:x:48:ILE:CG1	48:x:49:PRO:HD2	2.28	0.63
5:E:279:PRO:HD2	31:f:7:CYS:SG	2.38	0.63
45:u:1213:G:N1	45:u:1215:C:C2	2.67	0.63
48:x:33:LEU:CD1	53:3:118:PHE:CE1	2.81	0.63
55:5:87:THR:CA	55:5:256:PHE:CZ	2.60	0.63
5:E:254:LEU:HD23	5:E:257:ILE:CD1	2.13	0.63
30:e:108:ARG:HH22	30:e:127:ALA:HB3	1.63	0.63
48:x:42:PHE:CE1	48:x:45:CYS:CB	2.82	0.63
16:Q:65:ARG:NH1	45:u:1502:G:OP1	2.32	0.63
45:u:202:C:C2	45:u:214:G:C2	2.87	0.63
45:u:1550:G:C2	45:u:1579:C:C2	2.86	0.63
45:u:4723:A:C2	45:u:4724:A:C6	2.86	0.63
50:z:71:VAL:N	50:z:72:PRO:CD	2.62	0.63
55:5:395:THR:HG23	62:5:801:9UB:C02	2.29	0.63
6:F:161:TYR:CE2	6:F:170:ALA:HB2	2.34	0.63
9:I:204:GLY:O	9:I:205:PRO:C	2.41	0.63
45:u:465:G:C6	45:u:466:A:N7	2.67	0.63
7:G:87:LEU:CD2	7:G:184:LEU:CD2	2.77	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:22:G:C2	47:w:35:C:C2	2.87	0.63
45:u:1378:C:H3'	45:u:1379:C:H5'	1.81	0.63
45:u:2090:U:P	45:u:2090:U:O4'	2.56	0.63
45:u:2108:G:C6	45:u:2125:C:N4	2.67	0.63
48:x:236:ARG:HH12	48:x:238:ASN:HB2	1.64	0.63
11:L:65:ARG:HG2	11:L:66:TYR:CE2	2.34	0.62
45:u:468:U:O4	45:u:687:U:O4	2.17	0.62
45:u:2268:A:H4'	45:u:2269:C:H5'	1.80	0.62
55:5:175:CYS:HB3	55:5:205:MET:HB2	1.80	0.62
45:u:199:G:C4	45:u:201:C:C5	2.87	0.62
45:u:688:U:C4	45:u:689:U:C6	2.87	0.62
48:x:61:PRO:O	48:x:65:MET:CG	2.44	0.62
3:C:32:ILE:HD12	3:C:130:ALA:HB2	1.82	0.62
45:u:1983:A:C6	45:u:2008:U:O4	2.52	0.62
45:u:2409:U:O4	45:u:2783:A:C6	2.52	0.62
45:u:3900:G:N2	45:u:4562:C:C2	2.67	0.62
48:x:67:VAL:HG12	48:x:68:ILE:HD13	1.80	0.62
55:5:524:SER:HG	55:5:579:LEU:C	1.98	0.62
14:O:201:PHE:HB2	14:O:202:LEU:HD13	1.80	0.62
42:r:47:LYS:O	42:r:103:HIS:HD2	1.78	0.62
45:u:200:U:O4	45:u:238:C:H1'	1.98	0.62
45:u:4885:U:H2'	45:u:4886:C:O4'	1.99	0.62
48:x:186:ASN:HA	49:y:50:ILE:CG2	2.29	0.62
42:r:120:SER:CA	42:r:122:LYS:HZ2	2.13	0.62
45:u:1987:C:O2	45:u:1987:C:H2'	2.00	0.62
45:u:3783:A:H4'	45:u:3784:A:H5''	1.81	0.62
45:u:470:A:N7	45:u:471:A:N7	2.48	0.62
45:u:1081:C:C2	45:u:1220:G:C2	2.87	0.62
45:u:2547:G:N2	45:u:2548:C:C2	2.68	0.62
4:D:200:MET:CE	4:D:241:LYS:HG3	2.28	0.62
48:x:267:ILE:HG21	48:x:399:MET:HB3	1.82	0.62
5:E:202:VAL:HG13	5:E:256:LYS:HZ1	1.50	0.62
45:u:504:G:C6	45:u:654:C:C2	2.87	0.62
45:u:2758:G:O2'	45:u:2764:A:N3	2.26	0.62
48:x:61:PRO:O	48:x:65:MET:SD	2.51	0.62
12:M:81:ASP:OD1	12:M:84:THR:CG2	2.47	0.62
42:r:135:LYS:NZ	45:u:451:C:H3'	2.14	0.62
45:u:1983:A:C2	45:u:2008:U:C4	2.87	0.62
48:x:193:TRP:HZ2	49:y:53:PHE:C	2.07	0.62
9:I:204:GLY:O	9:I:205:PRO:O	2.16	0.62
45:u:1186:U:H2'	45:u:1187:G:O4'	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:3765:G:O2'	45:u:3766:A:C8	2.49	0.62
48:x:443:SER:H	48:x:447:ILE:HD12	1.63	0.62
2:B:163:LEU:HD23	2:B:182:GLU:CG	2.24	0.61
48:x:66:ARG:CD	48:x:72:ASN:HB3	2.30	0.61
50:z:83:SER:O	50:z:87:LEU:HB2	2.00	0.61
55:5:123:PHE:HZ	55:5:171:ILE:O	1.77	0.61
45:u:1339:U:H2'	45:u:1340:C:C6	2.34	0.61
45:u:1723:A:N1	45:u:1838:A:C2	2.67	0.61
48:x:59:ALA:HB3	48:x:65:MET:SD	2.40	0.61
24:Y:49:ILE:HD13	24:Y:80:ILE:HD13	1.82	0.61
45:u:209:U:C5	45:u:211:G:C5	2.89	0.61
45:u:472:C:O2	45:u:473:C:C6	2.52	0.61
45:u:680:G:C2	45:u:681:G:N9	2.68	0.61
45:u:2905:C:C2	45:u:3590:G:N2	2.68	0.61
45:u:969:C:O2'	45:u:970:G:N3	2.31	0.61
48:x:66:ARG:CD	48:x:72:ASN:CB	2.79	0.61
53:3:59:VAL:HA	53:3:71:PRO:HA	1.81	0.61
55:5:525:TRP:NE1	55:5:595:LYS:HD2	2.15	0.61
5:E:95:ASP:N	45:u:686:A:C8	2.69	0.61
42:r:120:SER:CA	42:r:122:LYS:NZ	2.63	0.61
48:x:33:LEU:CD1	53:3:122:PHE:HE1	2.11	0.61
37:l:5:LYS:NZ	45:u:2407:G:N7	2.48	0.61
45:u:77:U:H3	45:u:335:A:N6	1.97	0.61
45:u:977:C:C4	45:u:978:G:N7	2.69	0.61
45:u:1999:A:H1'	45:u:2017:A:N1	2.16	0.61
45:u:2623:A:C2	45:u:2624:G:C5	2.89	0.61
45:u:3723:A:C2	45:u:3724:A:C6	2.88	0.61
45:u:4769:G:H2'	45:u:4770:U:O4'	2.00	0.61
48:x:59:ALA:CB	48:x:65:MET:SD	2.89	0.61
55:5:123:PHE:CD1	55:5:171:ILE:CG2	2.71	0.61
55:5:525:TRP:NE1	55:5:595:LYS:CD	2.64	0.61
45:u:2127:C:H2'	45:u:2128:G:C8	2.36	0.61
48:x:288:ASN:HB3	48:x:291:ILE:HB	1.83	0.61
41:p:39:CYS:SG	41:p:41:PHE:HB2	2.41	0.61
45:u:1296:G:H1'	45:u:1297:U:P	2.41	0.61
45:u:1358:G:C8	45:u:1358:G:C3'	2.84	0.61
45:u:1672:U:H2'	45:u:1673:U:C6	2.36	0.61
45:u:3662:A:H61	45:u:3680:U:H3	1.48	0.61
45:u:4411:G:C2	45:u:4432:C:C2	2.89	0.61
48:x:66:ARG:HE	48:x:72:ASN:HB3	1.66	0.61
48:x:185:THR:OG1	49:y:50:ILE:HD13	1.95	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:211:GLY:HA3	48:x:240:PRO:HG2	1.81	0.61
55:5:553:SER:O	55:5:610:LYS:NZ	2.34	0.61
3:C:114:ARG:CZ	3:C:114:ARG:HB2	2.31	0.61
45:u:472:C:C2	45:u:473:C:C4	2.81	0.61
42:r:119:ARG:C	42:r:122:LYS:HE3	2.25	0.60
45:u:181:C:C2	45:u:256:G:N2	2.69	0.60
45:u:390:C:C4'	48:x:23:GLU:OE1	2.48	0.60
45:u:1839:U:H2'	45:u:1840:G:O4'	2.00	0.60
50:z:76:MET:N	50:z:76:MET:SD	2.65	0.60
23:X:83:THR:HG22	48:x:403:GLY:O	2.00	0.60
45:u:111:C:C2	45:u:331:G:C2	2.89	0.60
45:u:1241:C:N4	45:u:1270:A:O2'	2.34	0.60
45:u:2554:U:H4'	45:u:2555:G:OP1	2.01	0.60
55:5:528:TYR:CZ	55:5:581:ILE:HD12	2.36	0.60
45:u:2367:A:C2	45:u:2788:U:O4	2.53	0.60
45:u:2616:C:C2	45:u:2722:G:C2	2.89	0.60
48:x:48:ILE:N	49:y:61:ILE:CD1	2.63	0.60
45:u:209:U:C4	45:u:211:G:N9	2.68	0.60
45:u:216:C:C5	45:u:217:C:O2	2.52	0.60
45:u:2793:G:C5	45:u:2797:C:N4	2.69	0.60
45:u:3594:C:O2	45:u:3594:C:H2'	2.01	0.60
55:5:120:ALA:N	55:5:121:PRO:CD	2.65	0.60
3:C:45:ARG:NH2	45:u:2295:C:O2'	2.35	0.60
28:c:85:CYS:SG	28:c:94:LEU:HD22	2.42	0.60
42:r:47:LYS:CD	42:r:102:TYR:HD2	2.07	0.60
45:u:1213:G:C2	45:u:1215:C:O2	2.54	0.60
45:u:5000:G:C2	45:u:5051:C:C2	2.89	0.60
55:5:126:PHE:HB3	55:5:174:PHE:CE2	2.36	0.60
55:5:525:TRP:CB	55:5:592:ASP:OD2	2.49	0.60
14:O:18:ARG:NH2	45:u:2057:A:OP1	2.35	0.60
45:u:208:A:C5	45:u:233:U:N3	2.54	0.60
45:u:515:C:C2	45:u:647:G:C2	2.90	0.60
18:S:9:GLU:HG2	18:S:33:PHE:CE2	2.36	0.60
45:u:1957:U:H2'	45:u:1958:A:H8	1.67	0.60
45:u:2045:G:O6	45:u:3870:C:O2'	2.17	0.60
45:u:4207:C:C2	45:u:4226:G:C2	2.90	0.60
24:Y:91:ASN:O	48:x:26:ILE:HG22	2.01	0.60
48:x:46:CYS:CB	49:y:54:VAL:CG1	2.73	0.60
55:5:357:TRP:O	55:5:360:TYR:O	2.18	0.60
17:R:36:ASN:HD21	48:x:407:THR:CG2	2.14	0.60
18:S:53:LYS:NZ	46:v:74:A:O2'	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:17:LEU:HD23	42:r:18:ILE:N	2.17	0.60
45:u:4092:G:N2	45:u:4158:C:C2	2.70	0.60
48:x:66:ARG:CD	48:x:72:ASN:HD22	1.82	0.60
45:u:106:A:H1'	45:u:336:A:C8	2.36	0.60
48:x:48:ILE:CB	49:y:61:ILE:HD11	2.19	0.60
48:x:97:ALA:HB2	48:x:382:VAL:HG13	1.84	0.60
48:x:121:MET:HE1	48:x:156:PHE:CG	2.36	0.60
48:x:244:ASN:O	48:x:440:ALA:HA	2.02	0.60
42:r:132:ARG:HE	42:r:133:PRO:HD2	1.67	0.59
45:u:2288:G:N1	45:u:2290:C:C4	2.70	0.59
45:u:2827:G:H2'	45:u:2827:G:N3	2.17	0.59
45:u:4283:G:N2	45:u:4284:C:C2	2.70	0.59
45:u:4892:A:N1	45:u:4927:G:O6	2.35	0.59
55:5:212:TYR:OH	55:5:257:VAL:HG23	2.01	0.59
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.83	0.59
48:x:180:SER:CB	48:x:457:TYR:CG	2.74	0.59
48:x:444:GLY:O	48:x:447:ILE:N	2.31	0.59
54:4:7:LEU:HD23	55:5:36:PHE:HB3	1.82	0.59
18:S:84:TYR:CE2	18:S:93:MET:HE3	2.37	0.59
23:X:156:ILE:CG1	48:x:415:ARG:NH1	2.66	0.59
45:u:472:C:H2'	45:u:473:C:C6	2.37	0.59
45:u:1074:G:C2	45:u:1238:A:C2	2.91	0.59
45:u:1268:G:C2	45:u:1270:A:C8	2.90	0.59
45:u:1957:U:C2'	45:u:1958:A:H8	2.14	0.59
48:x:50:LEU:HD23	48:x:50:LEU:O	2.02	0.59
55:5:257:VAL:CG1	55:5:261:PRO:HD3	2.31	0.59
1:A:207:VAL:HG11	45:u:1633:G:C6	2.37	0.59
17:R:36:ASN:HD21	48:x:407:THR:HG23	1.65	0.59
45:u:2446:C:C2	45:u:2515:G:C2	2.90	0.59
45:u:3617:G:O2'	45:u:3620:G:N7	2.35	0.59
48:x:184:ALA:HB2	48:x:454:ILE:HG13	1.84	0.59
50:z:71:VAL:O	50:z:71:VAL:HG12	2.02	0.59
16:Q:104:ARG:NH2	45:u:1353:G:N7	2.51	0.59
45:u:4901:G:C2	45:u:4921:C:N3	2.70	0.59
48:x:54:MET:HE1	49:y:62:ASN:ND2	2.17	0.59
48:x:192:VAL:HG13	49:y:52:PHE:CD1	1.83	0.59
1:A:196:TRP:O	1:A:197:PRO:C	2.46	0.59
28:c:45:LEU:HD23	28:c:96:ILE:HD12	1.83	0.59
45:u:917:A:C2	45:u:919:C:C5	2.90	0.59
45:u:4441:A:H8	45:u:4441:A:H5''	1.68	0.59
48:x:244:ASN:CG	48:x:439:GLY:O	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:421:ALA:O	48:x:425:GLY:N	2.33	0.59
56:6:106:UNK:O	56:6:110:UNK:N	2.36	0.59
45:u:286:U:H2'	45:u:287:U:C6	2.37	0.59
45:u:466:A:C2	45:u:467:U:C4	2.90	0.59
45:u:4219:A:H2'	45:u:4220:A:C8	2.37	0.59
46:v:30:C:N3	46:v:48:G:C2	2.71	0.59
47:w:83:C:H4'	47:w:85:U:O2	2.03	0.59
55:5:525:TRP:HE1	55:5:595:LYS:CD	2.16	0.59
3:C:76:ILE:HG22	3:C:77:PRO:HD2	1.84	0.59
3:C:108:TRP:HZ2	11:L:19:GLN:HE21	1.51	0.59
3:C:114:ARG:NE	45:u:1358:G:O3'	2.36	0.59
3:C:357:ALA:O	3:C:361:LYS:HG3	2.03	0.59
17:R:10:LEU:O	17:R:14:VAL:HG23	2.03	0.59
26:a:25:HIS:CG	45:u:1338:G:H22	2.21	0.59
45:u:166:C:O2	45:u:166:C:C2'	2.49	0.59
23:X:156:ILE:HD12	48:x:415:ARG:HH12	1.63	0.59
48:x:185:THR:C	49:y:50:ILE:HB	2.28	0.59
45:u:1074:G:N2	45:u:1075:G:C2	2.71	0.59
45:u:1266:G:H5''	45:u:2112:G:C2	2.37	0.59
45:u:1541:C:C2	45:u:1619:G:C2	2.90	0.59
48:x:69:LEU:CB	48:x:80:GLY:HA2	2.33	0.59
45:u:1957:U:H2'	45:u:1958:A:C8	2.38	0.58
48:x:285:TYR:OH	48:x:385:SER:O	2.20	0.58
55:5:210:GLY:O	62:5:801:9UB:C16	2.50	0.58
55:5:374:GLY:O	55:5:378:CYS:N	2.36	0.58
41:p:42:CYS:HA	45:u:2674:A:N6	2.18	0.58
45:u:4757:C:O4'	45:u:4757:C:O2	2.21	0.58
50:z:78:LEU:CD1	50:z:78:LEU:H	2.14	0.58
55:5:600:VAL:O	55:5:615:HIS:HE1	1.85	0.58
45:u:113:A:H2'	45:u:114:G:O4'	2.03	0.58
48:x:191:ILE:HD12	49:y:44:PHE:HZ	1.68	0.58
45:u:463:A:N1	45:u:692:A:H2	2.00	0.58
45:u:3709:U:O2'	45:u:3710:G:O4'	2.21	0.58
49:y:58:HIS:HA	49:y:61:ILE:HG12	1.84	0.58
55:5:122:LEU:HD12	55:5:122:LEU:C	2.26	0.58
45:u:1358:G:H2'	45:u:1359:G:O4'	2.04	0.58
45:u:2084:C:H3'	45:u:2085:G:H5'	1.84	0.58
45:u:2654:C:C2	45:u:2681:G:N2	2.71	0.58
55:5:83:ILE:C	55:5:85:GLY:N	2.62	0.58
55:5:504:ASP:OD2	55:5:686:HIS:HB2	2.03	0.58
2:B:154:LYS:HB2	2:B:154:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:226:GLY:H	42:r:135:LYS:NZ	2.01	0.58
45:u:3751:G:O2'	45:u:3752:C:C5'	2.47	0.58
53:3:92:PHE:CE1	53:3:96:MET:CG	2.86	0.58
55:5:157:TYR:HB2	55:5:411:ALA:HB1	1.85	0.58
55:5:176:MET:O	55:5:179:THR:HG22	2.04	0.58
43:s:34:ASN:OD1	45:u:1968:G:O3'	2.21	0.58
45:u:642:G:N1	45:u:643:C:C4	2.71	0.58
45:u:2433:G:H4'	48:x:268:LYS:CD	2.34	0.58
45:u:300:A:C2	45:u:301:G:C5	2.92	0.58
55:5:530:TYR:CD1	55:5:543:ASP:OD1	2.56	0.58
7:G:156:VAL:CG1	7:G:184:LEU:CD1	2.78	0.58
45:u:245:C:O2	45:u:245:C:O4'	2.22	0.58
45:u:466:A:N3	45:u:467:U:C6	2.71	0.58
48:x:176:GLY:N	48:x:461:PHE:HD2	1.93	0.58
48:x:435:ALA:HB1	48:x:441:ILE:HG21	1.86	0.58
55:5:177:LEU:O	55:5:177:LEU:HD22	2.04	0.58
20:U:87:THR:HG23	20:U:102:VAL:HG21	1.85	0.57
45:u:212:A:C2	45:u:213:G:C5	2.91	0.57
45:u:1639:U:N3	45:u:1643:A:O2'	2.37	0.57
45:u:1757:U:H2'	45:u:1758:G:O4'	2.03	0.57
45:u:4754:G:C2	45:u:4880:C:C2	2.92	0.57
48:x:160:LEU:HA	48:x:163:LEU:HD12	1.84	0.57
48:x:392:LYS:O	48:x:396:GLU:HB2	2.04	0.57
53:3:92:PHE:HZ	53:3:96:MET:SD	2.23	0.57
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.34	0.57
10:J:83:LEU:CD1	10:J:170:TYR:CZ	2.87	0.57
10:J:119:TYR:HE2	10:J:125:ILE:HD11	1.68	0.57
45:u:472:C:C4	45:u:473:C:C5	2.91	0.57
45:u:1279:A:O3'	45:u:1279:A:OP1	2.22	0.57
45:u:1398:A:O2'	45:u:1399:G:OP2	2.20	0.57
45:u:4975:G:N2	45:u:4984:C:C2	2.72	0.57
48:x:184:ALA:HB2	48:x:454:ILE:HD11	1.84	0.57
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.86	0.57
45:u:919:C:C4	45:u:920:C:C5	2.92	0.57
45:u:3870:C:C2	45:u:3886:G:C2	2.92	0.57
55:5:525:TRP:CD1	55:5:592:ASP:OD1	2.57	0.57
3:C:313:VAL:CG1	6:F:172:THR:HG21	2.35	0.57
11:L:71:ARG:NH2	45:u:74:G:O3'	2.37	0.57
24:Y:84:ARG:HD2	53:3:112:ILE:CB	2.34	0.57
45:u:470:A:C6	45:u:471:A:N7	2.70	0.57
45:u:691:C:C2	45:u:692:A:N7	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:2256:C:O2	45:u:2256:C:H2'	2.04	0.57
47:w:155:C:H2'	47:w:156:U:O4'	2.05	0.57
55:5:260:GLN:O	55:5:267:HIS:NE2	2.32	0.57
14:O:7:LEU:HD22	14:O:9:LEU:HD21	1.86	0.57
42:r:135:LYS:NZ	45:u:451:C:C3'	2.68	0.57
45:u:390:C:H4'	48:x:23:GLU:OE2	2.05	0.57
45:u:976:G:C6	45:u:977:C:C4	2.93	0.57
45:u:1959:U:H1'	45:u:1961:G:C1'	2.35	0.57
48:x:185:THR:O	49:y:48:GLY:CA	2.52	0.57
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.86	0.57
40:o:66:ILE:HD13	40:o:91:PHE:CE1	2.40	0.57
43:s:14:PHE:HD2	43:s:62:ARG:HH11	1.53	0.57
45:u:199:G:C6	45:u:201:C:N4	2.73	0.57
45:u:976:G:C2	45:u:977:C:C2	2.91	0.57
45:u:1213:G:O6	45:u:1215:C:C4	2.57	0.57
45:u:1280:C:C2	45:u:1282:G:C5	2.92	0.57
47:w:55:U:C4	47:w:62:A:N1	2.72	0.57
48:x:223:ARG:NH1	48:x:232:GLU:OE1	2.38	0.57
9:I:184:MET:HE2	9:I:190:LEU:HD12	1.82	0.57
45:u:471:A:C2	45:u:472:C:H1'	2.40	0.57
45:u:1840:G:H3'	45:u:1842:G:P	2.44	0.57
45:u:2367:A:N6	45:u:2798:A:O4'	2.37	0.57
45:u:2408:U:C1'	45:u:2409:U:C5	2.88	0.57
45:u:3751:G:O2'	45:u:3775:A:N6	2.37	0.57
48:x:195:ALA:O	48:x:212:ALA:HB1	2.05	0.57
48:x:252:PHE:CZ	48:x:451:VAL:HG11	2.39	0.57
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.87	0.57
38:m:119:ASN:C	38:m:119:ASN:ND2	2.63	0.57
45:u:470:A:C6	45:u:471:A:C5	2.92	0.57
45:u:2640:G:N7	45:u:2694:G:O6	2.37	0.57
45:u:3593:C:H4'	45:u:3594:C:OP2	2.05	0.57
48:x:190:THR:N	49:y:51:GLY:HA3	1.83	0.57
3:C:114:ARG:CZ	45:u:1358:G:H5''	2.35	0.57
31:f:28:LEU:HG	31:f:101:ILE:HD11	1.85	0.57
48:x:33:LEU:HD11	53:3:122:PHE:HE1	1.65	0.57
48:x:71:SER:HB3	48:x:75:THR:H	1.68	0.57
55:5:593:ILE:CD1	55:5:639:MET:HG3	2.34	0.57
55:5:601:ARG:HB3	55:5:613:LYS:CD	2.34	0.57
45:u:1268:G:C4	45:u:2111:G:C2	2.93	0.56
23:X:83:THR:CG2	48:x:403:GLY:O	2.53	0.56
45:u:463:A:N1	45:u:692:A:N1	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:469:C:C4	45:u:470:A:C5	2.93	0.56
45:u:680:G:C6	45:u:681:G:N7	2.73	0.56
45:u:687:U:C4	45:u:688:U:C5	2.93	0.56
45:u:2524:U:H5''	45:u:2711:G:C2	2.40	0.56
45:u:4461:C:O2	45:u:4516:G:C2	2.58	0.56
48:x:375:PHE:O	48:x:379:TRP:HB2	2.03	0.56
3:C:336:ARG:O	3:C:340:ILE:HG12	2.05	0.56
38:m:119:ASN:C	38:m:119:ASN:HD22	2.12	0.56
45:u:209:U:O4	45:u:211:G:H1'	2.05	0.56
45:u:370:U:C6	45:u:1637:A:C2	2.93	0.56
45:u:422:C:C2	47:w:13:G:C2	2.94	0.56
45:u:516:C:N3	45:u:646:G:C2	2.74	0.56
45:u:707:C:C2	45:u:1291:G:C2	2.92	0.56
45:u:2409:U:C5	45:u:2783:A:C2	2.93	0.56
45:u:3641:U:H5	45:u:3646:A:N7	2.04	0.56
45:u:4260:U:H2'	45:u:4261:C:C6	2.40	0.56
48:x:121:MET:CE	48:x:156:PHE:HD1	2.04	0.56
48:x:301:LEU:HD23	48:x:304:ILE:HD12	1.87	0.56
55:5:601:ARG:HB3	55:5:613:LYS:NZ	2.17	0.56
14:O:18:ARG:NH1	45:u:2053:C:O3'	2.39	0.56
55:5:71:TRP:O	55:5:83:ILE:HD11	2.05	0.56
2:B:181:MET:HE2	2:B:183:ILE:HG12	1.88	0.56
6:F:91:LEU:HD22	6:F:92:ALA:N	2.20	0.56
6:F:146:TYR:CE2	6:F:239:GLU:HB3	2.41	0.56
11:L:42:ARG:HG3	11:L:45:ARG:HH12	1.69	0.56
11:L:161:PHE:CD1	26:a:105:ARG:HD2	2.40	0.56
17:R:60:ARG:NH1	17:R:63:CYS:SG	2.79	0.56
45:u:665:C:O2	45:u:665:C:H2'	2.05	0.56
45:u:680:G:N2	45:u:681:G:H1'	2.19	0.56
45:u:1485:C:O2	45:u:1485:C:O4'	2.23	0.56
48:x:186:ASN:HA	49:y:50:ILE:HB	1.86	0.56
55:5:601:ARG:HH11	55:5:601:ARG:HG3	1.71	0.56
45:u:471:A:N6	45:u:472:C:C5	2.73	0.56
45:u:1278:C:C6	45:u:1279:A:H1'	2.40	0.56
46:v:66:G:C2	46:v:67:C:C2	2.93	0.56
48:x:185:THR:HG23	49:y:47:MET:CG	2.35	0.56
50:z:74:LEU:C	50:z:78:LEU:CD1	2.70	0.56
45:u:4101:C:C2	45:u:4109:G:C2	2.94	0.56
46:v:30:C:C2	46:v:48:G:C2	2.94	0.56
48:x:97:ALA:HB2	48:x:382:VAL:CG1	2.36	0.56
45:u:465:G:N2	45:u:466:A:H1'	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:488:ILE:HG13	55:5:489:VAL:HG23	1.87	0.56
55:5:522:VAL:HG11	55:5:532:ILE:HD13	1.88	0.56
15:P:48:LEU:HD12	15:P:92:LEU:HD13	1.87	0.56
19:T:64:VAL:HG13	19:T:72:VAL:HG13	1.88	0.56
45:u:685:C:O2	45:u:685:C:C2'	2.53	0.56
45:u:1279:A:C3'	45:u:1280:C:C5'	2.78	0.56
45:u:1365:C:H4'	45:u:1366:G:OP1	2.05	0.56
45:u:1404:G:N2	45:u:1414:C:C2	2.74	0.56
45:u:2258:C:O2	45:u:2258:C:C2'	2.54	0.56
48:x:66:ARG:HD3	48:x:72:ASN:CG	2.26	0.56
48:x:121:MET:HE3	48:x:156:PHE:CE1	2.41	0.56
48:x:185:THR:HG21	49:y:46:ILE:HG22	1.88	0.56
53:3:93:LEU:HB3	53:3:133:PHE:HE1	1.71	0.56
55:5:127:THR:N	55:5:174:PHE:HE2	2.03	0.56
16:Q:69:LYS:O	16:Q:75:ARG:NH1	2.39	0.56
17:R:10:LEU:HB3	17:R:41:ILE:HD13	1.88	0.56
44:t:30:PRO:O	44:t:32:ILE:N	2.38	0.56
45:u:181:C:N4	45:u:256:G:C6	2.74	0.56
45:u:211:G:N2	45:u:212:A:C8	2.74	0.56
45:u:1269:G:C6	45:u:2111:G:N2	2.74	0.56
45:u:2773:G:N1	45:u:2774:C:C4	2.73	0.56
55:5:123:PHE:CZ	55:5:171:ILE:O	2.56	0.56
55:5:525:TRP:CD2	55:5:599:MET:HE2	2.41	0.56
3:C:158:VAL:HG22	3:C:161:TYR:HE2	1.71	0.55
7:G:86:VAL:HG22	7:G:183:ILE:HG22	1.87	0.55
42:r:47:LYS:CD	42:r:102:TYR:HE2	1.94	0.55
45:u:471:A:C6	45:u:472:C:N1	2.74	0.55
45:u:1968:G:O2'	45:u:1969:G:O5'	2.20	0.55
45:u:2547:G:N1	45:u:2548:C:C4	2.75	0.55
45:u:4416:G:N2	45:u:4417:C:C2	2.74	0.55
48:x:428:ILE:O	48:x:431:LEU:HB3	2.05	0.55
55:5:123:PHE:CD2	55:5:171:ILE:CG2	2.79	0.55
55:5:153:VAL:HA	55:5:158:ILE:HD11	1.88	0.55
55:5:570:MET:HB3	55:5:575:VAL:HG11	1.86	0.55
15:P:36:ILE:HD12	15:P:48:LEU:HD11	1.88	0.55
18:S:28:TYR:CD2	18:S:54:MET:HE1	2.41	0.55
45:u:1483:C:O2	45:u:1483:C:O4'	2.23	0.55
46:v:82:G:C2	46:v:95:C:C2	2.94	0.55
45:u:497:G:C2	45:u:657:C:C2	2.94	0.55
45:u:1279:A:C2	45:u:1280:C:C2	2.95	0.55
45:u:1743:A:C5	45:u:1744:U:C5	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:3612:C:H1'	45:u:5016:A:C8	2.41	0.55
48:x:189:GLU:CA	49:y:52:PHE:N	2.68	0.55
55:5:90:PRO:HA	55:5:93:MET:HE3	1.88	0.55
1:A:82:ILE:HD11	1:A:99:GLY:HA3	1.89	0.55
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.87	0.55
45:u:471:A:C2	45:u:472:C:O4'	2.59	0.55
45:u:472:C:H42	45:u:473:C:N4	2.03	0.55
45:u:1959:U:H1'	45:u:1961:G:N9	2.21	0.55
45:u:4717:A:H2'	45:u:4718:G:O4'	2.07	0.55
48:x:184:ALA:HB2	48:x:454:ILE:CG1	2.37	0.55
51:1:467:UNK:O	51:1:471:UNK:N	2.39	0.55
53:3:53:ILE:CD1	55:5:354:PRO:HG3	2.29	0.55
3:C:168:VAL:HG13	3:C:177:TRP:CZ3	2.41	0.55
23:X:87:MET:HE2	48:x:415:ARG:HH22	1.71	0.55
33:h:38:GLY:HA2	48:x:266:PRO:HB3	1.86	0.55
45:u:1277:G:N2	45:u:1278:C:C2	2.75	0.55
45:u:1975:G:O4'	45:u:1984:A:H1'	2.07	0.55
45:u:2557:G:C2	45:u:2571:C:C2	2.94	0.55
32:g:69:LYS:N	45:u:2769:U:OP1	2.40	0.55
45:u:4524:G:N2	45:u:4525:C:C2	2.75	0.55
19:T:87:LYS:NZ	45:u:4301:U:OP2	2.39	0.55
45:u:470:A:C6	45:u:471:A:C4	2.95	0.55
45:u:4586:G:H8	45:u:4586:G:H5''	1.70	0.55
45:u:5023:C:O2	45:u:5023:C:O4'	2.23	0.55
48:x:292:ILE:HD13	48:x:449:LEU:HB3	1.88	0.55
48:x:453:ILE:O	48:x:456:GLN:HG3	2.07	0.55
55:5:349:VAL:O	55:5:349:VAL:HG13	2.06	0.55
58:8:624:UNK:O	58:8:628:UNK:N	2.39	0.55
45:u:200:U:C5	45:u:238:C:O4'	2.60	0.55
45:u:1360:G:C6	45:u:1361:G:C5	2.94	0.55
45:u:4213:A:H61	45:u:4218:U:H3	1.55	0.55
50:z:68:VAL:C	50:z:70:PRO:HD2	2.32	0.55
54:4:22:VAL:HG11	55:5:146:LEU:HB3	1.88	0.55
55:5:127:THR:HA	55:5:174:PHE:CE2	2.42	0.55
7:G:156:VAL:HG13	7:G:184:LEU:HG	1.89	0.55
45:u:127:G:N2	45:u:128:C:C2	2.75	0.55
45:u:962:C:OP2	45:u:2264:C:N3	2.40	0.55
45:u:1959:U:H4'	45:u:1961:G:C4'	2.37	0.55
45:u:2256:C:O2	45:u:2256:C:C2'	2.54	0.55
45:u:2408:U:O4'	45:u:2409:U:C5	2.60	0.55
53:3:92:PHE:HE1	53:3:96:MET:CG	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:211:G:C2	45:u:212:A:C5	2.95	0.55
45:u:688:U:O4	45:u:689:U:C5	2.60	0.55
45:u:2688:G:N2	45:u:2689:C:C2	2.75	0.55
45:u:4730:C:O2	45:u:4730:C:O4'	2.25	0.55
48:x:297:LEU:HD13	48:x:300:ASN:HD22	1.70	0.55
55:5:641:LYS:NZ	55:5:674:GLU:OE1	2.39	0.55
45:u:919:C:N4	45:u:920:C:C5	2.75	0.54
45:u:937:U:O2	45:u:937:U:H2'	2.07	0.54
45:u:1380:G:H4'	45:u:1381:U:OP1	2.07	0.54
45:u:2481:G:C2	45:u:2498:C:C2	2.94	0.54
48:x:157:VAL:CG1	50:z:80:PHE:HE2	0.26	0.54
48:x:367:PHE:O	48:x:371:SER:OG	2.22	0.54
55:5:123:PHE:CE2	55:5:170:GLY:O	2.54	0.54
2:B:21:ARG:NH2	45:u:4568:A:O3'	2.41	0.54
41:p:41:PHE:O	45:u:2674:A:N6	2.40	0.54
45:u:1371:A:N6	47:w:28:C:O2'	2.40	0.54
48:x:66:ARG:HH22	48:x:69:LEU:C	2.15	0.54
55:5:357:TRP:O	55:5:360:TYR:CB	2.56	0.54
14:O:36:VAL:HG11	14:O:108:ILE:HD12	1.89	0.54
33:h:119:TYR:C	33:h:119:TYR:CD2	2.86	0.54
37:l:21:ARG:HH12	48:x:273:ARG:HH11	0.54	0.54
45:u:106:A:H2'	45:u:107:G:O4'	2.06	0.54
45:u:211:G:N1	45:u:212:A:C5	2.76	0.54
45:u:516:C:C2	45:u:646:G:C2	2.95	0.54
45:u:1249:C:C2	45:u:1262:G:C2	2.95	0.54
45:u:1279:A:H2'	45:u:1280:C:H5''	1.88	0.54
45:u:1398:A:H1'	45:u:1399:G:C8	2.43	0.54
45:u:2028:C:O2'	45:u:2029:A:O5'	2.24	0.54
48:x:121:MET:O	48:x:124:THR:OG1	2.25	0.54
48:x:184:ALA:O	49:y:47:MET:C	2.38	0.54
48:x:437:PHE:C	48:x:437:PHE:CD2	2.85	0.54
55:5:600:VAL:O	55:5:615:HIS:CE1	2.61	0.54
30:e:46:ARG:HA	30:e:55:MET:SD	2.48	0.54
45:u:470:A:C4	45:u:471:A:C8	2.95	0.54
45:u:1067:G:H2'	45:u:1068:G:O4'	2.07	0.54
6:F:230:VAL:HA	18:S:39:VAL:HG12	1.89	0.54
23:X:139:ARG:NH2	45:u:2533:C:OP1	2.41	0.54
24:Y:93:THR:CB	48:x:26:ILE:HD13	2.29	0.54
35:j:59:THR:O	35:j:60:GLY:C	2.50	0.54
45:u:301:G:C6	45:u:302:C:C4	2.96	0.54
45:u:471:A:N6	45:u:472:C:C4	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1563:A:C8	45:u:1563:A:O5'	2.60	0.54
48:x:121:MET:O	48:x:156:PHE:HE1	1.91	0.54
42:r:122:LYS:CB	42:r:123:PRO:CD	2.82	0.54
45:u:206:U:O2	45:u:208:A:H8	1.90	0.54
45:u:1664:U:H2'	45:u:1665:C:C6	2.42	0.54
45:u:933:G:C2	45:u:940:C:C6	2.95	0.54
45:u:1835:G:O2'	45:u:1836:G:OP2	2.21	0.54
48:x:64:TRP:CD1	48:x:64:TRP:N	2.73	0.54
55:5:234:HIS:O	55:5:237:TYR:N	2.39	0.54
55:5:359:SER:C	55:5:360:TYR:O	2.48	0.54
55:5:397:MET:HA	55:5:410:LEU:HD11	1.89	0.54
2:B:91:GLY:HA3	2:B:153:MET:HE3	1.88	0.54
2:B:116:ARG:HD2	2:B:122:TRP:CD2	2.43	0.54
13:N:67:ARG:NH1	45:u:2458:C:OP1	2.41	0.54
17:R:71:ARG:NH1	45:u:3605:C:OP2	2.36	0.54
48:x:121:MET:O	48:x:156:PHE:CE1	2.61	0.54
55:5:633:VAL:O	55:5:637:CYS:N	2.41	0.54
2:B:163:LEU:HD23	2:B:182:GLU:HA	1.90	0.54
45:u:472:C:O2	45:u:473:C:N1	2.41	0.54
45:u:1751:A:C2	45:u:1780:A:C2	2.95	0.54
45:u:3718:A:H2'	45:u:3719:A:C8	2.43	0.54
46:v:66:G:C6	46:v:67:C:C4	2.95	0.54
55:5:220:PRO:HG2	55:5:270:ALA:HB1	1.90	0.54
45:u:210:C:O5'	45:u:210:C:H6	1.91	0.54
45:u:1205:G:N2	45:u:1206:C:C2	2.76	0.54
45:u:1357:C:H5''	45:u:1358:G:OP1	2.08	0.54
54:4:14:LEU:HD22	55:5:29:LEU:HG	1.90	0.54
4:D:129:GLU:HG3	4:D:177:THR:HG21	1.90	0.53
7:G:29:ASN:HB2	7:G:32:PHE:CE2	2.43	0.53
45:u:2043:A:O2'	45:u:4461:C:O2	2.25	0.53
45:u:2301:G:N2	45:u:2302:C:C2	2.76	0.53
45:u:4895:C:H1'	45:u:4896:G:C8	2.43	0.53
47:w:15:G:C6	47:w:16:G:N1	2.76	0.53
55:5:601:ARG:HB2	55:5:613:LYS:HZ3	1.51	0.53
4:D:200:MET:HE2	4:D:241:LYS:CE	2.33	0.53
15:P:69:ARG:NH2	45:u:4568:A:N3	2.57	0.53
19:T:48:VAL:HG21	19:T:94:GLU:HG2	1.90	0.53
45:u:977:C:N3	45:u:978:G:N7	2.57	0.53
45:u:1430:C:C2	45:u:1455:G:C2	2.96	0.53
45:u:4759:C:H2'	45:u:4760:G:O4'	2.09	0.53
55:5:100:TYR:HB2	55:5:104:HIS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:525:TRP:CD2	55:5:599:MET:CE	2.91	0.53
17:R:59:SER:N	45:u:4646:U:OP1	2.42	0.53
32:g:61:PRO:HA	32:g:64:LEU:HD22	1.90	0.53
45:u:209:U:C6	45:u:211:G:N7	2.76	0.53
45:u:2089:G:N3	45:u:2089:G:H2'	2.23	0.53
45:u:2654:C:C2	45:u:2681:G:C2	2.97	0.53
45:u:3816:A:O2'	45:u:3819:G:N3	2.39	0.53
45:u:4138:C:C2	45:u:4147:G:C2	2.96	0.53
45:u:4977:A:H2'	45:u:4978:G:O4'	2.08	0.53
23:X:83:THR:HA	48:x:403:GLY:CA	2.37	0.53
45:u:1213:G:C6	45:u:1215:C:N3	2.77	0.53
45:u:1378:C:OP1	45:u:1379:C:H3'	2.09	0.53
45:u:2768:C:O2	45:u:2768:C:O4'	2.26	0.53
45:u:4635:A:C2	45:u:4664:A:C5	2.96	0.53
49:y:33:PHE:O	49:y:37:ALA:HB2	2.08	0.53
2:B:156:TYR:CD1	45:u:4909:A:C2'	2.89	0.53
8:H:26:ILE:HB	8:H:35:ARG:HG2	1.91	0.53
31:f:102:ARG:NH2	45:u:4947:U:O4	2.41	0.53
45:u:686:A:C3'	45:u:687:U:H5'	2.38	0.53
45:u:1468:C:C2	45:u:1498:G:C2	2.96	0.53
45:u:3662:A:N6	45:u:3680:U:H3	2.06	0.53
45:u:4389:C:H2'	45:u:4390:A:C8	2.43	0.53
48:x:189:GLU:CA	49:y:52:PHE:H	2.20	0.53
48:x:195:ALA:HB3	49:y:52:PHE:CZ	2.43	0.53
55:5:71:TRP:O	55:5:83:ILE:HG13	1.98	0.53
55:5:562:THR:HG21	55:5:565:LYS:HD2	1.91	0.53
5:E:202:VAL:HB	5:E:252:GLN:OE1	2.09	0.53
45:u:471:A:N1	45:u:472:C:H1'	2.23	0.53
45:u:746:A:O2'	45:u:747:A:O5'	2.20	0.53
45:u:1668:A:C4	45:u:2282:A:C2	2.96	0.53
45:u:4723:A:C2	45:u:4724:A:C5	2.97	0.53
48:x:61:PRO:HB2	48:x:65:MET:CB	2.38	0.53
51:1:533:UNK:O	51:1:537:UNK:CB	2.56	0.53
55:5:119:LEU:O	55:5:122:LEU:HB3	2.09	0.53
17:R:35:ALA:O	17:R:37:SER:N	2.41	0.53
24:Y:93:THR:CG2	48:x:26:ILE:HD12	2.32	0.53
45:u:1358:G:O2'	45:u:1359:G:O4'	2.20	0.53
55:5:83:ILE:HD12	55:5:84:ILE:H	1.73	0.53
5:E:202:VAL:HG12	5:E:256:LYS:HZ1	1.74	0.53
45:u:1899:G:N2	45:u:1900:C:C2	2.77	0.53
45:u:4583:C:C4	45:u:4718:G:C6	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:203:PHE:HA	55:5:206:VAL:HG12	1.91	0.53
55:5:468:LEU:O	55:5:471:TYR:CB	2.56	0.53
13:N:135:ILE:HD12	13:N:151:ILE:HD13	1.90	0.53
23:X:76:ILE:HG21	23:X:112:ALA:HB2	1.91	0.53
25:Z:29:ILE:HG21	25:Z:40:HIS:CE1	2.44	0.53
45:u:973:G:N2	45:u:1282:G:HO2'	2.04	0.53
45:u:1297:U:O4'	45:u:1297:U:OP2	2.27	0.53
45:u:2693:G:C6	45:u:2694:G:N1	2.77	0.53
55:5:30:SER:HG	55:5:124:SER:CB	1.91	0.53
6:F:244:ARG:NH1	45:u:942:G:OP2	2.41	0.53
8:H:180:TYR:HB2	38:m:85:LEU:HD11	1.90	0.53
11:L:58:ILE:HG23	11:L:70:VAL:CG1	2.39	0.53
45:u:2108:G:C2	45:u:2125:C:N3	2.77	0.53
7:G:34:LYS:O	45:u:4128:A:N3	2.42	0.52
31:f:48:ALA:HB2	31:f:71:TRP:CZ3	2.44	0.52
37:l:44:TRP:CZ3	37:l:45:ARG:HD3	2.44	0.52
45:u:4303:C:O2	45:u:4303:C:O4'	2.26	0.52
55:5:204:TYR:O	55:5:207:SER:OG	2.27	0.52
55:5:488:ILE:HG22	55:5:531:GLN:NE2	2.23	0.52
2:B:89:ILE:HD13	2:B:153:MET:HE1	1.91	0.52
45:u:93:G:O2'	45:u:94:A:O4'	2.25	0.52
45:u:472:C:N4	45:u:473:C:H41	2.06	0.52
45:u:1854:G:N2	45:u:4394:A:O4'	2.42	0.52
45:u:2089:G:O2'	45:u:2090:U:OP2	2.25	0.52
45:u:2905:C:C2	45:u:3590:G:C2	2.96	0.52
45:u:4579:U:H2'	45:u:4580:U:O4'	2.08	0.52
45:u:5028:G:C6	45:u:5029:C:N4	2.77	0.52
55:5:31:PHE:CZ	55:5:118:PHE:O	2.62	0.52
26:a:146:LEU:HD13	34:i:7:MET:HG2	1.91	0.52
40:o:63:THR:O	40:o:87:ARG:NH1	2.43	0.52
45:u:405:U:O2'	45:u:407:A:N7	2.40	0.52
45:u:680:G:N3	45:u:681:G:C8	2.78	0.52
45:u:4213:A:C2	45:u:4218:U:O4	2.57	0.52
47:w:119:C:C2	47:w:132:G:C2	2.98	0.52
48:x:191:ILE:HD12	49:y:44:PHE:CZ	2.42	0.52
55:5:31:PHE:CG	55:5:121:PRO:CB	2.69	0.52
55:5:83:ILE:C	55:5:85:GLY:H	2.18	0.52
2:B:29:VAL:HG13	2:B:348:ARG:HD3	1.91	0.52
11:L:9:ILE:O	11:L:9:ILE:HG23	2.09	0.52
45:u:256:G:N2	45:u:257:C:C2	2.77	0.52
45:u:707:C:O2	45:u:1291:G:C2	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:4281:A:C2	45:u:4283:G:C5	2.98	0.52
48:x:443:SER:HB2	48:x:447:ILE:HD11	1.91	0.52
45:u:12:A:H8	45:u:12:A:H5''	1.75	0.52
45:u:1086:C:C2	45:u:1212:G:C2	2.97	0.52
45:u:1447:C:H2'	45:u:1448:G:O4'	2.08	0.52
45:u:4966:A:H2'	45:u:4967:A:C8	2.45	0.52
48:x:50:LEU:HD11	50:z:88:HIS:HA	1.85	0.52
48:x:181:LEU:HD23	48:x:454:ILE:HD12	1.92	0.52
48:x:288:ASN:O	48:x:291:ILE:N	2.43	0.52
1:A:34:PHE:CD2	45:u:4087:G:C6	2.98	0.52
2:B:340:THR:OG1	2:B:341:LYS:N	2.43	0.52
12:M:69:ARG:O	12:M:71:LYS:N	2.42	0.52
45:u:52:G:N2	45:u:53:C:C2	2.78	0.52
45:u:2733:C:H2'	45:u:2734:U:O4'	2.10	0.52
55:5:178:LEU:HD23	55:5:179:THR:CA	2.39	0.52
2:B:56:ILE:HG12	2:B:365:LEU:HD22	1.92	0.52
23:X:147:LEU:CD2	49:y:20:ARG:NH2	2.70	0.52
45:u:181:C:C2	45:u:256:G:C2	2.98	0.52
45:u:2108:G:N1	45:u:2125:C:C4	2.77	0.52
45:u:2110:C:C6	45:u:2110:C:OP1	2.62	0.52
48:x:247:ALA:O	48:x:251:VAL:HG22	2.09	0.52
55:5:160:ARG:HB2	55:5:408:LEU:HD21	1.92	0.52
55:5:593:ILE:CD1	55:5:639:MET:CG	2.87	0.52
45:u:929:A:H3'	45:u:930:G:C5'	2.40	0.52
45:u:1771:U:H2'	45:u:1772:C:O4'	2.10	0.52
45:u:1891:A:O2'	45:u:1892:A:O4'	2.25	0.52
48:x:37:ILE:HA	48:x:40:PHE:HD2	1.75	0.52
5:E:250:ASP:O	5:E:254:LEU:HB2	2.10	0.52
10:J:53:ALA:HB2	10:J:68:ILE:HD12	1.91	0.52
45:u:671:G:C6	45:u:672:C:C4	2.98	0.52
45:u:986:C:C2	45:u:1068:G:C2	2.97	0.52
45:u:2363:A:C2	45:u:3860:A:C4	2.98	0.52
45:u:3594:C:O2	45:u:3594:C:C2'	2.56	0.52
55:5:36:PHE:HA	55:5:39:LEU:HB3	1.92	0.52
55:5:103:LEU:O	55:5:107:HIS:N	2.43	0.52
36:k:22:SER:HA	36:k:65:ALA:HB3	1.91	0.52
42:r:18:ILE:HG23	42:r:25:TYR:HB2	1.92	0.52
42:r:48:THR:N	42:r:102:TYR:OH	2.39	0.52
45:u:687:U:C5	45:u:688:U:C5	2.97	0.52
45:u:689:U:C2	45:u:690:C:C6	2.98	0.52
45:u:1266:G:H5''	45:u:2112:G:N3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1549:G:C2	45:u:1580:C:C2	2.98	0.52
45:u:2505:C:O2	45:u:2505:C:O4'	2.28	0.52
45:u:2517:A:N3	45:u:2539:C:O2'	2.43	0.52
48:x:188:CYS:SG	49:y:45:ALA:C	2.92	0.52
50:z:78:LEU:CD1	50:z:78:LEU:N	2.73	0.52
45:u:300:A:H2'	45:u:301:G:C8	2.45	0.51
45:u:691:C:H2'	45:u:692:A:H8	1.75	0.51
9:I:187:GLU:OE1	9:I:189:ARG:CD	2.58	0.51
20:U:46:ARG:O	20:U:47:ILE:C	2.53	0.51
45:u:112:C:C2	45:u:330:G:C2	2.97	0.51
45:u:691:C:H2'	45:u:692:A:C8	2.45	0.51
45:u:2297:G:N2	45:u:2338:C:C2	2.79	0.51
45:u:2525:U:P	45:u:2711:G:H1	2.33	0.51
48:x:48:ILE:CA	49:y:61:ILE:HD11	2.38	0.51
48:x:248:THR:N	48:x:440:ALA:CA	2.71	0.51
55:5:348:SER:CB	55:5:598:TRP:NE1	2.71	0.51
4:D:122:GLN:O	4:D:248:ARG:NH2	2.43	0.51
4:D:196:ARG:O	4:D:200:MET:HG2	2.10	0.51
30:e:7:LEU:HB2	30:e:93:LYS:HB3	1.92	0.51
44:t:121:LEU:HD22	44:t:132:ILE:HD13	1.92	0.51
45:u:220:C:H2'	45:u:221:C:C6	2.45	0.51
45:u:476:G:N2	45:u:679:C:C2	2.79	0.51
45:u:677:G:N2	45:u:678:C:C2	2.77	0.51
45:u:1874:A:H5'	45:u:4218:U:O2	2.10	0.51
45:u:1912:G:N2	45:u:1913:C:C2	2.78	0.51
45:u:3628:G:C2	45:u:3834:C:C2	2.98	0.51
45:u:4441:A:H5''	45:u:4441:A:C8	2.44	0.51
50:z:84:VAL:O	50:z:88:HIS:HB2	2.09	0.51
2:B:378:ARG:HE	22:W:32:LEU:HD21	1.75	0.51
45:u:2301:G:N1	45:u:2302:C:C4	2.79	0.51
45:u:4305:G:N3	45:u:4305:G:C2'	2.73	0.51
45:u:4913:G:O2'	45:u:4914:C:O4'	2.28	0.51
48:x:41:ILE:O	48:x:45:CYS:N	2.30	0.51
50:z:69:GLY:H	50:z:70:PRO:CD	2.17	0.51
55:5:52:PHE:CB	55:5:530:TYR:CD1	2.83	0.51
55:5:221:LEU:O	55:5:224:LEU:HB3	2.11	0.51
3:C:130:ALA:HB1	3:C:136:LEU:HD12	1.91	0.51
26:a:25:HIS:ND1	45:u:1338:G:N2	2.58	0.51
35:j:63:ARG:NH2	47:w:58:G:N7	2.58	0.51
45:u:2712:G:N2	45:u:2713:C:C2	2.79	0.51
45:u:4338:G:C4	45:u:4372:U:C5	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:106:G:N2	47:w:107:C:C2	2.79	0.51
48:x:33:LEU:HD13	53:3:121:LEU:HD12	1.91	0.51
48:x:48:ILE:HD12	49:y:61:ILE:C	2.36	0.51
2:B:36:ASP:OD1	2:B:36:ASP:N	2.44	0.51
5:E:126:ARG:HH12	45:u:712:C:H2'	1.69	0.51
8:H:111:LEU:HD11	8:H:125:ARG:HB2	1.92	0.51
14:O:72:HIS:N	45:u:4586:G:OP1	2.41	0.51
42:r:85:ASN:O	42:r:87:ARG:N	2.44	0.51
45:u:205:C:N3	45:u:209:U:C5	2.79	0.51
45:u:1723:A:N1	45:u:1838:A:N1	2.58	0.51
45:u:1929:A:C2	45:u:2054:U:O4	2.60	0.51
45:u:4735:G:C2	45:u:4736:C:C2	2.98	0.51
55:5:286:LEU:CD2	55:5:286:LEU:N	2.74	0.51
55:5:470:THR:HA	55:5:473:PHE:HD2	1.76	0.51
2:B:220:ILE:HG12	2:B:278:THR:HG23	1.93	0.51
9:I:76:MET:HG3	9:I:87:ILE:HD11	1.93	0.51
9:I:97:ILE:HD13	9:I:126:VAL:HG11	1.92	0.51
14:O:70:PRO:O	14:O:72:HIS:CE1	2.64	0.51
42:r:119:ARG:CG	42:r:122:LYS:CE	2.88	0.51
43:s:54:LEU:HD23	43:s:60:MET:HE1	1.93	0.51
45:u:43:U:H2'	45:u:44:A:O5'	2.09	0.51
45:u:1412:G:N2	45:u:1413:C:C2	2.79	0.51
45:u:1904:G:C2	45:u:2073:C:C2	2.98	0.51
45:u:4966:A:C2	45:u:4967:A:C2	2.99	0.51
48:x:187:ILE:CG2	49:y:44:PHE:HE1	2.24	0.51
48:x:443:SER:CB	48:x:447:ILE:HD12	2.39	0.51
51:1:465:UNK:O	51:1:469:UNK:N	2.44	0.51
55:5:212:TYR:HE2	55:5:257:VAL:CG2	2.20	0.51
48:x:30:GLU:HG2	48:x:33:LEU:HD12	1.88	0.51
48:x:61:PRO:HB2	48:x:65:MET:HB2	1.93	0.51
48:x:132:VAL:HG23	48:x:133:MET:HG3	1.91	0.51
55:5:645:TYR:O	55:5:690:ARG:NH2	2.43	0.51
5:E:226:GLY:N	42:r:135:LYS:CE	2.74	0.51
45:u:463:A:C2	45:u:692:A:H2	2.29	0.51
45:u:3723:A:C2	45:u:3724:A:C5	2.99	0.51
45:u:4758:U:O2	45:u:4758:U:O4'	2.29	0.51
45:u:4906:C:C2	45:u:4916:G:C2	2.99	0.51
48:x:66:ARG:HH21	48:x:70:ALA:CA	2.01	0.51
48:x:175:LEU:CD2	48:x:462:VAL:HA	2.40	0.51
55:5:31:PHE:CG	55:5:121:PRO:HB2	2.16	0.51
45:u:1959:U:H4'	45:u:1961:G:C5'	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:4093:G:C3'	45:u:4094:G:H5'	2.41	0.51
45:u:4281:A:C2	45:u:4283:G:C6	2.99	0.51
45:u:5000:G:N2	45:u:5051:C:C2	2.78	0.51
48:x:48:ILE:H	49:y:61:ILE:CD1	2.22	0.51
55:5:528:TYR:CZ	55:5:581:ILE:CD1	2.94	0.51
4:D:3:PHE:HB2	45:u:1755:C:C6	2.47	0.50
45:u:224:U:O2	45:u:224:U:O4'	2.27	0.50
45:u:504:G:C2	45:u:654:C:C2	2.99	0.50
45:u:1072:C:O2	45:u:1072:C:C2'	2.60	0.50
45:u:1171:G:C2	45:u:1191:C:C2	2.99	0.50
45:u:1400:G:C6	45:u:1401:C:C4	2.99	0.50
45:u:1822:U:O4'	45:u:1822:U:O2	2.27	0.50
45:u:1960:A:H4'	45:u:1961:G:OP2	2.11	0.50
45:u:2028:C:O2'	45:u:2029:A:C5'	2.60	0.50
45:u:3782:C:C2	45:u:3811:G:N2	2.79	0.50
47:w:125:C:O2	47:w:125:C:O4'	2.29	0.50
48:x:186:ASN:HA	49:y:50:ILE:HG22	1.92	0.50
50:z:70:PRO:HB2	50:z:72:PRO:HD2	1.92	0.50
55:5:413:VAL:HA	55:5:416:ILE:HD12	1.92	0.50
2:B:302:ASN:HB2	2:B:313:SER:HA	1.94	0.50
25:Z:5:MET:HG2	25:Z:77:TYR:CE1	2.46	0.50
37:l:21:ARG:CZ	48:x:273:ARG:HH22	2.23	0.50
45:u:1265:G:C2'	45:u:1266:G:H5'	2.41	0.50
45:u:1268:G:C2	45:u:2111:G:N2	2.78	0.50
45:u:1358:G:H2'	45:u:1359:G:H8	1.75	0.50
45:u:1998:A:O2'	45:u:1999:A:O4'	2.30	0.50
45:u:2638:G:C2	45:u:2639:U:C4	2.98	0.50
48:x:185:THR:O	49:y:48:GLY:C	2.55	0.50
7:G:95:LEU:HD13	7:G:184:LEU:HD11	1.93	0.50
25:Z:15:ALA:HB3	25:Z:79:HIS:HB3	1.93	0.50
45:u:105:A:C2	45:u:336:A:C8	3.00	0.50
45:u:1400:G:C2	45:u:1401:C:C2	2.99	0.50
45:u:1776:A:C6	45:u:1777:C:C4	2.99	0.50
45:u:2297:G:C2	45:u:2338:C:N3	2.79	0.50
55:5:345:ILE:HA	55:5:598:TRP:CD1	2.46	0.50
55:5:619:THR:N	55:5:623:GLU:O	2.32	0.50
56:6:80:UNK:O	56:6:82:UNK:N	2.45	0.50
5:E:95:ASP:N	45:u:686:A:N7	2.59	0.50
45:u:1736:A:N3	46:v:78:C:O2'	2.42	0.50
45:u:3641:U:C2	45:u:3645:U:C5	2.99	0.50
48:x:64:TRP:H	48:x:64:TRP:HD1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:z:69:GLY:H	50:z:70:PRO:HD3	1.76	0.50
51:1:446:PHE:HA	51:1:449:LEU:HD12	1.92	0.50
55:5:365:GLN:HG3	55:5:474:HIS:CG	2.46	0.50
55:5:616:ASP:OD2	55:5:634:LEU:N	2.36	0.50
3:C:334:THR:HG21	6:F:53:TYR:OH	2.11	0.50
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.47	0.50
42:r:47:LYS:HD3	42:r:102:TYR:CD2	2.44	0.50
42:r:122:LYS:N	42:r:122:LYS:CD	2.73	0.50
45:u:222:C:H2'	45:u:223:G:O4'	2.11	0.50
45:u:325:U:H2'	45:u:326:C:C6	2.47	0.50
45:u:471:A:N1	45:u:472:C:C1'	2.74	0.50
45:u:1214:C:H1'	45:u:1215:C:OP2	2.10	0.50
45:u:2028:C:O2'	45:u:2029:A:O4'	2.29	0.50
45:u:2494:U:H2'	45:u:2495:U:O4'	2.12	0.50
45:u:4094:G:H2'	45:u:4095:G:O4'	2.12	0.50
55:5:212:TYR:CE2	55:5:257:VAL:CG2	2.92	0.50
55:5:642:MET:O	55:5:692:TYR:OH	2.20	0.50
5:E:226:GLY:H	42:r:135:LYS:CE	2.25	0.50
17:R:61:ALA:HB2	45:u:2633:U:H5''	1.93	0.50
45:u:1886:G:C2	45:u:1894:C:C2	3.00	0.50
45:u:5031:G:N2	45:u:5032:C:C2	2.80	0.50
48:x:193:TRP:CZ2	49:y:53:PHE:C	2.89	0.50
48:x:437:PHE:CE2	48:x:438:LEU:HD21	2.44	0.50
50:z:81:ILE:C	50:z:81:ILE:HD12	2.36	0.50
2:B:4:ARG:HG3	45:u:4458:C:N4	2.27	0.50
2:B:43:LEU:HD13	2:B:196:TRP:CH2	2.46	0.50
25:Z:51:ARG:HB2	25:Z:65:ARG:HD2	1.92	0.50
32:g:60:ARG:HG3	32:g:61:PRO:HD2	1.94	0.50
45:u:77:U:C4	45:u:335:A:N1	2.76	0.50
45:u:466:A:N1	45:u:467:U:C5	2.79	0.50
45:u:1263:A:C6	45:u:1264:C:C4	3.00	0.50
45:u:3717:A:N1	45:u:3933:G:H1'	2.26	0.50
45:u:4389:C:H2'	45:u:4390:A:H8	1.76	0.50
45:u:4462:C:C2	45:u:4515:G:C2	3.00	0.50
48:x:61:PRO:O	48:x:65:MET:HE3	1.96	0.50
50:z:85:PHE:HE1	53:3:136:ARG:NH1	2.09	0.50
55:5:645:TYR:HD1	55:5:673:PHE:HA	1.77	0.50
5:E:134:ARG:NH1	5:E:165:SER:O	2.45	0.50
45:u:125:C:O2'	45:u:126:C:OP1	2.22	0.50
45:u:462:G:O2'	45:u:463:A:H5'	2.12	0.50
45:u:977:C:H2'	45:u:978:G:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1358:G:C2'	45:u:1359:G:O4'	2.59	0.50
45:u:1983:A:C2	45:u:2010:A:H5''	2.47	0.50
45:u:2368:A:N6	45:u:2788:U:O2	2.45	0.50
45:u:4583:C:N4	45:u:4718:G:C6	2.80	0.50
48:x:441:ILE:HD12	48:x:444:GLY:HA2	1.93	0.50
17:R:109:TYR:HB3	17:R:115:ILE:HG12	1.94	0.50
23:X:156:ILE:HD11	48:x:415:ARG:HH11	1.62	0.50
30:e:108:ARG:NH2	30:e:127:ALA:HB3	2.26	0.50
42:r:47:LYS:HB3	42:r:102:TYR:CZ	2.46	0.50
43:s:14:PHE:CZ	45:u:1960:A:N3	2.79	0.50
45:u:1754:U:O2	45:u:1754:U:O4'	2.30	0.50
45:u:2108:G:N2	45:u:2125:C:C2	2.80	0.50
45:u:2311:C:C2	45:u:2328:G:C2	3.00	0.50
48:x:248:THR:O	48:x:251:VAL:HG23	2.10	0.50
42:r:107:ARG:HD2	42:r:108:MET:CA	2.42	0.49
45:u:2752:G:H2'	45:u:2753:G:O4'	2.12	0.49
50:z:79:LEU:C	50:z:79:LEU:CD2	2.85	0.49
42:r:119:ARG:O	42:r:122:LYS:CD	2.59	0.49
45:u:211:G:N2	45:u:212:A:N9	2.60	0.49
45:u:467:U:C2	45:u:468:U:C6	3.00	0.49
45:u:1400:G:H2'	45:u:1401:C:O4'	2.13	0.49
45:u:1910:G:N2	45:u:1911:C:C2	2.80	0.49
45:u:2588:C:OP1	45:u:2767:U:O2'	2.30	0.49
45:u:4079:C:C2	45:u:4168:G:C2	3.00	0.49
45:u:4579:U:O2	45:u:4580:U:C2	2.65	0.49
45:u:4989:U:O2	45:u:4989:U:O4'	2.30	0.49
55:5:521:LYS:N	55:5:576:SER:OG	2.45	0.49
1:A:180:LEU:HD21	41:p:26:VAL:HG21	1.93	0.49
13:N:169:ARG:NH1	45:u:63:G:OP2	2.41	0.49
17:R:105:LEU:HD12	17:R:138:LEU:HD13	1.94	0.49
42:r:135:LYS:HD2	42:r:135:LYS:C	2.37	0.49
45:u:93:G:H2'	45:u:94:A:C8	2.48	0.49
45:u:971:U:H2'	45:u:972:C:H5'	1.95	0.49
45:u:1613:A:C2	45:u:1630:A:C2	3.00	0.49
45:u:2056:G:C8	45:u:2058:G:C8	3.00	0.49
45:u:2090:U:O4'	45:u:2090:U:OP2	2.30	0.49
45:u:2463:G:N2	45:u:2464:C:C2	2.80	0.49
45:u:3752:C:H2'	45:u:3777:G:C8	2.47	0.49
45:u:3914:U:N3	45:u:4378:A:N6	2.48	0.49
45:u:4213:A:N6	45:u:4218:U:H3	2.10	0.49
45:u:4691:A:C2	45:u:4700:A:C4	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:244:ASN:ND2	48:x:439:GLY:C	2.63	0.49
4:D:111:ASN:ND2	4:D:111:ASN:C	2.70	0.49
14:O:54:TYR:CE1	14:O:145:VAL:HG11	2.47	0.49
45:u:975:C:C3'	45:u:976:G:O4'	2.60	0.49
45:u:1167:C:C2	45:u:1195:G:C2	3.00	0.49
45:u:2123:C:O2'	45:u:2124:G:OP2	2.20	0.49
45:u:2257:C:O2'	45:u:2258:C:O5'	2.25	0.49
55:5:130:VAL:HG21	55:5:177:LEU:HD12	1.87	0.49
3:C:213:GLU:OE1	3:C:213:GLU:N	2.46	0.49
5:E:62:LYS:HE2	45:u:979:C:OP2	2.13	0.49
11:L:9:ILE:HG21	26:a:52:TYR:CE2	2.48	0.49
15:P:54:GLN:HA	15:P:83:TRP:CD1	2.47	0.49
20:U:80:LYS:HD3	20:U:110:TYR:CE2	2.47	0.49
42:r:82:ILE:HD11	42:r:96:MET:HE3	1.94	0.49
45:u:1235:G:H2'	45:u:1236:C:H5'	1.93	0.49
45:u:1245:C:C4	45:u:1269:G:O6	2.66	0.49
45:u:1956:A:C2'	45:u:1957:U:H5'	2.43	0.49
55:5:176:MET:HE1	55:5:215:LEU:HD22	1.94	0.49
55:5:222:HIS:O	55:5:225:VAL:HB	2.13	0.49
55:5:361:TYR:O	55:5:365:GLN:NE2	2.45	0.49
4:D:146:LEU:HD11	4:D:159:VAL:HG11	1.94	0.49
9:I:46:PHE:CD1	9:I:140:THR:HA	2.48	0.49
9:I:181:PHE:O	9:I:185:VAL:HG23	2.12	0.49
45:u:166:C:C2	45:u:167:C:H5	2.30	0.49
45:u:230:G:C2	45:u:239:C:C2	3.01	0.49
45:u:703:G:O6	45:u:706:C:N4	2.45	0.49
45:u:1170:G:C2	45:u:1192:C:C2	3.00	0.49
45:u:1811:G:N2	45:u:1812:C:C2	2.80	0.49
45:u:2477:A:H2'	45:u:2478:C:C6	2.48	0.49
45:u:4099:G:C6	45:u:4100:C:C4	3.01	0.49
45:u:4411:G:C2	45:u:4432:C:O2	2.65	0.49
46:v:71:G:C2	46:v:105:C:C2	3.00	0.49
48:x:30:GLU:OE1	53:3:117:ARG:CB	2.60	0.49
4:D:68:ARG:HG3	4:D:73:MET:HE3	1.95	0.49
4:D:195:HIS:CE1	4:D:199:ILE:HD11	2.48	0.49
11:L:66:TYR:O	11:L:68:THR:N	2.46	0.49
21:V:82:ILE:HD12	21:V:104:VAL:HG22	1.93	0.49
23:X:127:LEU:HD12	23:X:127:LEU:C	2.38	0.49
43:s:112:ARG:NH1	45:u:1968:G:OP1	2.45	0.49
45:u:986:C:N3	45:u:1068:G:C2	2.81	0.49
45:u:990:C:C4	45:u:1064:G:C2	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1301:C:O4'	45:u:1301:C:O2	2.29	0.49
45:u:1666:C:O2'	45:u:1688:G:OP1	2.21	0.49
45:u:1699:A:N6	45:u:2094:G:O2'	2.46	0.49
45:u:2468:U:O2	45:u:2469:C:C5	2.66	0.49
55:5:126:PHE:C	55:5:174:PHE:CE2	2.82	0.49
55:5:127:THR:N	55:5:174:PHE:CE2	2.80	0.49
5:E:208:LEU:HD12	5:E:208:LEU:O	2.12	0.49
10:J:156:ARG:NH2	46:v:17:C:OP1	2.46	0.49
16:Q:11:ARG:NH2	45:u:1690:C:OP2	2.45	0.49
42:r:47:LYS:O	42:r:103:HIS:NE2	2.45	0.49
44:t:94:LYS:HA	44:t:95:GLN:C	2.38	0.49
45:u:100:C:H2'	45:u:101:A:O4'	2.13	0.49
45:u:465:G:N1	45:u:466:A:C8	2.81	0.49
45:u:956:A:H3'	45:u:957:G:C8	2.48	0.49
45:u:1269:G:C5	45:u:2111:G:C2	3.01	0.49
45:u:1345:A:H2'	45:u:1346:C:C6	2.48	0.49
45:u:1787:A:N3	45:u:4210:U:O2'	2.44	0.49
45:u:1987:C:O2	45:u:1987:C:C2'	2.61	0.49
45:u:2730:U:H2'	45:u:2731:C:C6	2.48	0.49
45:u:4093:G:H3'	45:u:4094:G:H5'	1.95	0.49
45:u:4136:G:C6	45:u:4137:C:C4	3.01	0.49
45:u:4489:G:C6	45:u:4490:C:C4	3.00	0.49
48:x:82:SER:O	48:x:86:THR:OG1	2.24	0.49
55:5:463:VAL:HG22	55:5:467:PHE:HB2	1.93	0.49
1:A:44:ILE:HG22	1:A:87:PHE:CD2	2.48	0.49
4:D:258:LYS:O	4:D:259:ARG:HG3	2.13	0.49
5:E:202:VAL:HG12	5:E:256:LYS:NZ	2.17	0.49
45:u:1449:C:H2'	45:u:1450:C:O4'	2.12	0.49
45:u:1726:U:H3	45:u:1836:G:H1	1.61	0.49
45:u:2468:U:C4	45:u:2473:A:N6	2.77	0.49
45:u:4735:G:C6	45:u:4736:C:C4	3.01	0.49
45:u:4932:U:H2'	45:u:4933:C:O4'	2.13	0.49
2:B:252:ALA:HB3	45:u:4457:U:O2	2.13	0.49
27:b:45:PHE:CE1	45:u:1815:G:N7	2.81	0.49
37:l:21:ARG:NH2	48:x:273:ARG:NH1	2.55	0.49
45:u:1328:G:O2'	45:u:2349:A:OP1	2.31	0.49
45:u:1381:U:O2	45:u:1381:U:O4'	2.28	0.49
45:u:1399:G:H2'	45:u:1400:G:O4'	2.12	0.49
45:u:2726:G:C6	45:u:2727:C:N4	2.81	0.49
48:x:189:GLU:HA	49:y:52:PHE:N	2.28	0.49
50:z:75:VAL:HA	50:z:78:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:31:PHE:O	55:5:35:LEU:HG	2.12	0.49
32:g:46:CYS:SG	32:g:47:GLY:N	2.85	0.48
45:u:356:G:O2'	47:w:25:G:N3	2.44	0.48
45:u:919:C:N4	45:u:920:C:N4	2.61	0.48
45:u:4767:C:C2	45:u:4868:G:C2	3.01	0.48
48:x:189:GLU:C	49:y:51:GLY:C	2.72	0.48
55:5:84:ILE:HD12	55:5:87:THR:HG23	1.95	0.48
55:5:155:PRO:HA	55:5:158:ILE:HD12	1.95	0.48
1:A:107:MET:SD	1:A:113:VAL:HG11	2.53	0.48
45:u:384:A:C6	45:u:386:A:C6	3.01	0.48
45:u:467:U:N3	45:u:468:U:C6	2.80	0.48
45:u:1279:A:O2'	45:u:1280:C:OP1	2.30	0.48
45:u:1448:G:N2	45:u:1449:C:C2	2.81	0.48
45:u:2026:A:H2'	45:u:2027:U:H5'	1.93	0.48
45:u:3782:C:N3	45:u:3811:G:C2	2.81	0.48
45:u:3896:C:O2	45:u:4564:A:N1	2.46	0.48
45:u:4303:C:O2	45:u:4303:C:O5'	2.32	0.48
45:u:4574:U:H3'	45:u:4575:G:H5''	1.94	0.48
48:x:69:LEU:HD22	48:x:81:ILE:HG13	1.95	0.48
55:5:95:THR:OG1	55:5:204:TYR:OH	2.29	0.48
17:R:44:LEU:HD22	17:R:49:LEU:HD12	1.96	0.48
31:f:79:GLY:O	31:f:81:SER:N	2.45	0.48
45:u:984:C:C2	45:u:1070:G:C2	3.01	0.48
45:u:1878:G:N2	45:u:1879:C:C2	2.81	0.48
45:u:2729:C:H2'	45:u:2730:U:O4'	2.13	0.48
45:u:2909:C:C2	45:u:3586:G:C2	3.01	0.48
45:u:3626:G:C6	45:u:3836:A:C2	3.01	0.48
45:u:3860:A:H61	45:u:4560:C:H5	1.61	0.48
45:u:4129:G:H2'	45:u:4130:C:O4'	2.14	0.48
48:x:186:ASN:CG	49:y:50:ILE:CG2	2.62	0.48
55:5:590:SER:CA	55:5:591:ASP:N	2.76	0.48
55:5:675:LEU:HD13	55:5:679:GLU:HA	1.94	0.48
2:B:49:TYR:CE1	2:B:168:MET:HE1	2.47	0.48
7:G:100:HIS:HA	7:G:103:ARG:HD2	1.95	0.48
26:a:61:TYR:N	45:u:4354:U:O4	2.46	0.48
43:s:128:THR:HG22	43:s:178:LEU:HD21	1.96	0.48
45:u:300:A:C2	45:u:301:G:C6	3.01	0.48
45:u:505:G:C2	45:u:506:C:C2	3.01	0.48
45:u:1367:C:O2	45:u:1367:C:H2'	2.14	0.48
45:u:3715:U:O2'	45:u:3716:C:O4'	2.28	0.48
45:u:4724:A:C6	45:u:4725:C:C4	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:175:LEU:N	48:x:461:PHE:CZ	2.66	0.48
48:x:200:THR:N	48:x:208:GLU:OE1	2.46	0.48
55:5:645:TYR:HE1	55:5:674:GLU:H	1.60	0.48
2:B:165:HIS:HB3	2:B:180:LEU:HG	1.95	0.48
5:E:254:LEU:O	5:E:258:LYS:HG3	2.13	0.48
11:L:65:ARG:HG2	11:L:66:TYR:CD2	2.48	0.48
13:N:65:ARG:HG3	13:N:129:PHE:CE1	2.49	0.48
16:Q:86:ILE:HB	16:Q:105:VAL:HG13	1.95	0.48
45:u:106:A:O2'	45:u:335:A:N3	2.43	0.48
45:u:1383:G:C5	45:u:1384:C:C4	3.02	0.48
45:u:2539:C:H2'	45:u:2540:C:C6	2.48	0.48
45:u:2557:G:C6	45:u:2558:C:C4	3.01	0.48
53:3:88:LEU:N	53:3:88:LEU:HD13	2.27	0.48
1:A:49:ILE:HG22	1:A:58:LEU:HB2	1.94	0.48
3:C:303:ARG:O	16:Q:38:ARG:NH1	2.42	0.48
5:E:254:LEU:O	5:E:257:ILE:HG12	2.14	0.48
12:M:36:ALA:HB2	12:M:52:PHE:CE1	2.49	0.48
40:o:24:THR:HG23	40:o:69:ARG:HB3	1.94	0.48
45:u:1252:C:C2	45:u:1259:G:C2	3.01	0.48
45:u:1297:U:P	45:u:1297:U:O4'	2.71	0.48
45:u:1448:G:C6	45:u:1449:C:N4	2.82	0.48
45:u:2336:G:C6	45:u:2337:C:C4	3.02	0.48
48:x:93:LEU:O	48:x:97:ALA:N	2.43	0.48
48:x:212:ALA:HB3	48:x:215:ALA:H	1.79	0.48
48:x:254:VAL:O	48:x:257:TYR:HB3	2.13	0.48
55:5:652:THR:O	55:5:655:LYS:NZ	2.46	0.48
2:B:252:ALA:HB1	45:u:4524:G:N3	2.29	0.48
5:E:62:LYS:HE2	45:u:978:G:OP1	2.08	0.48
7:G:32:PHE:CZ	25:Z:55:ALA:HA	2.48	0.48
35:j:45:ARG:NH1	45:u:372:A:O3'	2.46	0.48
45:u:80:C:C2	45:u:104:G:C2	3.01	0.48
45:u:499:G:N3	45:u:499:G:H2'	2.28	0.48
45:u:2336:G:C2	45:u:2337:C:C2	3.01	0.48
45:u:3724:A:N6	45:u:3725:G:C6	2.81	0.48
45:u:4489:G:C2	45:u:4490:C:C2	3.02	0.48
45:u:4916:G:C2	45:u:4917:C:C2	3.02	0.48
48:x:176:GLY:HA2	48:x:457:TYR:C	2.28	0.48
55:5:376:TYR:O	55:5:380:SER:N	2.46	0.48
3:C:193:LYS:HD2	3:C:196:MET:HE3	1.94	0.48
28:c:82:GLY:HA2	28:c:91:VAL:CG1	2.44	0.48
45:u:28:C:C2	45:u:55:G:C2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:351:C:C2	47:w:25:G:N2	2.82	0.48
45:u:965:G:N3	45:u:965:G:H2'	2.29	0.48
45:u:2557:G:C2	45:u:2558:C:C2	3.01	0.48
45:u:2844:A:O2'	45:u:4631:G:H4'	2.14	0.48
48:x:33:LEU:HD22	53:3:121:LEU:HD12	1.96	0.48
55:5:48:PHE:HA	55:5:531:GLN:HE21	1.78	0.48
55:5:126:PHE:HB3	55:5:174:PHE:CZ	2.49	0.48
5:E:254:LEU:N	5:E:255:PRO:HD2	2.28	0.48
9:I:184:MET:HE3	9:I:189:ARG:HB3	1.95	0.48
42:r:118:LEU:HD12	42:r:121:GLN:HE22	1.77	0.48
45:u:499:G:C2	45:u:656:C:N3	2.82	0.48
45:u:1995:G:C2	45:u:1996:C:C2	3.02	0.48
45:u:2519:U:C2	45:u:2520:C:C5	3.01	0.48
45:u:2586:G:C8	45:u:2770:C:H1'	2.49	0.48
45:u:2618:G:N2	45:u:2720:C:C2	2.82	0.48
45:u:5020:G:H2'	45:u:5021:C:O4'	2.13	0.48
48:x:68:ILE:HD13	48:x:68:ILE:N	2.28	0.48
48:x:157:VAL:CG2	50:z:80:PHE:CE2	2.84	0.48
50:z:75:VAL:CA	50:z:78:LEU:HD13	2.43	0.48
3:C:290:SER:O	3:C:294:LYS:HG2	2.14	0.48
16:Q:67:ILE:HD12	16:Q:96:PRO:HD2	1.96	0.48
28:c:34:THR:HG21	28:c:93:THR:CG2	2.44	0.48
32:g:5:LEU:HD13	32:g:32:TYR:CE2	2.49	0.48
40:o:68:LEU:HD11	40:o:85:ILE:CD1	2.44	0.48
41:p:49:ARG:HB2	41:p:55:TRP:CZ3	2.49	0.48
45:u:472:C:H2'	45:u:473:C:O4'	2.14	0.48
45:u:2627:C:O2	45:u:2627:C:O4'	2.30	0.48
45:u:3714:G:C6	45:u:3715:U:C4	3.02	0.48
45:u:4378:A:O2'	45:u:4379:A:H2'	2.14	0.48
48:x:173:TYR:CZ	48:x:461:PHE:CD1	2.72	0.48
48:x:187:ILE:CG2	49:y:44:PHE:CE1	2.97	0.48
53:3:141:MET:HE2	55:5:362:PHE:HB2	1.96	0.48
55:5:175:CYS:SG	55:5:204:TYR:C	2.97	0.48
5:E:59:TYR:CZ	5:E:64:LEU:HB2	2.49	0.47
8:H:39:ASN:O	8:H:40:HIS:HB3	2.14	0.47
13:N:124:ASP:OD1	13:N:125:SER:N	2.46	0.47
24:Y:52:ASP:OD1	24:Y:52:ASP:N	2.47	0.47
45:u:1176:C:HO2'	45:u:1177:U:C4'	2.26	0.47
45:u:1958:A:H3'	45:u:1958:A:P	2.54	0.47
45:u:4099:G:C2	45:u:4100:C:C2	3.02	0.47
45:u:4492:U:O2'	45:u:4512:U:O2	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:44:VAL:HG22	55:5:45:ILE:HG13	1.96	0.47
55:5:146:LEU:HD21	55:5:423:SER:HB2	1.96	0.47
55:5:387:ILE:HA	55:5:390:ILE:HD12	1.96	0.47
2:B:105:VAL:HG11	2:B:150:PHE:CZ	2.49	0.47
37:l:21:ARG:NH1	48:x:273:ARG:HH12	0.18	0.47
42:r:10:VAL:HG13	42:r:14:SER:HB3	1.96	0.47
45:u:199:G:N2	45:u:201:C:C2	2.82	0.47
45:u:508:G:C2	45:u:510:U:C5	3.02	0.47
45:u:671:G:C2	45:u:672:C:C2	3.01	0.47
45:u:689:U:C4	45:u:690:C:C5	3.03	0.47
45:u:967:C:N3	45:u:2254:G:C6	2.83	0.47
45:u:1246:G:H2'	45:u:1247:U:O4'	2.14	0.47
45:u:1872:G:O2'	45:u:4219:A:N3	2.38	0.47
45:u:5020:G:C2	45:u:5021:C:C2	3.02	0.47
48:x:54:MET:HE1	49:y:62:ASN:HD21	1.78	0.47
2:B:234:ARG:HA	2:B:272:LYS:HD2	1.95	0.47
3:C:268:ARG:NH2	45:u:655:C:OP2	2.47	0.47
4:D:64:ILE:HG13	4:D:105:LEU:HD21	1.95	0.47
13:N:5:LYS:HG2	34:i:40:VAL:HG11	1.96	0.47
33:h:88:THR:O	33:h:89:ARG:C	2.57	0.47
42:r:135:LYS:HZ1	45:u:451:C:H3'	1.77	0.47
45:u:977:C:H2'	45:u:978:G:H5'	1.96	0.47
45:u:1383:G:C6	45:u:1384:C:C4	3.02	0.47
45:u:1910:G:C6	45:u:1911:C:N4	2.82	0.47
45:u:2496:G:C2	45:u:2497:C:C2	3.02	0.47
45:u:3938:G:O6	45:u:4172:A:N1	2.48	0.47
45:u:4730:C:O5'	45:u:4731:G:N2	2.47	0.47
45:u:4919:G:C2	45:u:4920:C:C2	3.02	0.47
48:x:59:ALA:HB1	48:x:65:MET:SD	2.54	0.47
48:x:62:PHE:N	48:x:65:MET:CE	2.66	0.47
55:5:127:THR:HA	55:5:130:VAL:HG22	1.95	0.47
55:5:134:LEU:HD13	55:5:177:LEU:CD2	2.42	0.47
55:5:567:TYR:OH	55:5:695:LYS:O	2.32	0.47
6:F:211:TRP:CD1	6:F:212:PRO:HD2	2.50	0.47
23:X:84:GLU:N	48:x:403:GLY:C	2.61	0.47
37:l:41:ARG:NH1	45:u:2431:A:OP1	2.48	0.47
45:u:298:G:N2	45:u:299:C:C2	2.83	0.47
45:u:1279:A:H2'	45:u:1280:C:C6	2.49	0.47
45:u:1584:G:C6	45:u:1585:C:C4	3.02	0.47
45:u:1661:C:C2	45:u:2345:G:N1	2.82	0.47
48:x:69:LEU:HD23	48:x:80:GLY:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:GLY:CA	2:B:153:MET:HE3	2.45	0.47
5:E:123:SER:O	5:E:126:ARG:HG2	2.15	0.47
5:E:124:HIS:NE2	45:u:1282:G:N7	2.63	0.47
9:I:45:GLU:O	9:I:46:PHE:CD1	2.67	0.47
14:O:109:PRO:HB2	14:O:110:PRO:CD	2.43	0.47
17:R:11:ALA:HB1	17:R:50:ILE:HD13	1.96	0.47
20:U:100:LEU:HD22	20:U:112:LEU:HB3	1.96	0.47
23:X:156:ILE:CD1	48:x:415:ARG:CZ	2.89	0.47
27:b:8:THR:OG1	27:b:9:THR:N	2.46	0.47
30:e:35:TRP:CZ2	30:e:56:PRO:HD2	2.50	0.47
32:g:63:VAL:O	32:g:66:ARG:N	2.45	0.47
42:r:119:ARG:O	42:r:122:LYS:HD2	2.15	0.47
45:u:2459:G:N2	45:u:2462:C:OP2	2.47	0.47
45:u:4092:G:C2	45:u:4158:C:C2	3.02	0.47
55:5:14:GLN:HA	55:5:17:LEU:HB2	1.97	0.47
55:5:31:PHE:CZ	55:5:121:PRO:CG	2.97	0.47
55:5:65:PHE:O	55:5:69:HIS:N	2.47	0.47
55:5:99:ILE:HG23	55:5:103:LEU:HD13	1.95	0.47
55:5:154:VAL:HG13	55:5:157:TYR:HB3	1.96	0.47
55:5:353:GLN:HB3	55:5:354:PRO:HD2	1.95	0.47
2:B:119:TYR:OH	2:B:129:ALA:N	2.48	0.47
5:E:226:GLY:CA	42:r:135:LYS:HD3	2.41	0.47
11:L:65:ARG:HD3	26:a:69:PHE:CD1	2.49	0.47
14:O:84:VAL:HG11	14:O:102:LEU:HD22	1.96	0.47
29:d:38:PHE:CE1	45:u:4634:U:C2	3.03	0.47
45:u:211:G:N2	45:u:212:A:C4	2.83	0.47
45:u:721:G:C2	45:u:948:C:C2	3.03	0.47
45:u:1280:C:N3	45:u:1282:G:C6	2.83	0.47
45:u:4119:C:O2	45:u:4119:C:O4'	2.30	0.47
47:w:56:G:C6	47:w:57:C:C4	3.02	0.47
2:B:241:PRO:O	2:B:244:THR:OG1	2.30	0.47
2:B:312:LYS:HD2	2:B:370:THR:HG21	1.97	0.47
9:I:153:ARG:HA	9:I:165:ILE:HD11	1.96	0.47
27:b:13:SER:HA	27:b:16:TRP:CE3	2.49	0.47
29:d:46:LEU:HD12	29:d:72:VAL:HG11	1.97	0.47
45:u:120:A:H2'	45:u:149:A:N6	2.29	0.47
45:u:177:G:C6	45:u:178:C:C4	3.03	0.47
45:u:177:G:C2	45:u:178:C:C2	3.03	0.47
45:u:208:A:C2	45:u:233:U:C2	3.03	0.47
45:u:497:G:C2	45:u:657:C:N3	2.82	0.47
45:u:1189:G:C6	45:u:1190:C:C4	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1308:C:H2'	45:u:1309:C:C6	2.49	0.47
45:u:1468:C:C2	45:u:1498:G:N2	2.82	0.47
45:u:1643:A:H2'	45:u:1644:C:C6	2.50	0.47
45:u:1957:U:O2'	45:u:1958:A:O4'	2.33	0.47
45:u:2128:G:C6	45:u:2129:C:C4	3.03	0.47
45:u:2618:G:C2	45:u:2720:C:C2	3.03	0.47
45:u:2818:C:OP1	45:u:4655:A:H4'	2.15	0.47
45:u:3586:G:C6	45:u:3587:C:C4	3.02	0.47
45:u:4152:G:N2	45:u:4153:C:C2	2.82	0.47
45:u:4525:C:H2'	45:u:4526:U:O4'	2.15	0.47
55:5:348:SER:HB2	55:5:598:TRP:CZ2	2.42	0.47
55:5:348:SER:O	55:5:349:VAL:C	2.53	0.47
55:5:567:TYR:OH	55:5:696:ASP:O	2.32	0.47
16:Q:186:TYR:CD2	45:u:4307:A:H4'	2.50	0.47
24:Y:93:THR:N	48:x:26:ILE:CG2	2.78	0.47
35:j:9:GLY:HA2	45:u:2792:C:O2	2.14	0.47
45:u:484:U:C4	45:u:486:C:C5	3.02	0.47
45:u:505:G:C6	45:u:506:C:C4	3.02	0.47
45:u:1198:G:H2'	45:u:1199:G:C8	2.49	0.47
45:u:2907:G:H2'	45:u:2908:U:O4'	2.15	0.47
45:u:3715:U:H2'	45:u:3716:C:C6	2.49	0.47
45:u:4942:C:O3'	45:u:4944:C:P	2.73	0.47
48:x:37:ILE:HG21	50:z:74:LEU:HD13	1.97	0.47
55:5:644:TYR:OH	55:5:664:ARG:NH1	2.48	0.47
4:D:76:CYS:SG	4:D:77:ALA:N	2.87	0.47
11:L:100:PRO:O	34:i:25:ARG:NH2	2.47	0.47
17:R:124:TYR:OH	45:u:2666:U:OP2	2.23	0.47
45:u:77:U:H3	45:u:336:A:N6	2.13	0.47
45:u:211:G:H4'	45:u:234:G:H8	1.76	0.47
45:u:384:A:N6	45:u:386:A:C6	2.83	0.47
45:u:1240:G:C2	45:u:1241:C:C2	3.03	0.47
45:u:2771:G:C6	45:u:2772:C:C4	3.03	0.47
45:u:2858:A:O2'	45:u:2859:G:C8	2.65	0.47
48:x:33:LEU:CD2	53:3:122:PHE:HE1	2.28	0.47
48:x:69:LEU:HD23	48:x:80:GLY:N	2.29	0.47
55:5:561:SER:HA	55:5:637:CYS:HA	1.96	0.47
7:G:58:PRO:HD3	23:X:46:PHE:HD2	1.80	0.47
15:P:32:THR:HG21	15:P:87:SER:HB3	1.96	0.47
23:X:52:LEU:HD22	23:X:53:ARG:N	2.30	0.47
45:u:465:G:C2	45:u:466:A:N9	2.83	0.47
45:u:967:C:OP1	45:u:2254:G:N1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1075:G:C2	45:u:1076:C:C2	3.02	0.47
45:u:1099:C:H2'	45:u:1100:U:O4'	2.15	0.47
45:u:1189:G:C2	45:u:1190:C:C2	3.03	0.47
45:u:1270:A:H2'	45:u:1271:G:O5'	2.15	0.47
45:u:1995:G:C6	45:u:1996:C:C4	3.03	0.47
45:u:3597:G:C2	45:u:3598:C:C2	3.03	0.47
45:u:4461:C:C2	45:u:4516:G:C2	3.02	0.47
45:u:4661:G:C6	45:u:4662:C:C4	3.03	0.47
48:x:193:TRP:HE1	49:y:54:VAL:HG22	1.79	0.47
4:D:43:LYS:HB3	4:D:46:THR:CG2	2.46	0.46
14:O:160:ARG:NH2	45:u:4759:C:OP1	2.47	0.46
17:R:99:MET:HE3	17:R:127:VAL:HG12	1.96	0.46
21:V:38:TYR:N	21:V:64:THR:O	2.47	0.46
45:u:218:A:N3	45:u:218:A:C2'	2.78	0.46
45:u:2065:G:C6	45:u:2066:C:C4	3.03	0.46
45:u:2814:C:O2	45:u:2814:C:C2'	2.62	0.46
45:u:3586:G:C2	45:u:3587:C:C2	3.03	0.46
45:u:4246:G:N2	45:u:4263:C:C2	2.83	0.46
45:u:4537:C:H2'	45:u:4538:G:C8	2.50	0.46
46:v:117:G:C2	46:v:118:C:C2	3.03	0.46
47:w:127:U:C4	47:w:128:C:C5	3.03	0.46
48:x:33:LEU:HG	53:3:118:PHE:CE1	2.50	0.46
55:5:472:THR:O	55:5:476:THR:OG1	2.27	0.46
3:C:161:TYR:CD1	3:C:166:GLU:HB3	2.49	0.46
19:T:64:VAL:HG22	19:T:72:VAL:HG11	1.97	0.46
26:a:59:ARG:NH2	45:u:294:G:O2'	2.48	0.46
45:u:22:G:N1	47:w:35:C:C4	2.83	0.46
45:u:108:A:N1	45:u:333:U:O2'	2.41	0.46
45:u:1541:C:C2	45:u:1619:G:N2	2.82	0.46
45:u:2089:G:HO2'	45:u:2090:U:P	2.38	0.46
45:u:5017:G:C6	45:u:5018:C:C4	3.04	0.46
48:x:48:ILE:N	49:y:61:ILE:HD11	2.31	0.46
48:x:88:GLY:HA2	48:x:116:GLN:HE22	1.79	0.46
50:z:71:VAL:O	50:z:75:VAL:HG23	2.15	0.46
50:z:79:LEU:HD23	50:z:79:LEU:O	2.14	0.46
6:F:98:ARG:HH21	6:F:226:THR:HG22	1.80	0.46
14:O:26:GLN:OE1	14:O:31:ARG:NH1	2.48	0.46
30:e:31:ILE:HD11	45:u:2347:A:C5	2.50	0.46
42:r:82:ILE:HD11	42:r:96:MET:CE	2.46	0.46
42:r:118:LEU:CD1	42:r:121:GLN:NE2	2.79	0.46
45:u:120:A:C2	45:u:148:C:O2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:984:C:C2	45:u:1070:G:N2	2.84	0.46
45:u:1732:C:C2	45:u:1798:G:C2	3.03	0.46
45:u:2046:G:C2	45:u:2047:A:C2	3.03	0.46
45:u:2496:G:C6	45:u:2497:C:C4	3.02	0.46
45:u:3941:G:H2'	45:u:3942:A:O4'	2.15	0.46
48:x:248:THR:N	48:x:440:ALA:CB	2.38	0.46
53:3:118:PHE:HD1	53:3:122:PHE:HZ	1.64	0.46
55:5:426:LEU:HG	55:5:430:MET:HE2	1.97	0.46
13:N:68:ARG:CG	45:u:302:C:OP1	2.64	0.46
15:P:41:ILE:HD12	15:P:150:LEU:CD1	2.46	0.46
18:S:47:PHE:HE1	18:S:125:GLN:HG2	1.81	0.46
45:u:499:G:C2	45:u:500:G:C8	3.03	0.46
45:u:1928:C:C4	45:u:2054:U:O2	2.69	0.46
45:u:1984:A:N6	45:u:2011:C:O2'	2.48	0.46
45:u:3717:A:O2'	45:u:3718:A:O4'	2.33	0.46
45:u:3900:G:H5''	45:u:3901:A:H4'	1.97	0.46
48:x:375:PHE:O	48:x:379:TRP:CB	2.62	0.46
55:5:286:LEU:N	55:5:286:LEU:HD22	2.31	0.46
6:F:41:GLN:CG	45:u:2095:A:N1	2.79	0.46
18:S:84:TYR:CD1	18:S:84:TYR:C	2.94	0.46
37:l:20:ASN:O	37:l:41:ARG:NE	2.48	0.46
45:u:479:G:N2	45:u:480:C:C2	2.83	0.46
45:u:698:G:N2	45:u:699:C:C2	2.83	0.46
45:u:747:A:C2	45:u:749:G:H1'	2.50	0.46
45:u:1322:A:N6	45:u:4446:U:OP1	2.48	0.46
45:u:2089:G:C6	45:u:2262:G:H2'	2.50	0.46
45:u:2297:G:C2	45:u:2338:C:C2	3.03	0.46
45:u:2569:G:H2'	45:u:2570:U:O4'	2.15	0.46
45:u:2743:A:C2	45:u:2744:A:C4	3.03	0.46
45:u:3600:G:C6	45:u:3601:C:C4	3.04	0.46
45:u:4102:C:C2	45:u:4108:G:C2	3.03	0.46
5:E:41:SER:HA	45:u:978:G:H4'	1.97	0.46
12:M:119:ARG:NH2	14:O:189:ILE:HD12	2.31	0.46
14:O:133:ARG:CZ	45:u:1928:C:C4	2.98	0.46
14:O:196:LEU:HB3	14:O:202:LEU:HD22	1.97	0.46
45:u:279:A:OP1	45:u:279:A:H3'	2.15	0.46
45:u:302:C:N4	45:u:303:C:N4	2.64	0.46
45:u:384:A:C6	45:u:386:A:C5	3.04	0.46
45:u:978:G:C6	45:u:979:C:C4	3.04	0.46
45:u:1221:G:O2'	45:u:1222:A:O5'	2.22	0.46
45:u:1826:G:C6	45:u:1827:C:C4	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1855:G:C2	45:u:1856:C:C2	3.04	0.46
45:u:2122:G:O2'	45:u:2123:C:P	2.74	0.46
45:u:3662:A:N6	45:u:3680:U:N3	2.57	0.46
45:u:4473:A:C2	45:u:4474:A:C5	3.04	0.46
5:E:250:ASP:O	5:E:254:LEU:N	2.46	0.46
8:H:126:VAL:HG11	8:H:161:ILE:HG22	1.97	0.46
11:L:150:LEU:HD22	33:h:121:VAL:CG2	2.46	0.46
33:h:60:VAL:O	33:h:64:THR:HG23	2.16	0.46
42:r:17:LEU:HD21	42:r:19:LYS:HG3	1.97	0.46
45:u:35:U:O2'	45:u:1525:A:N1	2.46	0.46
45:u:691:C:O2	45:u:692:A:C8	2.69	0.46
45:u:917:A:C6	45:u:919:C:N4	2.84	0.46
45:u:1886:G:N2	45:u:1894:C:C2	2.83	0.46
45:u:2743:A:H2'	45:u:2744:A:C8	2.50	0.46
45:u:4737:G:C2	45:u:4738:C:C2	3.04	0.46
47:w:126:C:O2'	47:w:127:U:C5	2.64	0.46
48:x:155:LEU:O	48:x:159:GLY:N	2.49	0.46
55:5:14:GLN:HA	55:5:17:LEU:HD13	1.97	0.46
55:5:126:PHE:O	55:5:129:ILE:HG22	2.16	0.46
2:B:29:VAL:CG2	2:B:346:THR:HG21	2.46	0.46
4:D:200:MET:HE1	4:D:241:LYS:HG2	1.93	0.46
9:I:202:ASN:N	9:I:202:ASN:OD1	2.49	0.46
25:Z:28:ASN:C	25:Z:29:ILE:HD12	2.41	0.46
25:Z:55:ALA:O	25:Z:57:MET:N	2.49	0.46
29:d:28:ASN:C	29:d:28:ASN:OD1	2.57	0.46
35:j:27:TYR:HA	35:j:34:CYS:HA	1.98	0.46
42:r:132:ARG:NE	42:r:132:ARG:HA	2.31	0.46
45:u:181:C:C4	45:u:256:G:N1	2.84	0.46
45:u:497:G:H3'	45:u:498:C:H5''	1.98	0.46
45:u:680:G:N1	45:u:681:G:C5	2.84	0.46
45:u:705:G:N2	45:u:706:C:C2	2.84	0.46
45:u:751:G:C2	45:u:752:G:N7	2.84	0.46
45:u:1404:G:C6	45:u:1405:C:C4	3.04	0.46
45:u:2065:G:H2'	45:u:2066:C:O4'	2.16	0.46
45:u:2847:G:N2	45:u:3842:C:C2	2.84	0.46
45:u:4283:G:N1	45:u:4284:C:C4	2.84	0.46
45:u:4740:G:C2	45:u:4741:C:C2	3.04	0.46
45:u:4881:U:O2	45:u:4881:U:O4'	2.34	0.46
47:w:71:A:C2	47:w:88:A:H1'	2.50	0.46
47:w:139:G:C6	47:w:140:C:C4	3.02	0.46
48:x:189:GLU:O	49:y:51:GLY:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:175:CYS:SG	55:5:205:MET:N	2.89	0.46
16:Q:14:ARG:NH2	45:u:2083:C:OP2	2.48	0.46
45:u:1237:C:O2	45:u:1237:C:O4'	2.33	0.46
45:u:1358:G:H2'	45:u:1359:G:C8	2.50	0.46
45:u:1591:U:N3	45:u:4555:U:OP1	2.47	0.46
45:u:1613:A:H3'	45:u:1614:C:C5'	2.46	0.46
45:u:2020:U:O2	45:u:2020:U:H2'	2.14	0.46
45:u:3918:G:C6	45:u:3919:C:C4	3.04	0.46
47:w:55:U:N3	47:w:62:A:C2	2.83	0.46
48:x:401:MET:H	48:x:409:MET:HE2	1.80	0.46
55:5:72:PHE:HA	55:5:83:ILE:CG1	2.42	0.46
55:5:176:MET:HE2	55:5:176:MET:HA	1.97	0.46
55:5:182:MET:HB3	55:5:198:CYS:HA	1.98	0.46
1:A:193:ARG:NH2	45:u:3685:C:OP1	2.48	0.46
7:G:159:HIS:CE1	7:G:185:LYS:HE2	2.51	0.46
16:Q:17:GLU:HB2	16:Q:18:PRO:HD2	1.98	0.46
31:f:45:LYS:HD3	31:f:107:PRO:HD2	1.97	0.46
45:u:726:G:C6	45:u:727:C:N4	2.84	0.46
45:u:918:G:H2'	45:u:918:G:N3	2.31	0.46
45:u:1269:G:C8	45:u:2111:G:C6	3.04	0.46
45:u:1416:G:N2	45:u:1417:C:C2	2.84	0.46
45:u:1448:G:C2	45:u:1449:C:C2	3.04	0.46
45:u:1983:A:C2	45:u:2008:U:O4	2.65	0.46
45:u:1995:G:C6	45:u:1996:C:N3	2.84	0.46
45:u:2245:G:C2	45:u:2246:C:C2	3.04	0.46
45:u:2270:G:C6	45:u:2271:C:C4	3.04	0.46
45:u:2559:G:C6	45:u:2560:C:C4	3.04	0.46
45:u:2698:G:C6	45:u:2699:C:C4	3.03	0.46
45:u:4423:U:O2	45:u:4423:U:O4'	2.34	0.46
45:u:4473:A:H2'	45:u:4474:A:C8	2.51	0.46
48:x:196:PHE:HA	48:x:214:ILE:HD12	1.10	0.46
55:5:145:LEU:HA	55:5:145:LEU:HD23	1.80	0.46
55:5:199:ALA:HB2	55:5:243:VAL:HA	1.98	0.46
5:E:169:LEU:HD21	5:E:187:GLN:HG3	1.98	0.45
6:F:41:GLN:HG3	45:u:2095:A:N1	2.31	0.45
45:u:190:G:C2	45:u:252:C:C2	3.04	0.45
45:u:978:G:C2	45:u:979:C:C2	3.05	0.45
45:u:2465:C:H2'	45:u:2466:G:C8	2.51	0.45
45:u:2594:C:C2	45:u:2752:G:C2	3.04	0.45
45:u:3727:A:H2'	45:u:3728:A:C8	2.51	0.45
45:u:4372:U:O2	45:u:4377:G:H1'	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:4919:G:C6	45:u:4920:C:C4	3.04	0.45
48:x:76:LEU:HD21	48:x:154:GLN:HE21	1.80	0.45
48:x:78:GLU:CG	48:x:155:LEU:HD22	2.44	0.45
48:x:157:VAL:CG2	50:z:80:PHE:CZ	2.89	0.45
48:x:248:THR:O	48:x:251:VAL:CG2	2.64	0.45
1:A:209:HIS:CG	1:A:210:PRO:HD2	2.51	0.45
18:S:84:TYR:C	18:S:84:TYR:HD1	2.24	0.45
23:X:156:ILE:CG1	48:x:415:ARG:CZ	2.89	0.45
26:a:79:TRP:CZ2	26:a:122:VAL:HG13	2.51	0.45
40:o:43:ARG:NH2	45:u:294:G:OP2	2.48	0.45
42:r:103:HIS:ND1	42:r:106:LEU:CD2	2.73	0.45
43:s:180:ILE:HG22	43:s:182:PRO:HD3	1.98	0.45
45:u:746:A:H4'	45:u:747:A:OP1	2.16	0.45
45:u:751:G:N2	45:u:912:G:C4	2.85	0.45
45:u:1240:G:C6	45:u:1241:C:C4	3.04	0.45
45:u:1855:G:C6	45:u:1856:C:C4	3.04	0.45
45:u:2128:G:C2	45:u:2129:C:C2	3.03	0.45
45:u:4916:G:C6	45:u:4917:C:C4	3.04	0.45
47:w:56:G:C2	47:w:57:C:C2	3.03	0.45
48:x:376:SER:OG	48:x:377:LYS:N	2.50	0.45
55:5:130:VAL:CG2	55:5:177:LEU:CD1	2.78	0.45
55:5:601:ARG:CG	55:5:601:ARG:NH1	2.72	0.45
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.51	0.45
42:r:8:MET:HA	42:r:8:MET:HE2	1.97	0.45
45:u:351:C:C2	47:w:25:G:C2	3.04	0.45
45:u:467:U:C4	45:u:468:U:C5	3.05	0.45
45:u:1270:A:H2'	45:u:1271:G:O4'	2.16	0.45
45:u:1279:A:C4	45:u:1280:C:C4	3.04	0.45
45:u:1357:C:O2'	45:u:1358:G:O4'	2.29	0.45
45:u:1379:C:H4'	45:u:1380:G:C8	2.50	0.45
45:u:1549:G:N2	45:u:1580:C:C2	2.84	0.45
45:u:1826:G:C2	45:u:1827:C:C2	3.04	0.45
45:u:1995:G:C5	45:u:1996:C:C4	3.05	0.45
45:u:2315:G:C2	45:u:2325:C:C2	3.05	0.45
45:u:3942:A:H2'	45:u:3943:A:O4'	2.17	0.45
45:u:4773:C:C2	45:u:4863:G:C2	3.04	0.45
46:v:86:G:C2	46:v:92:C:C2	3.03	0.45
48:x:54:MET:HE2	49:y:66:VAL:CG2	2.47	0.45
53:3:92:PHE:CZ	53:3:96:MET:HE2	1.87	0.45
55:5:507:GLU:OE2	55:5:685:GLU:CG	2.62	0.45
3:C:181:LYS:HD2	45:u:2300:A:N1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:31:SER:OG	45:u:239:C:O3'	2.34	0.45
26:a:75:LEU:HD11	26:a:133:ALA:HA	1.98	0.45
26:a:84:GLU:O	26:a:88:VAL:HG23	2.16	0.45
34:i:39:PHE:O	34:i:43:MET:HB2	2.16	0.45
45:u:994:G:C6	45:u:995:C:C4	3.05	0.45
45:u:2097:U:O2	45:u:2097:U:O4'	2.33	0.45
45:u:2245:G:C6	45:u:2246:C:C4	3.05	0.45
45:u:4644:G:C6	45:u:4645:C:C4	3.05	0.45
45:u:4699:U:C4	45:u:4702:G:C6	3.05	0.45
48:x:48:ILE:CG1	49:y:61:ILE:CD1	2.78	0.45
55:5:52:PHE:CD1	55:5:530:TYR:CD1	3.00	0.45
2:B:240:LEU:HB3	2:B:241:PRO:HD2	1.96	0.45
3:C:86:ARG:HD3	45:u:376:A:OP1	2.16	0.45
4:D:146:LEU:HD11	4:D:159:VAL:CG1	2.47	0.45
5:E:113:PRO:O	42:r:112:ARG:NE	2.50	0.45
14:O:116:LYS:HD3	18:S:169:THR:HG21	1.98	0.45
45:u:1904:G:N2	45:u:2073:C:C2	2.84	0.45
45:u:1925:G:C6	45:u:1926:C:C4	3.05	0.45
45:u:3900:G:C2	45:u:4562:C:N3	2.84	0.45
45:u:4472:G:C6	45:u:4473:A:N7	2.84	0.45
45:u:4740:G:C6	45:u:4741:C:C4	3.04	0.45
48:x:194:LYS:O	48:x:212:ALA:HB2	2.16	0.45
53:3:99:LEU:HA	53:3:102:ILE:HD12	1.98	0.45
5:E:174:PRO:O	5:E:177:LEU:N	2.50	0.45
6:F:171:LEU:HB2	6:F:189:MET:HE1	1.98	0.45
14:O:12:ARG:O	18:S:171:ARG:NH2	2.49	0.45
17:R:119:MET:HG3	17:R:123:LEU:HD22	1.97	0.45
45:u:1196:G:C2	45:u:1197:C:C2	3.05	0.45
45:u:2567:G:C2	45:u:2568:C:C2	3.04	0.45
45:u:3690:U:H2'	45:u:3691:G:O4'	2.17	0.45
45:u:3782:C:C2	45:u:3811:G:C2	3.05	0.45
45:u:4587:G:C2	45:u:4716:C:C2	3.04	0.45
55:5:125:SER:O	55:5:128:THR:HG22	2.17	0.45
55:5:593:ILE:HD12	55:5:639:MET:HG2	1.99	0.45
55:5:625:ARG:HH11	55:5:629:GLU:HB3	1.82	0.45
2:B:100:ARG:NH1	45:u:4911:A:OP2	2.49	0.45
2:B:154:LYS:HB2	2:B:154:LYS:HZ2	1.79	0.45
8:H:95:VAL:HG12	38:m:78:ILE:HD11	1.97	0.45
17:R:36:ASN:ND2	48:x:407:THR:HG23	2.28	0.45
24:Y:10:ASP:O	24:Y:11:ARG:C	2.59	0.45
31:f:35:ALA:O	31:f:37:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:88:THR:O	33:h:91:MET:N	2.50	0.45
36:k:37:ARG:NH2	45:u:2537:A:OP2	2.50	0.45
45:u:467:U:H2'	45:u:467:U:O2	2.17	0.45
45:u:1072:C:O2	45:u:1072:C:H2'	2.17	0.45
45:u:1171:G:C6	45:u:1172:C:C4	3.04	0.45
45:u:1959:U:H1'	45:u:1961:G:O4'	2.16	0.45
45:u:2433:G:C4'	48:x:268:LYS:CE	2.93	0.45
45:u:4183:G:H2'	45:u:4183:G:N3	2.32	0.45
45:u:5001:U:H2'	45:u:5002:U:O4'	2.16	0.45
55:5:345:ILE:CD1	55:5:525:TRP:HE1	2.29	0.45
7:G:221:ALA:O	7:G:224:THR:OG1	2.34	0.45
45:u:199:G:C2	45:u:201:C:C2	3.05	0.45
45:u:504:G:O6	45:u:654:C:C4	2.70	0.45
45:u:994:G:C2	45:u:1050:C:C2	3.04	0.45
45:u:1070:G:C6	45:u:1071:C:N4	2.85	0.45
45:u:1365:C:O2	45:u:1366:G:C8	2.69	0.45
45:u:2711:G:H3'	45:u:2712:G:H5''	1.99	0.45
55:5:280:HIS:O	55:5:284:ASP:CG	2.59	0.45
18:S:83:ARG:HH21	18:S:83:ARG:CG	2.29	0.45
32:g:26:PRO:HG2	45:u:2521:G:O2'	2.17	0.45
45:u:1277:G:N1	45:u:1278:C:C4	2.85	0.45
45:u:1946:G:O2'	45:u:1948:G:OP1	2.24	0.45
45:u:2322:G:C6	45:u:2323:C:C4	3.05	0.45
45:u:2698:G:C2	45:u:2699:C:C2	3.04	0.45
45:u:4136:G:C2	45:u:4137:C:C2	3.04	0.45
45:u:4240:G:C6	45:u:4241:C:C4	3.05	0.45
46:v:27:G:C2	46:v:28:C:C2	3.05	0.45
48:x:115:ALA:HA	48:x:118:LEU:HD12	1.97	0.45
55:5:504:ASP:CG	55:5:688:LEU:HG	2.30	0.45
55:5:654:ALA:HB1	55:5:667:GLU:HG2	1.97	0.45
5:E:157:ARG:HD3	5:E:266:TYR:CZ	2.52	0.45
5:E:173:GLY:O	5:E:174:PRO:C	2.60	0.45
42:r:17:LEU:HD23	42:r:17:LEU:C	2.42	0.45
45:u:100:C:O2	45:u:100:C:O4'	2.33	0.45
45:u:179:G:C2	45:u:180:C:C2	3.05	0.45
45:u:488:G:N2	45:u:489:C:C2	2.85	0.45
45:u:973:G:N2	45:u:974:C:C2	2.85	0.45
45:u:2715:G:C6	45:u:2716:C:C4	3.05	0.45
45:u:4109:G:C6	45:u:4110:C:C4	3.05	0.45
45:u:4666:G:C6	45:u:4667:C:C4	3.05	0.45
45:u:5017:G:C2	45:u:5018:C:C2	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:35:THR:O	48:x:38:THR:OG1	2.28	0.45
48:x:38:THR:HG21	48:x:169:LEU:HD11	1.98	0.45
48:x:39:LEU:CD1	49:y:46:ILE:HG23	2.47	0.45
6:F:49:ARG:NH1	45:u:974:C:O3'	2.49	0.44
9:I:14:ASN:O	9:I:128:ARG:NH2	2.45	0.44
11:L:74:ARG:NH2	45:u:76:A:N7	2.65	0.44
19:T:80:VAL:O	19:T:82:GLY:N	2.51	0.44
23:X:96:LEU:HG	23:X:140:LEU:HD11	1.99	0.44
25:Z:29:ILE:HD12	25:Z:29:ILE:N	2.32	0.44
30:e:53:ILE:HG22	45:u:437:G:H5'	1.99	0.44
45:u:994:G:C2	45:u:995:C:C2	3.05	0.44
45:u:1639:U:O2	45:u:1639:U:H2'	2.16	0.44
45:u:1823:G:C3'	45:u:1825:A:P	3.05	0.44
45:u:1840:G:C3'	45:u:1842:G:P	3.05	0.44
45:u:2065:G:C2	45:u:2066:C:C2	3.04	0.44
45:u:2659:A:N1	45:u:2672:C:O2'	2.40	0.44
45:u:2898:G:C6	45:u:2899:C:C4	3.05	0.44
45:u:4091:G:N2	45:u:4159:C:C2	2.85	0.44
45:u:4883:C:O2'	45:u:4884:G:P	2.74	0.44
46:v:117:G:C6	46:v:118:C:C4	3.05	0.44
48:x:35:THR:OG1	48:x:36:ALA:N	2.50	0.44
48:x:62:PHE:O	48:x:66:ARG:N	2.49	0.44
48:x:66:ARG:HA	48:x:66:ARG:NE	2.29	0.44
55:5:32:SER:HA	55:5:35:LEU:HD12	1.98	0.44
55:5:52:PHE:CB	55:5:530:TYR:CZ	2.89	0.44
9:I:93:PRO:HB2	9:I:125:THR:HB	1.99	0.44
25:Z:54:THR:O	25:Z:56:ALA:N	2.50	0.44
44:t:97:ASN:N	44:t:98:ILE:HA	2.32	0.44
45:u:977:C:O2'	45:u:978:G:H5'	2.17	0.44
45:u:2793:G:H5''	45:u:2794:C:H5''	1.99	0.44
45:u:4147:G:C6	45:u:4148:C:C4	3.05	0.44
45:u:4713:G:C6	45:u:4714:C:C4	3.05	0.44
45:u:4874:A:H3'	45:u:4875:G:C5'	2.47	0.44
45:u:4904:G:N2	45:u:4905:C:C2	2.85	0.44
48:x:61:PRO:HB2	48:x:65:MET:HB3	2.00	0.44
48:x:69:LEU:CD2	48:x:80:GLY:CA	2.95	0.44
48:x:78:GLU:OE2	48:x:155:LEU:HD22	2.17	0.44
48:x:177:SER:OG	48:x:180:SER:N	2.36	0.44
48:x:284:PHE:HB3	48:x:287:SER:HA	2.00	0.44
50:z:83:SER:O	50:z:87:LEU:CB	2.65	0.44
55:5:131:THR:HG21	55:5:151:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:19:GLN:HA	11:L:22:VAL:HG23	1.99	0.44
26:a:19:HIS:NE2	45:u:1338:G:N2	2.65	0.44
31:f:11:PHE:CE2	31:f:97:ILE:HD13	2.51	0.44
42:r:47:LYS:C	42:r:103:HIS:HD2	2.25	0.44
44:t:85:LEU:HD13	44:t:109:ILE:CG2	2.48	0.44
45:u:278:G:H4'	45:u:279:A:OP2	2.17	0.44
45:u:1098:G:C2	45:u:1099:C:C2	3.05	0.44
45:u:2270:G:C2	45:u:2271:C:C2	3.06	0.44
45:u:2481:G:C6	45:u:2482:C:C4	3.05	0.44
45:u:2594:C:O2	45:u:2752:G:C2	2.71	0.44
45:u:2715:G:C2	45:u:2716:C:C2	3.05	0.44
45:u:3729:U:H2'	45:u:3730:U:C6	2.52	0.44
45:u:4129:G:C6	45:u:4130:C:C4	3.05	0.44
45:u:4451:G:C6	45:u:4522:G:C8	3.05	0.44
46:v:111:C:H2'	46:v:112:U:O4'	2.18	0.44
47:w:94:G:H5'	47:w:94:G:C8	2.52	0.44
55:5:151:ILE:HA	55:5:154:VAL:HG12	1.98	0.44
2:B:56:ILE:CG1	2:B:365:LEU:HD22	2.47	0.44
2:B:154:LYS:NZ	2:B:154:LYS:CB	2.81	0.44
12:M:37:LEU:HD23	18:S:100:LEU:HD11	1.98	0.44
30:e:23:HIS:HB2	30:e:53:ILE:HD11	1.99	0.44
35:j:9:GLY:HA3	45:u:2800:G:H1'	1.98	0.44
45:u:654:C:O2	45:u:654:C:H2'	2.16	0.44
45:u:1679:A:N1	45:u:4391:G:O2'	2.46	0.44
45:u:2288:G:C2	45:u:2290:C:C4	3.05	0.44
45:u:2609:G:C2	45:u:2731:C:O2	2.70	0.44
45:u:4349:C:H3'	45:u:4350:C:C5'	2.48	0.44
45:u:4749:C:O2	45:u:4749:C:O4'	2.32	0.44
48:x:174:GLY:CA	48:x:461:PHE:CE2	2.99	0.44
55:5:688:LEU:HD13	55:5:689:VAL:HG23	1.99	0.44
3:C:86:ARG:HA	3:C:89:GLN:HG3	2.00	0.44
7:G:30:PRO:HG2	7:G:31:LEU:HD22	2.00	0.44
17:R:99:MET:O	17:R:103:ARG:HB2	2.17	0.44
35:j:13:ASN:OD1	35:j:13:ASN:N	2.50	0.44
41:p:17:ARG:NH2	45:u:1577:G:OP1	2.50	0.44
45:u:686:A:H3'	45:u:687:U:H5'	2.00	0.44
45:u:689:U:C2	45:u:690:C:C5	3.05	0.44
45:u:1744:U:H2'	45:u:1745:G:O4'	2.17	0.44
45:u:2909:C:O2	45:u:3586:G:C2	2.71	0.44
45:u:3670:C:O2'	45:u:3671:G:O4'	2.36	0.44
45:u:4088:C:H2'	45:u:4089:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:4240:G:C2	45:u:4241:C:C2	3.06	0.44
45:u:4320:G:H2'	45:u:4321:U:O4'	2.18	0.44
45:u:5008:C:H2'	45:u:5009:G:O4'	2.16	0.44
47:w:68:G:H2'	47:w:69:U:O4'	2.17	0.44
1:A:90:CYS:CB	1:A:101:VAL:HG13	2.47	0.44
1:A:152:SER:OG	45:u:3661:G:N7	2.47	0.44
2:B:261:ARG:HB2	14:O:64:THR:HG21	2.00	0.44
11:L:104:ASN:OD1	11:L:110:LEU:HB2	2.18	0.44
13:N:198:LEU:HD23	13:N:198:LEU:HA	1.94	0.44
33:h:21:LEU:HD11	33:h:54:ILE:HG23	2.00	0.44
42:r:17:LEU:HD12	42:r:36:ASN:HD21	1.82	0.44
45:u:1241:C:C2'	45:u:1242:G:OP1	2.65	0.44
45:u:1874:A:C5'	45:u:4218:U:O2	2.66	0.44
45:u:4666:G:C2	45:u:4667:C:C2	3.06	0.44
45:u:4754:G:N2	45:u:4880:C:C2	2.86	0.44
45:u:5020:G:C6	45:u:5021:C:C4	3.04	0.44
48:x:69:LEU:HD22	48:x:80:GLY:C	2.42	0.44
48:x:417:ILE:HD13	48:x:417:ILE:HA	1.85	0.44
53:3:92:PHE:CD1	53:3:92:PHE:O	2.70	0.44
2:B:385:LYS:NZ	45:u:5002:U:OP2	2.48	0.44
8:H:117:PHE:CE1	8:H:118:LEU:HD23	2.53	0.44
9:I:47:PRO:HB3	9:I:171:TRP:CE2	2.53	0.44
17:R:99:MET:N	17:R:99:MET:SD	2.91	0.44
45:u:52:G:N1	45:u:53:C:C4	2.86	0.44
45:u:1048:G:C2	45:u:1049:C:C2	3.06	0.44
45:u:2275:G:H8	45:u:2275:G:H5''	1.82	0.44
45:u:2559:G:C2	45:u:2560:C:C2	3.06	0.44
45:u:3900:G:C2	45:u:4562:C:C2	3.06	0.44
45:u:4109:G:C2	45:u:4110:C:C2	3.06	0.44
45:u:4207:C:C2	45:u:4226:G:N2	2.85	0.44
45:u:4482:U:N3	45:u:4483:C:C5	2.86	0.44
45:u:4890:G:C2	45:u:4930:C:C2	3.06	0.44
47:w:134:G:C6	47:w:135:C:C4	3.05	0.44
48:x:247:ALA:O	48:x:440:ALA:HB3	2.13	0.44
55:5:9:LEU:HG	55:5:13:LYS:HB3	2.00	0.44
55:5:52:PHE:CG	55:5:530:TYR:CD1	3.04	0.44
55:5:245:CYS:O	55:5:248:THR:OG1	2.35	0.44
1:A:207:VAL:HG12	45:u:3919:C:C5'	2.48	0.44
5:E:262:GLN:N	45:u:4930:C:OP1	2.48	0.44
32:g:8:ARG:HB2	32:g:34:TYR:HE2	1.83	0.44
45:u:2:G:C2	45:u:3:C:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:322:C:O2	45:u:4356:G:C2	2.71	0.44
45:u:952:G:C6	45:u:953:C:C4	3.06	0.44
45:u:1354:A:N1	45:u:1385:G:O2'	2.45	0.44
45:u:2315:G:C2	45:u:2325:C:O2	2.71	0.44
45:u:2457:G:C6	45:u:2458:C:C4	3.06	0.44
45:u:2612:G:C2	45:u:2613:C:C2	3.06	0.44
45:u:2612:G:C6	45:u:2613:C:C4	3.05	0.44
45:u:2738:C:O2'	45:u:2740:U:O2	2.35	0.44
45:u:3600:G:C2	45:u:3601:C:C2	3.06	0.44
45:u:3882:C:H2'	45:u:3883:U:C6	2.53	0.44
45:u:3891:A:H2'	45:u:3892:U:O4'	2.18	0.44
45:u:4142:C:C4	45:u:4143:G:N1	2.86	0.44
45:u:4904:G:C2	45:u:4905:C:C2	3.06	0.44
45:u:5038:A:H2'	45:u:5039:U:O4'	2.18	0.44
48:x:207:MET:SD	48:x:207:MET:N	2.89	0.44
48:x:401:MET:HG2	48:x:409:MET:HE2	2.00	0.44
55:5:19:LYS:HE3	55:5:19:LYS:HB2	1.83	0.44
55:5:349:VAL:CG1	55:5:352:HIS:HD2	2.27	0.44
55:5:611:HIS:HB3	55:5:612:ILE:HD12	2.00	0.44
3:C:224:ILE:HG22	3:C:227:ILE:HD13	1.99	0.44
3:C:262:ASP:O	3:C:271:ALA:O	2.36	0.44
6:F:92:ALA:HB3	6:F:127:LEU:HD21	2.00	0.44
15:P:41:ILE:HD12	15:P:150:LEU:HD13	1.99	0.44
41:p:4:ARG:NH1	45:u:1554:A:OP2	2.51	0.44
44:t:143:VAL:O	44:t:145:GLY:N	2.51	0.44
45:u:43:U:C2'	45:u:44:A:O5'	2.66	0.44
45:u:680:G:C6	45:u:681:G:C5	3.06	0.44
45:u:977:C:C3'	45:u:978:G:H5'	2.46	0.44
45:u:1326:A:OP2	45:u:4445:U:O2'	2.35	0.44
45:u:1691:G:C2	45:u:1692:C:C2	3.06	0.44
45:u:2490:U:O2'	45:u:2491:C:O4'	2.23	0.44
45:u:2654:C:N3	45:u:2681:G:C2	2.86	0.44
45:u:2664:G:N2	45:u:2671:C:C2	2.85	0.44
45:u:2816:G:C6	45:u:2817:C:C4	3.06	0.44
45:u:3861:A:H2'	45:u:3862:A:C8	2.53	0.44
45:u:4216:G:C2'	45:u:4217:G:H5'	2.48	0.44
45:u:5016:A:N6	45:u:5033:G:O2'	2.50	0.44
47:w:10:G:C2	47:w:11:C:C2	3.06	0.44
48:x:185:THR:OG1	49:y:50:ILE:HD11	2.05	0.44
48:x:450:ALA:HA	48:x:453:ILE:HD12	2.00	0.44
55:5:610:LYS:HA	55:5:615:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:18:ARG:HA	15:P:147:GLU:HA	1.99	0.43
22:W:44:ARG:HG2	22:W:44:ARG:HH11	1.81	0.43
45:u:217:C:H6	45:u:217:C:H2'	1.67	0.43
45:u:218:A:H1'	45:u:219:G:H8	1.83	0.43
45:u:469:C:N4	45:u:470:A:C6	2.86	0.43
45:u:1064:G:C2	45:u:1065:G:C4	3.06	0.43
45:u:1171:G:C2	45:u:1172:C:C2	3.05	0.43
45:u:1213:G:C6	45:u:1215:C:C4	3.06	0.43
45:u:2021:G:C2	45:u:2022:C:C2	3.06	0.43
45:u:2042:A:N3	45:u:4462:C:O2'	2.49	0.43
45:u:2376:A:H2'	45:u:2377:C:O4'	2.17	0.43
45:u:2468:U:C2	45:u:2473:A:N6	2.85	0.43
45:u:2871:A:H2'	45:u:2872:C:O4'	2.18	0.43
45:u:4232:U:H1'	45:u:4233:A:OP2	2.18	0.43
45:u:4408:G:C6	45:u:4409:C:C4	3.06	0.43
46:v:25:G:C6	46:v:26:C:C4	3.06	0.43
53:3:136:ARG:HD2	53:3:136:ARG:HA	1.81	0.43
55:5:176:MET:SD	55:5:215:LEU:HD13	2.58	0.43
55:5:455:GLU:O	55:5:458:SER:OG	2.27	0.43
6:F:146:TYR:CE2	6:F:239:GLU:CB	3.01	0.43
12:M:116:LYS:HE3	14:O:201:PHE:CE2	2.53	0.43
14:O:27:VAL:CG1	14:O:98:ALA:HB1	2.47	0.43
32:g:5:LEU:HD21	32:g:22:LEU:HD12	2.00	0.43
45:u:476:G:C2	45:u:679:C:C2	3.06	0.43
45:u:723:A:C2	45:u:724:C:C6	3.06	0.43
45:u:1196:G:C6	45:u:1197:C:C4	3.05	0.43
45:u:1358:G:N3	45:u:1359:G:N7	2.66	0.43
45:u:1724:G:C4'	45:u:1725:U:OP2	2.63	0.43
45:u:3705:G:C6	45:u:3706:C:C4	3.06	0.43
45:u:4681:A:H2'	45:u:4682:U:O4'	2.18	0.43
47:w:118:C:C2	47:w:133:G:C2	3.06	0.43
48:x:33:LEU:HD13	53:3:122:PHE:CE1	2.52	0.43
55:5:67:LYS:NZ	58:8:600:UNK:H2	2.16	0.43
5:E:132:HIS:CE1	45:u:711:A:H1'	2.52	0.43
26:a:97:ALA:O	26:a:98:ALA:HB3	2.18	0.43
45:u:192:G:C2	45:u:250:C:C2	3.05	0.43
45:u:254:G:C2	45:u:255:C:C2	3.06	0.43
45:u:744:G:H2'	45:u:745:G:C8	2.53	0.43
45:u:1265:G:OP1	45:u:2115:G:N1	2.51	0.43
45:u:1268:G:C4	45:u:2111:G:N2	2.86	0.43
45:u:1358:G:O6	45:u:1379:C:N3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1691:G:C6	45:u:1692:C:C4	3.06	0.43
45:u:1846:G:C2	45:u:1847:C:C2	3.07	0.43
45:u:2358:G:H2'	45:u:2359:U:O4'	2.19	0.43
45:u:2682:G:N2	45:u:2683:C:C2	2.85	0.43
45:u:4416:G:N1	45:u:4417:C:C4	2.86	0.43
45:u:4737:G:C6	45:u:4738:C:C4	3.07	0.43
45:u:4919:G:N2	45:u:4920:C:C2	2.87	0.43
48:x:37:ILE:CD1	53:3:121:LEU:CD2	2.76	0.43
48:x:268:LYS:HG3	48:x:402:ARG:HD2	2.00	0.43
55:5:345:ILE:HD11	55:5:595:LYS:CD	2.36	0.43
55:5:357:TRP:O	55:5:360:TYR:HB2	2.19	0.43
1:A:30:ARG:O	1:A:163:ARG:NH2	2.52	0.43
13:N:68:ARG:HG2	45:u:302:C:OP1	2.18	0.43
17:R:4:LEU:HD22	17:R:32:ILE:HG22	1.99	0.43
26:a:13:GLY:HA2	45:u:1660:U:H3'	2.00	0.43
29:d:28:ASN:HB3	45:u:4996:C:OP1	2.18	0.43
45:u:218:A:N3	45:u:218:A:H2'	2.32	0.43
45:u:307:A:N3	45:u:310:G:O2'	2.41	0.43
45:u:469:C:C4	45:u:470:A:N7	2.86	0.43
45:u:744:G:H2'	45:u:745:G:H8	1.83	0.43
45:u:1072:C:H1'	45:u:1073:G:C8	2.54	0.43
45:u:1271:G:H3'	45:u:1272:C:H5'	2.00	0.43
45:u:1374:G:C6	45:u:1375:C:C4	3.06	0.43
45:u:1436:C:O5'	45:u:2119:C:N4	2.51	0.43
45:u:1655:C:H2'	45:u:1656:U:H5''	2.00	0.43
45:u:1947:U:O2	45:u:1947:U:H2'	2.17	0.43
45:u:4187:G:H2'	45:u:4188:U:O4'	2.19	0.43
48:x:441:ILE:HB	48:x:444:GLY:H	1.84	0.43
48:x:462:VAL:O	48:x:465:GLN:N	2.50	0.43
52:2:15:UNK:O	52:2:17:UNK:N	2.51	0.43
54:4:9:ILE:HA	54:4:12:ASN:HD22	1.83	0.43
55:5:214:PHE:CB	62:5:801:9UB:C06	2.97	0.43
55:5:378:CYS:HB3	55:5:390:ILE:HD11	1.99	0.43
55:5:525:TRP:CZ3	55:5:599:MET:HE2	2.52	0.43
3:C:28:PHE:HA	3:C:129:ALA:HA	2.00	0.43
8:H:55:LEU:HD22	8:H:77:VAL:HG11	2.00	0.43
11:L:29:PRO:CB	45:u:1371:A:H2'	2.49	0.43
16:Q:89:ASP:OD1	16:Q:91:ARG:NH2	2.51	0.43
19:T:85:LEU:HD13	45:u:4305:G:C2	2.53	0.43
29:d:22:THR:HG22	29:d:89:SER:HB2	2.01	0.43
35:j:72:ARG:NH2	47:w:94:G:OP2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1430:C:O2	45:u:1455:G:C2	2.70	0.43
45:u:1912:G:C2	45:u:1913:C:C2	3.07	0.43
45:u:1928:C:N4	45:u:2054:U:O2	2.51	0.43
45:u:2021:G:C6	45:u:2022:C:C4	3.06	0.43
45:u:2050:G:C6	45:u:2051:C:C4	3.07	0.43
45:u:2898:G:C2	45:u:2899:C:C2	3.06	0.43
45:u:4913:G:HO2'	45:u:4914:C:C1'	2.32	0.43
49:y:33:PHE:O	49:y:37:ALA:CB	2.66	0.43
55:5:31:PHE:CE1	55:5:121:PRO:CD	2.93	0.43
1:A:233:ARG:O	1:A:235:VAL:HB	2.17	0.43
2:B:10:ARG:C	2:B:10:ARG:CD	2.91	0.43
7:G:87:LEU:HD11	7:G:91:THR:HG21	2.01	0.43
21:V:20:LEU:HD13	21:V:26:ILE:HG21	2.01	0.43
40:o:77:CYS:SG	61:o:201:ZN:ZN	1.79	0.43
45:u:1048:G:C6	45:u:1049:C:C4	3.06	0.43
45:u:1270:A:C2'	45:u:1271:G:O5'	2.67	0.43
45:u:1280:C:C2	45:u:1282:G:C4	3.06	0.43
45:u:4129:G:C2	45:u:4130:C:C2	3.06	0.43
45:u:4948:C:H3'	45:u:4949:G:N2	2.33	0.43
45:u:5060:A:O2'	45:u:5061:A:OP1	2.30	0.43
55:5:357:TRP:CA	55:5:360:TYR:CB	2.65	0.43
2:B:378:ARG:NE	22:W:32:LEU:HD21	2.34	0.43
6:F:92:ALA:CB	6:F:127:LEU:HD21	2.49	0.43
13:N:180:PHE:O	13:N:182:HIS:N	2.52	0.43
15:P:118:GLN:NE2	45:u:423:G:N3	2.66	0.43
19:T:14:MET:HE1	19:T:55:LYS:HB2	2.00	0.43
26:a:17:HIS:CE1	45:u:1338:G:H2'	2.53	0.43
45:u:125:C:C2	45:u:145:G:C2	3.06	0.43
45:u:174:C:C2	45:u:263:G:C2	3.07	0.43
45:u:642:G:C2	45:u:643:C:C4	3.06	0.43
45:u:744:G:C2	45:u:921:C:C2	3.06	0.43
45:u:972:C:H2'	45:u:973:G:H8	1.84	0.43
45:u:1280:C:C4	45:u:1282:G:O6	2.72	0.43
45:u:1296:G:C1'	45:u:1297:U:P	3.06	0.43
45:u:2606:G:C2	45:u:2607:C:C2	3.07	0.43
45:u:4090:G:N2	45:u:4160:C:C2	2.86	0.43
45:u:4222:G:C6	45:u:4223:C:C4	3.07	0.43
45:u:4250:G:C2	45:u:4259:C:C2	3.06	0.43
46:v:110:G:C2	46:v:111:C:C2	3.06	0.43
48:x:61:PRO:O	48:x:65:MET:N	2.51	0.43
1:A:207:VAL:HG12	45:u:3919:C:H4'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:LEU:HD13	2:B:196:TRP:HH2	1.83	0.43
17:R:36:ASN:ND2	48:x:407:THR:HG21	2.32	0.43
23:X:119:ILE:HG23	23:X:120:ASP:N	2.33	0.43
27:b:36:ASP:N	27:b:36:ASP:OD1	2.52	0.43
45:u:76:A:C5	45:u:77:U:C5	3.06	0.43
45:u:212:A:C4	45:u:213:G:N7	2.87	0.43
45:u:468:U:O2	45:u:468:U:H2'	2.18	0.43
45:u:686:A:C2'	45:u:687:U:H5'	2.49	0.43
45:u:691:C:N3	45:u:692:A:C5	2.87	0.43
45:u:1959:U:H4'	45:u:1961:G:O4'	2.19	0.43
45:u:2088:A:O2'	45:u:2089:G:P	2.76	0.43
45:u:2256:C:H1'	45:u:2257:C:OP2	2.19	0.43
45:u:2712:G:N1	45:u:2713:C:C4	2.87	0.43
45:u:4731:G:H4'	45:u:4732:G:H5'	1.99	0.43
48:x:175:LEU:HD12	48:x:461:PHE:O	2.11	0.43
48:x:373:ALA:O	48:x:376:SER:OG	2.27	0.43
48:x:431:LEU:HD23	48:x:448:LEU:HD21	2.00	0.43
55:5:177:LEU:HD13	55:5:177:LEU:O	2.19	0.43
55:5:526:TRP:CE3	55:5:544:ASN:CA	2.83	0.43
55:5:544:ASN:O	55:5:546:THR:HG23	2.16	0.43
1:A:103:PRO:HA	1:A:163:ARG:HA	2.00	0.43
5:E:95:ASP:OD1	5:E:96:LYS:N	2.49	0.43
13:N:94:PHE:CE2	13:N:96:ARG:HB2	2.54	0.43
35:j:81:GLY:O	35:j:82:THR:CG2	2.67	0.43
45:u:156:G:N2	45:u:157:U:O4	2.52	0.43
45:u:1090:G:C2	45:u:1091:C:C2	3.06	0.43
45:u:1404:G:C2	45:u:1405:C:C2	3.06	0.43
45:u:2076:G:C6	45:u:2077:C:C4	3.07	0.43
47:w:51:U:OP2	48:x:273:ARG:NH2	2.51	0.43
47:w:134:G:C2	47:w:135:C:C2	3.06	0.43
48:x:241:ASN:HB3	48:x:244:ASN:HB2	2.01	0.43
53:3:93:LEU:C	53:3:133:PHE:CE1	2.95	0.43
55:5:127:THR:CA	55:5:174:PHE:CE2	3.02	0.43
5:E:43:ASN:HB3	5:E:58:MET:SD	2.59	0.43
6:F:175:ALA:O	6:F:179:ARG:HB2	2.19	0.43
11:L:163:LYS:NZ	45:u:509:A:H5'	2.34	0.43
22:W:44:ARG:HH11	22:W:44:ARG:CG	2.32	0.43
25:Z:136:PHE:OXT	32:g:90:ARG:NH1	2.51	0.43
36:k:32:VAL:HG11	36:k:53:ALA:HB1	2.00	0.43
45:u:158:A:H5''	45:u:159:C:H2'	1.99	0.43
45:u:179:G:C6	45:u:180:C:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:202:C:C2	45:u:214:G:N2	2.87	0.43
45:u:301:G:C2	45:u:302:C:C2	3.07	0.43
45:u:1757:U:C2	45:u:1758:G:C8	3.07	0.43
45:u:1942:A:N3	45:u:4432:C:O2'	2.44	0.43
45:u:1959:U:OP1	45:u:1960:A:O3'	2.37	0.43
45:u:2567:G:C6	45:u:2568:C:C4	3.07	0.43
45:u:2703:G:C2	45:u:2704:C:C2	3.06	0.43
45:u:4508:C:N3	45:u:4512:U:H5	2.16	0.43
15:P:118:GLN:HE22	45:u:423:G:H21	1.66	0.42
42:r:46:ARG:HH22	42:r:67:ARG:HH11	1.67	0.42
45:u:258:G:C2	45:u:259:C:C2	3.06	0.42
45:u:687:U:C4	45:u:688:U:C4	3.07	0.42
45:u:1270:A:C5	45:u:1271:G:H1'	2.53	0.42
45:u:1379:C:O2	45:u:1379:C:O4'	2.37	0.42
45:u:1539:G:C6	45:u:1540:C:C4	3.06	0.42
45:u:1755:C:O2	45:u:1755:C:O2'	2.22	0.42
45:u:1811:G:C6	45:u:1812:C:C4	3.07	0.42
45:u:2542:G:C2	45:u:2775:C:C2	3.07	0.42
45:u:4124:G:O2'	45:u:4125:C:OP1	2.29	0.42
45:u:4139:G:C6	45:u:4140:C:C4	3.06	0.42
45:u:4147:G:C2	45:u:4148:C:C2	3.07	0.42
45:u:4898:G:N2	45:u:4923:C:C2	2.87	0.42
45:u:4904:G:C6	45:u:4905:C:C4	3.07	0.42
47:w:60:G:N2	47:w:64:U:C2	2.87	0.42
48:x:289:ILE:H	48:x:289:ILE:HG13	1.63	0.42
48:x:458:PHE:CE2	49:y:36:ILE:HG22	2.53	0.42
50:z:82:ALA:HA	50:z:85:PHE:HB3	2.01	0.42
55:5:139:LYS:HG2	55:5:140:ASP:HB2	2.01	0.42
55:5:635:LEU:HA	55:5:640:TYR:CD2	2.54	0.42
2:B:2:SER:N	45:u:4517:A:OP2	2.53	0.42
3:C:114:ARG:HB3	13:N:203:TYR:CD1	2.54	0.42
14:O:48:TYR:CE2	14:O:52:LEU:HD11	2.54	0.42
45:u:127:G:C2	45:u:128:C:C2	3.07	0.42
45:u:469:C:N4	45:u:470:A:C5	2.87	0.42
45:u:504:G:H22	45:u:654:C:H1'	1.84	0.42
45:u:681:G:C6	45:u:682:G:C5	3.07	0.42
45:u:689:U:C3'	45:u:690:C:H5''	2.49	0.42
45:u:702:U:H2'	45:u:703:G:H4'	2.01	0.42
45:u:747:A:C2	45:u:918:G:N1	2.87	0.42
45:u:976:G:C6	45:u:977:C:N3	2.88	0.42
45:u:1466:G:N2	45:u:1467:C:C2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1484:G:H2'	45:u:1484:G:N3	2.34	0.42
45:u:1584:G:C2	45:u:1585:C:C2	3.08	0.42
45:u:1811:G:C2	45:u:1812:C:C2	3.07	0.42
45:u:2034:G:C6	45:u:2035:C:C4	3.06	0.42
45:u:2468:U:N3	45:u:2473:A:C6	2.83	0.42
45:u:2468:U:C4	45:u:2473:A:C6	3.07	0.42
45:u:3590:G:N1	45:u:3591:C:C2	2.86	0.42
45:u:3597:G:C6	45:u:3598:C:C4	3.07	0.42
45:u:4713:G:C2	45:u:4714:C:C2	3.08	0.42
47:w:2:G:N3	47:w:2:G:H2'	2.34	0.42
47:w:10:G:C6	47:w:11:C:C4	3.07	0.42
48:x:48:ILE:CD1	49:y:61:ILE:CG1	2.90	0.42
48:x:54:MET:HE2	49:y:66:VAL:HG23	2.02	0.42
48:x:394:LEU:HD23	48:x:394:LEU:HA	1.78	0.42
55:5:177:LEU:C	55:5:177:LEU:HD22	2.41	0.42
5:E:116:ASP:N	5:E:116:ASP:OD1	2.52	0.42
30:e:81:ASN:HA	30:e:111:ILE:HD11	2.01	0.42
35:j:70:VAL:HG22	35:j:73:ARG:NH2	2.33	0.42
42:r:130:ARG:C	42:r:130:ARG:CD	2.86	0.42
45:u:298:G:C2	45:u:299:C:C2	3.07	0.42
45:u:681:G:C2	45:u:682:G:H1'	2.54	0.42
45:u:742:G:C2	45:u:923:C:C2	3.07	0.42
45:u:1416:G:C6	45:u:1417:C:C4	3.08	0.42
45:u:1431:C:C2	45:u:1454:G:N2	2.87	0.42
45:u:1550:G:C2	45:u:1579:C:O2	2.72	0.42
45:u:2294:G:N2	45:u:2295:C:C2	2.87	0.42
45:u:2468:U:C2	45:u:2469:C:C5	3.08	0.42
45:u:2481:G:C2	45:u:2482:C:C2	3.07	0.42
45:u:2862:G:N3	45:u:3624:A:H2'	2.34	0.42
48:x:66:ARG:NE	48:x:72:ASN:CB	2.67	0.42
55:5:19:LYS:HD3	55:5:145:LEU:HD11	2.01	0.42
55:5:52:PHE:CE1	55:5:530:TYR:CE1	3.03	0.42
55:5:144:GLY:HA2	55:5:147:ALA:HB3	2.01	0.42
6:F:92:ALA:HA	6:F:147:PRO:HD3	2.02	0.42
14:O:27:VAL:HG13	14:O:98:ALA:HB1	2.01	0.42
30:e:87:VAL:HG13	42:r:25:TYR:CD1	2.53	0.42
31:f:30:ILE:HD11	31:f:84:VAL:HG11	2.01	0.42
31:f:93:PRO:O	31:f:94:ALA:HB3	2.19	0.42
40:o:19:GLN:NE2	40:o:72:CYS:SG	2.92	0.42
45:u:5:A:C6	45:u:6:C:C4	3.07	0.42
45:u:76:A:C6	45:u:77:U:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:93:G:O2'	45:u:94:A:O5'	2.37	0.42
45:u:963:G:H2'	45:u:963:G:N3	2.35	0.42
45:u:1234:G:H2'	45:u:1235:G:C8	2.55	0.42
45:u:1925:G:C2	45:u:1926:C:C2	3.06	0.42
45:u:4139:G:C2	45:u:4140:C:C2	3.07	0.42
45:u:4212:A:C2	45:u:4218:U:C5	3.07	0.42
45:u:4462:C:C2	45:u:4515:G:N2	2.88	0.42
48:x:186:ASN:HA	49:y:50:ILE:CB	2.49	0.42
55:5:34:ARG:NH2	55:5:124:SER:HB3	2.34	0.42
3:C:342:ARG:HG3	3:C:342:ARG:HH11	1.84	0.42
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.53	0.42
4:D:207:TYR:CE1	46:v:33:U:C6	3.08	0.42
5:E:149:LEU:HD11	5:E:191:ILE:HG13	2.02	0.42
9:I:87:ILE:HG12	9:I:138:ILE:CG1	2.45	0.42
9:I:184:MET:CE	9:I:190:LEU:CG	2.78	0.42
24:Y:19:PHE:O	24:Y:26:ARG:NH2	2.52	0.42
44:t:162:CYS:N	44:t:163:PRO:CD	2.83	0.42
45:u:209:U:N3	45:u:211:G:C8	2.88	0.42
45:u:517:C:C2	45:u:645:G:N2	2.88	0.42
45:u:978:G:OP2	45:u:979:C:OP2	2.37	0.42
45:u:2052:G:C6	45:u:2053:C:C4	3.08	0.42
45:u:2609:G:N1	45:u:2731:C:C2	2.88	0.42
45:u:2703:G:C6	45:u:2704:C:C4	3.08	0.42
45:u:4213:A:N6	45:u:4218:U:N3	2.61	0.42
45:u:5031:G:C6	45:u:5032:C:C4	3.08	0.42
46:v:93:G:C2	46:v:94:C:C2	3.07	0.42
53:3:63:THR:O	53:3:65:GLU:N	2.53	0.42
2:B:114:CYS:SG	2:B:180:LEU:HD11	2.59	0.42
3:C:161:TYR:HD1	3:C:166:GLU:OE2	2.02	0.42
3:C:354:ALA:O	3:C:358:LEU:HG	2.20	0.42
5:E:48:ARG:NH2	45:u:1281:G:C4	2.88	0.42
12:M:34:ASN:ND2	45:u:1925:G:OP1	2.52	0.42
17:R:4:LEU:HD11	17:R:29:THR:HG23	2.02	0.42
42:r:64:MET:HE1	42:r:102:TYR:CD1	2.54	0.42
44:t:22:VAL:HG13	44:t:48:LYS:HE2	2.00	0.42
45:u:199:G:C2	45:u:201:C:C4	3.07	0.42
45:u:1090:G:C6	45:u:1091:C:C4	3.08	0.42
45:u:1416:G:C2	45:u:1417:C:C2	3.07	0.42
45:u:1431:C:C2	45:u:1454:G:C2	3.06	0.42
45:u:1612:G:N3	45:u:1612:G:C2'	2.83	0.42
45:u:2526:C:N4	45:u:2527:A:N6	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:2712:G:C2	45:u:2713:C:C2	3.08	0.42
45:u:3753:G:O2'	45:u:3754:G:H5'	2.20	0.42
47:w:53:G:C6	47:w:54:C:C4	3.07	0.42
48:x:46:CYS:SG	49:y:54:VAL:CG1	3.07	0.42
48:x:58:SER:HA	48:x:73:ARG:HE	1.83	0.42
55:5:661:ASP:HB2	55:5:666:ALA:HB3	2.02	0.42
4:D:44:TYR:CD1	45:u:1823:G:H4'	2.55	0.42
5:E:225:GLU:HG3	42:r:135:LYS:HE2	1.21	0.42
6:F:164:ILE:HB	6:F:169:ILE:HD12	2.02	0.42
8:H:117:PHE:CZ	8:H:118:LEU:HD23	2.54	0.42
8:H:134:CYS:SG	8:H:144:LEU:HD23	2.59	0.42
11:L:50:PRO:HD2	33:h:119:TYR:HE2	1.85	0.42
14:O:85:ARG:NH2	45:u:3887:C:OP2	2.45	0.42
24:Y:55:VAL:HG13	24:Y:104:VAL:HG13	2.02	0.42
31:f:18:LEU:HD23	31:f:19:ARG:NH1	2.34	0.42
36:k:11:PHE:HB3	36:k:45:LEU:HD22	2.02	0.42
37:l:38:ASN:O	45:u:362:A:N1	2.53	0.42
38:m:94:MET:HG2	38:m:105:PRO:HA	2.01	0.42
45:u:165:A:H3'	45:u:166:C:H6	1.85	0.42
45:u:472:C:N3	45:u:473:C:N3	2.63	0.42
45:u:709:C:H2'	45:u:710:G:O4'	2.20	0.42
45:u:952:G:H2'	45:u:953:C:O4'	2.20	0.42
45:u:1098:G:C6	45:u:1099:C:C4	3.08	0.42
45:u:1806:G:C2	45:u:1807:C:C2	3.08	0.42
45:u:2831:G:C2	45:u:3855:C:C2	3.08	0.42
45:u:3724:A:C6	45:u:3725:G:C5	3.08	0.42
45:u:3868:G:N2	45:u:3900:G:O2'	2.53	0.42
45:u:3870:C:C2	45:u:3886:G:N2	2.87	0.42
45:u:4072:C:H2'	45:u:4073:A:O4'	2.20	0.42
45:u:4094:G:H2'	45:u:4095:G:C1'	2.50	0.42
45:u:4274:A:H2'	45:u:4275:G:C8	2.54	0.42
45:u:4901:G:C2	45:u:4921:C:C2	3.08	0.42
45:u:4920:C:H2'	45:u:4921:C:C6	2.55	0.42
48:x:376:SER:O	48:x:379:TRP:N	2.47	0.42
2:B:242:ARG:NH2	45:u:1591:U:OP2	2.41	0.42
4:D:111:ASN:C	4:D:111:ASN:HD22	2.28	0.42
5:E:43:ASN:HD22	5:E:43:ASN:C	2.28	0.42
5:E:208:LEU:HA	5:E:212:TYR:HD2	1.84	0.42
6:F:168:ARG:HD2	6:F:211:TRP:CD1	2.55	0.42
19:T:40:VAL:HG13	19:T:96:ILE:HG23	2.01	0.42
35:j:39:TYR:O	35:j:40:PRO:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:23:VAL:HG22	36:k:23:VAL:O	2.20	0.42
43:s:145:THR:HG22	43:s:154:ILE:HG13	2.01	0.42
45:u:689:U:O2	45:u:689:U:H2'	2.20	0.42
45:u:952:G:C2	45:u:953:C:C2	3.07	0.42
45:u:1075:G:C6	45:u:1076:C:C4	3.07	0.42
45:u:1736:A:C2	45:u:1794:A:C4	3.08	0.42
45:u:1755:C:C3'	45:u:1756:U:H5''	2.50	0.42
45:u:1969:G:O2'	45:u:1970:A:C5'	2.66	0.42
45:u:2793:G:C6	45:u:2797:C:N4	2.86	0.42
45:u:3769:C:H2'	45:u:3770:U:O4'	2.20	0.42
45:u:4093:G:C6	45:u:4094:G:N7	2.88	0.42
45:u:4269:G:C2	45:u:4270:C:C2	3.08	0.42
45:u:4326:G:C6	45:u:4327:C:C4	3.07	0.42
45:u:4530:U:H2'	45:u:4531:U:C6	2.55	0.42
45:u:4891:G:C2	45:u:4929:C:C2	3.07	0.42
45:u:4931:G:N3	45:u:4931:G:H2'	2.35	0.42
48:x:69:LEU:HD23	48:x:80:GLY:CA	2.49	0.42
48:x:236:ARG:H	48:x:241:ASN:ND2	2.17	0.42
53:3:118:PHE:HD1	53:3:122:PHE:CZ	2.38	0.42
1:A:196:TRP:CG	1:A:197:PRO:N	2.86	0.42
1:A:243:THR:HG21	45:u:3748:A:O4'	2.20	0.42
2:B:36:ASP:OD2	2:B:39:LYS:CE	2.62	0.42
5:E:225:GLU:HG3	42:r:135:LYS:HE3	1.35	0.42
8:H:5:LEU:HD22	8:H:60:TRP:CH2	2.55	0.42
13:N:179:LYS:O	45:u:298:G:H5'	2.20	0.42
42:r:33:LYS:HD2	42:r:40:TYR:CE2	2.54	0.42
42:r:118:LEU:CB	42:r:121:GLN:HE21	2.32	0.42
45:u:116:G:C2	45:u:117:C:C2	3.08	0.42
45:u:284:G:C2	45:u:304:C:O2	2.73	0.42
45:u:479:G:C2	45:u:480:C:C2	3.07	0.42
45:u:707:C:H42	45:u:1290:G:H1	1.68	0.42
45:u:1075:G:N2	45:u:1076:C:C2	2.88	0.42
45:u:1374:G:C2	45:u:1375:C:C2	3.07	0.42
45:u:4395:U:C6	45:u:4395:U:H5'	2.55	0.42
45:u:4901:G:N1	45:u:4921:C:C4	2.88	0.42
45:u:5028:G:C2	45:u:5029:C:C2	3.07	0.42
47:w:139:G:C2	47:w:140:C:C2	3.08	0.42
55:5:117:VAL:HG23	55:5:164:GLY:HA2	2.00	0.42
55:5:420:ILE:O	55:5:424:GLN:N	2.53	0.42
10:J:15:LEU:HD11	10:J:157:ILE:HG23	2.01	0.42
19:T:109:VAL:HG13	45:u:1803:G:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:258:G:C6	45:u:259:C:C4	3.08	0.42
45:u:685:C:O2	45:u:685:C:H2'	2.20	0.42
45:u:1367:C:H1'	45:u:1370:G:C8	2.54	0.42
45:u:1448:G:C6	45:u:1449:C:C4	3.08	0.42
45:u:1557:C:C2	45:u:1571:G:N2	2.87	0.42
45:u:1557:C:C2	45:u:1571:G:C2	3.07	0.42
45:u:2771:G:C2	45:u:2772:C:C2	3.08	0.42
45:u:3590:G:C6	45:u:3591:C:C4	3.07	0.42
45:u:4181:U:O4	45:u:4182:G:C6	2.73	0.42
45:u:4247:G:C2	45:u:4262:C:C2	3.08	0.42
45:u:4283:G:C6	45:u:4284:C:N4	2.88	0.42
45:u:4371:G:C5	45:u:4372:U:C4	3.07	0.42
45:u:4583:C:C2	45:u:4718:G:C2	3.08	0.42
47:w:31:G:C2	47:w:32:C:C2	3.08	0.42
48:x:34:TRP:HZ3	50:z:74:LEU:HD11	1.84	0.42
48:x:175:LEU:O	48:x:460:ILE:HG22	2.19	0.42
49:y:61:ILE:HA	49:y:64:ILE:HD12	2.02	0.42
53:3:90:SER:CB	55:5:357:TRP:CD1	3.03	0.42
2:B:41:VAL:HG21	2:B:196:TRP:CG	2.55	0.41
14:O:15:LEU:HD11	14:O:129:LEU:HD13	2.01	0.41
15:P:36:ILE:CD1	15:P:48:LEU:HD11	2.48	0.41
21:V:20:LEU:HB2	21:V:55:ALA:O	2.19	0.41
27:b:45:PHE:CD1	45:u:1815:G:N7	2.88	0.41
40:o:55:ILE:HD12	40:o:57:ARG:NH2	2.35	0.41
45:u:127:G:C6	45:u:128:C:C4	3.08	0.41
45:u:1075:G:C6	45:u:1076:C:N4	2.88	0.41
45:u:1205:G:C2	45:u:1206:C:C2	3.08	0.41
45:u:1329:G:C8	45:u:1329:G:H3'	2.55	0.41
45:u:1781:U:C4	45:u:1782:U:C5	3.08	0.41
45:u:2313:A:O2'	45:u:2314:G:OP1	2.22	0.41
45:u:2463:G:C2	45:u:2464:C:C2	3.07	0.41
45:u:2606:G:C6	45:u:2607:C:C4	3.08	0.41
45:u:2645:G:C6	45:u:2646:C:C4	3.07	0.41
45:u:4966:A:N1	45:u:4967:A:C6	2.88	0.41
48:x:189:GLU:OE1	49:y:50:ILE:HG23	2.06	0.41
55:5:9:LEU:HD23	55:5:9:LEU:H	1.85	0.41
55:5:502:PHE:C	55:5:503:ASP:N	2.78	0.41
55:5:586:THR:HG23	55:5:687:TRP:HZ2	1.85	0.41
5:E:62:LYS:NZ	45:u:978:G:P	2.83	0.41
6:F:111:LEU:HD23	6:F:111:LEU:HA	1.92	0.41
7:G:157:ILE:HG23	7:G:167:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:CYS:HB2	9:I:172:GLY:O	2.21	0.41
20:U:21:PHE:CD1	20:U:80:LYS:HG2	2.55	0.41
25:Z:36:ARG:CD	25:Z:74:VAL:HG11	2.50	0.41
25:Z:38:TYR:CE1	25:Z:76:ASN:OD1	2.73	0.41
29:d:78:ARG:HG2	29:d:78:ARG:HH11	1.83	0.41
45:u:212:A:C2	45:u:213:G:C6	3.08	0.41
45:u:742:G:N2	45:u:923:C:C2	2.88	0.41
45:u:1275:G:C2	45:u:1276:C:C2	3.08	0.41
45:u:1359:G:C5	45:u:1360:G:C5	3.07	0.41
45:u:1484:G:N3	45:u:1484:G:C2'	2.82	0.41
45:u:1615:C:H2'	45:u:1616:U:O4'	2.19	0.41
45:u:1958:A:C4'	45:u:1962:A:O2'	2.63	0.41
45:u:2050:G:C2	45:u:2051:C:C2	3.08	0.41
45:u:2273:G:C2	45:u:2274:C:C2	3.08	0.41
45:u:2311:C:C2	45:u:2328:G:N2	2.89	0.41
45:u:2661:U:HO2'	45:u:2662:G:P	2.43	0.41
45:u:4131:G:C6	45:u:4132:C:C4	3.08	0.41
45:u:4433:G:C2	45:u:4434:C:C2	3.09	0.41
45:u:4583:C:N3	45:u:4718:G:C2	2.88	0.41
45:u:5031:G:C2	45:u:5032:C:C2	3.09	0.41
47:w:46:G:N2	47:w:47:C:C2	2.88	0.41
48:x:192:VAL:HG21	49:y:49:PHE:CD1	2.54	0.41
48:x:196:PHE:O	49:y:55:LYS:NZ	2.53	0.41
48:x:244:ASN:HA	48:x:439:GLY:O	2.20	0.41
48:x:288:ASN:ND2	48:x:428:ILE:HG13	2.35	0.41
53:3:52:VAL:HG13	53:3:53:ILE:HG13	2.01	0.41
1:A:107:MET:SD	1:A:113:VAL:CG1	3.09	0.41
3:C:229:LEU:HD22	3:C:229:LEU:N	2.35	0.41
4:D:64:ILE:CD1	4:D:109:LEU:HD22	2.50	0.41
8:H:95:VAL:CG1	38:m:78:ILE:HD11	2.51	0.41
15:P:10:ASN:N	15:P:10:ASN:OD1	2.53	0.41
24:Y:93:THR:HG22	48:x:26:ILE:HD13	0.48	0.41
40:o:39:ARG:NH1	45:u:295:A:OP2	2.52	0.41
45:u:29:G:C2	45:u:30:C:C2	3.08	0.41
45:u:196:C:C2	45:u:246:G:C2	3.08	0.41
45:u:385:A:C2	45:u:386:A:C5	3.08	0.41
45:u:1819:G:H5''	45:u:1819:G:C8	2.55	0.41
45:u:1959:U:O2'	45:u:1960:A:P	2.78	0.41
45:u:2793:G:O6	45:u:2797:C:C5	2.73	0.41
45:u:2889:G:C6	45:u:2890:C:C4	3.08	0.41
45:u:3752:C:O2'	45:u:3753:G:P	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:379:PHE:HD1	55:5:379:PHE:HA	1.73	0.41
9:I:49:CYS:SG	9:I:49:CYS:O	2.78	0.41
18:S:173:ASN:HA	45:u:4762:A:H2	1.86	0.41
31:f:13:GLY:HA2	31:f:97:ILE:CD1	2.50	0.41
35:j:55:ARG:NH2	45:u:364:G:O6	2.52	0.41
40:o:31:ASP:O	40:o:33:LEU:N	2.53	0.41
42:r:97:ILE:HG22	42:r:107:ARG:HB2	1.91	0.41
45:u:674:G:C2	45:u:675:C:C2	3.08	0.41
45:u:682:G:H2'	45:u:682:G:N3	2.35	0.41
45:u:975:C:H5''	45:u:976:G:OP2	2.20	0.41
45:u:1203:G:C2	45:u:1204:C:C2	3.08	0.41
45:u:1268:G:O4'	45:u:2111:G:C5	2.73	0.41
45:u:1277:G:C2	45:u:1278:C:C2	3.08	0.41
45:u:1349:G:C6	45:u:1350:C:C4	3.08	0.41
45:u:1412:G:C2	45:u:1413:C:C2	3.09	0.41
45:u:1721:G:C6	45:u:1722:C:C4	3.08	0.41
45:u:2076:G:C2	45:u:2077:C:C2	3.08	0.41
45:u:2465:C:H2'	45:u:2466:G:O4'	2.20	0.41
45:u:3937:C:H2'	45:u:3938:G:N2	2.35	0.41
45:u:4182:G:H5''	45:u:4183:G:OP2	2.20	0.41
45:u:4305:G:N3	45:u:4305:G:H2'	2.35	0.41
45:u:4349:C:H3'	45:u:4350:C:H5'	2.03	0.41
45:u:4595:G:C6	45:u:4596:C:C4	3.08	0.41
45:u:4911:A:H3'	45:u:4912:G:H5''	2.01	0.41
46:v:27:G:C6	46:v:28:C:C4	3.08	0.41
48:x:127:GLN:HA	48:x:130:VAL:HG12	2.02	0.41
48:x:417:ILE:O	48:x:421:ALA:N	2.52	0.41
48:x:443:SER:CB	48:x:447:ILE:HG13	2.31	0.41
55:5:355:THR:HB	55:5:359:SER:OG	2.20	0.41
55:5:488:ILE:CG2	55:5:531:GLN:NE2	2.84	0.41
2:B:116:ARG:HB3	2:B:177:LYS:HA	2.03	0.41
6:F:118:GLN:HG3	16:Q:3:VAL:HG22	2.03	0.41
8:H:5:LEU:HD13	8:H:60:TRP:CD2	2.56	0.41
13:N:200:LEU:HD23	13:N:200:LEU:HA	1.96	0.41
16:Q:148:VAL:HG13	16:Q:152:PHE:CZ	2.56	0.41
23:X:151:ASN:HD21	49:y:20:ARG:CZ	2.34	0.41
32:g:59:VAL:HG21	32:g:63:VAL:HG11	2.02	0.41
45:u:80:C:C2	45:u:104:G:N2	2.89	0.41
45:u:369:G:N2	45:u:372:A:OP2	2.50	0.41
45:u:479:G:C6	45:u:480:C:C4	3.08	0.41
45:u:1085:C:C2	45:u:1213:G:N1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1466:G:C2	45:u:1467:C:C2	3.09	0.41
45:u:2396:A:N6	45:u:2814:C:O2	2.54	0.41
45:u:3923:A:H2'	45:u:3924:C:C6	2.55	0.41
45:u:4152:G:C2	45:u:4153:C:C2	3.08	0.41
46:v:93:G:C6	46:v:94:C:C4	3.07	0.41
47:w:128:C:C5	47:w:129:C:C5	3.08	0.41
48:x:13:CYS:HB3	48:x:118:LEU:HD21	2.02	0.41
48:x:46:CYS:SG	49:y:54:VAL:HG11	2.61	0.41
48:x:453:ILE:O	48:x:457:TYR:HB2	2.20	0.41
50:z:68:VAL:HA	50:z:70:PRO:HD2	2.02	0.41
2:B:89:ILE:CD1	2:B:153:MET:HE1	2.50	0.41
7:G:58:PRO:CD	23:X:46:PHE:HD2	2.34	0.41
9:I:35:ASP:OD1	9:I:35:ASP:N	2.54	0.41
12:M:55:MET:O	18:S:157:ARG:NH2	2.53	0.41
13:N:64:ILE:HD11	13:N:102:ALA:HA	2.03	0.41
18:S:95:ARG:HD3	18:S:97:TYR:OH	2.19	0.41
45:u:169:G:C2	45:u:170:C:C2	3.09	0.41
45:u:209:U:C6	45:u:211:G:C8	3.08	0.41
45:u:235:A:C2	45:u:238:C:C5	3.08	0.41
45:u:689:U:O2	45:u:690:C:C6	2.73	0.41
45:u:715:G:H1	45:u:953:C:H42	1.68	0.41
45:u:931:C:C2'	45:u:932:A:O5'	2.68	0.41
45:u:1422:G:C2	45:u:1464:C:C2	3.09	0.41
45:u:1633:G:H5'	45:u:1634:A:OP1	2.20	0.41
45:u:1912:G:C6	45:u:1913:C:N4	2.89	0.41
45:u:2547:G:C2	45:u:2548:C:C2	3.09	0.41
45:u:4276:G:N2	45:u:4333:C:C2	2.88	0.41
45:u:4586:G:H5''	45:u:4586:G:C8	2.52	0.41
48:x:39:LEU:HD13	49:y:46:ILE:HG23	2.02	0.41
55:5:70:ASN:HB3	55:5:84:ILE:HG21	2.03	0.41
55:5:682:TYR:CE2	55:5:684:THR:HA	2.54	0.41
3:C:266:THR:HG22	3:C:269:LYS:HB3	2.02	0.41
13:N:11:TRP:CE3	13:N:44:ARG:NH2	2.89	0.41
23:X:147:LEU:HD21	49:y:20:ARG:NH2	2.36	0.41
31:f:72:GLY:HA3	31:f:88:PHE:CD2	2.56	0.41
32:g:63:VAL:O	32:g:64:LEU:C	2.63	0.41
33:h:6:ALA:O	33:h:7:ARG:C	2.64	0.41
35:j:59:THR:HG22	47:w:41:A:O2'	2.20	0.41
42:r:135:LYS:HZ1	45:u:451:C:C3'	2.30	0.41
45:u:167:C:C2	45:u:269:G:C2	3.08	0.41
45:u:197:A:H2'	45:u:198:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:684:G:HO2'	45:u:685:C:P	2.42	0.41
45:u:684:G:O2'	45:u:685:C:O5'	2.37	0.41
45:u:976:G:H2'	45:u:977:C:C1'	2.37	0.41
45:u:1439:C:O2	45:u:1439:C:O4'	2.39	0.41
45:u:2625:U:C4	45:u:2626:U:C4	3.09	0.41
45:u:4269:G:C6	45:u:4270:C:C4	3.09	0.41
48:x:33:LEU:HD22	53:3:121:LEU:CD1	2.51	0.41
55:5:638:LEU:HD23	55:5:638:LEU:HA	1.91	0.41
55:5:677:VAL:HG23	55:5:678:LEU:HG	2.02	0.41
1:A:117:GLU:OE1	1:A:121:GLY:N	2.52	0.41
3:C:190:ARG:NE	3:C:199:ARG:O	2.44	0.41
25:Z:73:LYS:HG2	25:Z:75:TYR:CZ	2.56	0.41
29:d:79:ASN:OD1	29:d:79:ASN:N	2.53	0.41
45:u:28:C:C2	45:u:55:G:N2	2.88	0.41
45:u:303:C:H2'	45:u:304:C:O4'	2.21	0.41
45:u:1264:C:C4	45:u:1265:G:N7	2.88	0.41
45:u:1424:G:H2'	45:u:1425:G:O4'	2.21	0.41
45:u:1441:C:N4	45:u:1442:C:N4	2.69	0.41
45:u:2433:G:H4'	48:x:268:LYS:HD3	2.02	0.41
45:u:2645:G:C2	45:u:2646:C:C2	3.08	0.41
45:u:3786:U:O4'	45:u:4537:C:O2'	2.36	0.41
45:u:4408:G:C2	45:u:4409:C:C2	3.08	0.41
47:w:56:G:C4	47:w:62:A:C2	3.08	0.41
48:x:418:PRO:O	48:x:421:ALA:HB3	2.20	0.41
55:5:41:PHE:CZ	55:5:489:VAL:HG11	2.56	0.41
55:5:582:PHE:CE1	55:5:643:CYS:HB3	2.55	0.41
55:5:626:VAL:HG11	55:5:664:ARG:CZ	2.50	0.41
1:A:236:GLY:N	45:u:3687:A:O2'	2.52	0.41
3:C:76:ILE:HG22	3:C:77:PRO:CD	2.51	0.41
3:C:228:THR:OG1	3:C:248:ARG:NH2	2.54	0.41
4:D:43:LYS:O	4:D:46:THR:HG22	2.20	0.41
5:E:157:ARG:NH2	12:M:106:ASP:OD2	2.53	0.41
6:F:181:LEU:HD11	6:F:209:PHE:HB2	2.02	0.41
7:G:140:VAL:HG13	7:G:200:THR:OG1	2.21	0.41
8:H:109:GLY:O	8:H:110:SER:C	2.63	0.41
10:J:15:LEU:HD21	10:J:157:ILE:HD13	2.03	0.41
11:L:146:LEU:HB2	11:L:148:THR:HG22	2.01	0.41
12:M:116:LYS:HG2	14:O:196:LEU:CD2	2.35	0.41
13:N:124:ASP:OD1	45:u:3937:C:O2'	2.37	0.41
16:Q:24:TYR:CE1	42:r:5:LEU:HD13	2.56	0.41
16:Q:41:SER:OG	16:Q:44:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:123:LYS:O	25:Z:124:THR:HG23	2.20	0.41
26:a:90:ALA:O	26:a:91:ALA:HB3	2.21	0.41
26:a:98:ALA:HB2	26:a:121:PRO:HB2	2.03	0.41
28:c:30:GLY:O	28:c:34:THR:HG22	2.20	0.41
29:d:30:HIS:CG	29:d:82:TYR:CD1	3.09	0.41
30:e:100:ALA:HB3	30:e:103:VAL:HG23	2.02	0.41
30:e:104:SER:HB3	45:u:2303:C:OP1	2.21	0.41
36:k:28:ASN:ND2	45:u:2695:A:OP2	2.50	0.41
44:t:85:LEU:HD13	44:t:109:ILE:HG21	2.03	0.41
45:u:29:G:C6	45:u:30:C:C4	3.09	0.41
45:u:206:U:O2	45:u:206:U:H2'	2.20	0.41
45:u:254:G:C6	45:u:255:C:C4	3.09	0.41
45:u:258:G:N2	45:u:259:C:C2	2.89	0.41
45:u:462:G:C2'	45:u:463:A:H5'	2.51	0.41
45:u:933:G:C2	45:u:939:G:C2	3.09	0.41
45:u:960:A:N6	45:u:1283:G:O6	2.54	0.41
45:u:976:G:OP1	45:u:976:G:C4'	2.68	0.41
45:u:1205:G:N1	45:u:1206:C:C4	2.89	0.41
45:u:1279:A:C4	45:u:1280:C:N3	2.89	0.41
45:u:1431:C:H2'	45:u:1432:G:O4'	2.20	0.41
45:u:1466:G:C6	45:u:1467:C:C4	3.09	0.41
45:u:1721:G:C2	45:u:1722:C:C2	3.09	0.41
45:u:2052:G:C2	45:u:2053:C:C2	3.09	0.41
45:u:2301:G:C6	45:u:2302:C:C4	3.09	0.41
45:u:2613:C:N4	45:u:2614:C:N4	2.68	0.41
45:u:2623:A:C2	45:u:2624:G:C6	3.08	0.41
45:u:4131:G:C2	45:u:4132:C:C2	3.09	0.41
45:u:4595:G:C2	45:u:4596:C:C2	3.08	0.41
45:u:4661:G:C2	45:u:4662:C:C2	3.09	0.41
45:u:4868:G:H3'	45:u:4869:U:H5''	2.03	0.41
47:w:49:G:C6	47:w:50:C:C4	3.09	0.41
47:w:112:G:C6	47:w:113:C:C4	3.09	0.41
48:x:406:GLU:OE1	48:x:407:THR:HB	2.21	0.41
48:x:449:LEU:HA	48:x:449:LEU:HD23	1.70	0.41
55:5:122:LEU:HD11	55:5:126:PHE:CD2	2.56	0.41
55:5:178:LEU:C	55:5:178:LEU:CD2	2.85	0.41
55:5:207:SER:OG	55:5:208:SER:N	2.53	0.41
3:C:27:VAL:HG11	3:C:128:LEU:HD13	2.03	0.41
3:C:143:ARG:N	3:C:179:ASP:OD1	2.54	0.41
4:D:17:GLN:O	45:u:4265:U:N3	2.46	0.41
5:E:90:LYS:N	5:E:91:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:ALA:HB2	10:J:68:ILE:CD1	2.51	0.41
14:O:42:ASN:OD1	14:O:42:ASN:N	2.54	0.41
23:X:156:ILE:HG22	49:y:24:ARG:HE	1.86	0.41
28:c:31:TYR:HA	28:c:34:THR:HG22	2.02	0.41
45:u:22:G:C2	47:w:35:C:C4	3.09	0.41
45:u:119:G:H3'	45:u:120:A:H5'	2.03	0.41
45:u:119:G:H5''	45:u:119:G:C8	2.56	0.41
45:u:2630:U:O2'	45:u:2632:U:H4'	2.21	0.41
45:u:3717:A:O2'	45:u:3718:A:O5'	2.38	0.41
45:u:4326:G:C2	45:u:4327:C:C2	3.08	0.41
45:u:4473:A:C2	45:u:4474:A:C4	3.09	0.41
46:v:51:G:C2	46:v:52:C:C2	3.09	0.41
55:5:209:TRP:NE1	62:5:801:9UB:O27	2.54	0.41
55:5:488:ILE:CG2	55:5:531:GLN:HE22	2.33	0.41
55:5:631:SER:HA	55:5:632:PRO:HD3	1.81	0.41
1:A:27:ALA:HB1	1:A:77:ILE:HG13	2.03	0.40
5:E:59:TYR:CE2	5:E:64:LEU:HD12	2.48	0.40
9:I:204:GLY:C	9:I:205:PRO:O	2.64	0.40
16:Q:72:LEU:HB2	16:Q:75:ARG:HD3	2.03	0.40
42:r:47:LYS:HD3	42:r:102:TYR:CE2	2.50	0.40
45:u:368:C:C2	45:u:374:G:C2	3.09	0.40
45:u:933:G:N1	45:u:939:G:N2	2.69	0.40
45:u:1075:G:H2'	45:u:1076:C:C6	2.56	0.40
45:u:1351:G:C2	45:u:1352:C:C2	3.10	0.40
45:u:1412:G:C6	45:u:1413:C:C4	3.09	0.40
45:u:1834:U:O2	45:u:1834:U:H2'	2.20	0.40
45:u:2083:C:H4'	45:u:2084:C:OP2	2.21	0.40
45:u:2273:G:C6	45:u:2274:C:C4	3.10	0.40
45:u:2322:G:C2	45:u:2323:C:C2	3.09	0.40
45:u:2463:G:C6	45:u:2464:C:N4	2.89	0.40
45:u:2517:A:N1	45:u:2518:G:C2	2.89	0.40
45:u:2628:U:C4	45:u:2629:C:C5	3.09	0.40
45:u:2661:U:O2'	45:u:2662:G:O5'	2.40	0.40
45:u:2889:G:C2	45:u:2890:C:C2	3.09	0.40
45:u:3723:A:C2	45:u:3730:U:N3	2.89	0.40
45:u:4201:G:C6	45:u:4202:U:C4	3.09	0.40
45:u:4614:G:C6	45:u:4615:C:C4	3.09	0.40
46:v:16:A:H2'	46:v:17:C:C6	2.56	0.40
47:w:32:C:H2'	47:w:33:G:O4'	2.20	0.40
54:4:25:TYR:CE2	55:5:145:LEU:HD12	2.56	0.40
55:5:122:LEU:HD11	55:5:126:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:5:348:SER:OG	55:5:598:TRP:NE1	2.54	0.40
55:5:491:SER:O	55:5:588:TYR:OH	2.32	0.40
55:5:554:ARG:HB2	55:5:557:GLN:HE21	1.86	0.40
2:B:30:LYS:NZ	45:u:4717:A:OP2	2.49	0.40
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.56	0.40
4:D:200:MET:CE	4:D:241:LYS:CE	2.98	0.40
6:F:94:VAL:HG13	6:F:142:ILE:HD12	2.04	0.40
14:O:48:TYR:CE2	45:u:1930:U:C2	3.09	0.40
20:U:87:THR:CG2	20:U:102:VAL:HG21	2.51	0.40
21:V:98:PHE:O	21:V:99:GLU:HB3	2.21	0.40
31:f:15:LYS:HB3	31:f:25:THR:HB	2.03	0.40
35:j:81:GLY:C	35:j:82:THR:HG23	2.46	0.40
45:u:93:G:C2'	45:u:94:A:C8	3.04	0.40
45:u:465:G:N1	45:u:466:A:C5	2.89	0.40
45:u:1448:G:C2	45:u:2097:U:C4	3.10	0.40
45:u:1506:G:C2	45:u:1507:C:C2	3.09	0.40
45:u:1932:A:H2'	45:u:1933:G:C8	2.57	0.40
45:u:2862:G:H2'	45:u:3619:G:O6	2.21	0.40
45:u:3705:G:C2	45:u:3706:C:C2	3.09	0.40
45:u:4154:G:C2	45:u:4155:C:C2	3.09	0.40
45:u:4486:C:H2'	45:u:4487:A:O4'	2.21	0.40
46:v:66:G:C6	46:v:67:C:N3	2.89	0.40
47:w:154:G:C2	47:w:155:C:C2	3.09	0.40
55:5:593:ILE:HD13	55:5:639:MET:CG	2.42	0.40
1:A:181:LYS:HB3	45:u:1577:G:N7	2.36	0.40
3:C:173:LYS:NZ	45:u:218:A:N6	2.69	0.40
6:F:147:PRO:HA	6:F:243:ASN:OD1	2.22	0.40
8:H:137:SER:HB3	8:H:145:VAL:HG23	2.04	0.40
9:I:76:MET:HB3	9:I:85:PHE:CD2	2.56	0.40
12:M:81:ASP:O	12:M:84:THR:OG1	2.32	0.40
20:U:82:TYR:CZ	20:U:86:LEU:HD11	2.56	0.40
22:W:9:SER:HA	22:W:52:THR:HG22	2.04	0.40
31:f:8:LYS:HB3	31:f:100:ARG:CZ	2.52	0.40
45:u:2:G:C6	45:u:3:C:C4	3.09	0.40
45:u:247:G:C2	45:u:248:C:C2	3.09	0.40
45:u:301:G:C5	45:u:302:C:C4	3.08	0.40
45:u:488:G:C6	45:u:489:C:C4	3.09	0.40
45:u:695:G:H3'	45:u:696:C:H5'	2.02	0.40
45:u:730:G:N2	45:u:939:G:N2	2.69	0.40
45:u:751:G:N2	45:u:752:G:C5	2.89	0.40
45:u:971:U:C2'	45:u:972:C:H5'	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:1573:G:C6	45:u:1574:G:N1	2.89	0.40
45:u:1959:U:C1'	45:u:1961:G:O4'	2.70	0.40
45:u:2316:G:C2	45:u:2317:C:C2	3.10	0.40
45:u:2316:G:C6	45:u:2317:C:C4	3.09	0.40
45:u:2533:C:C2	45:u:2534:C:C5	3.08	0.40
45:u:4395:U:H5'	45:u:4395:U:H6	1.85	0.40
45:u:4411:G:C6	45:u:4412:C:C4	3.10	0.40
45:u:4476:C:O2	45:u:4476:C:O4'	2.39	0.40
45:u:4495:G:C2	45:u:4506:C:C2	3.09	0.40
45:u:4900:C:O2'	45:u:4901:G:P	2.80	0.40
48:x:61:PRO:O	48:x:65:MET:CA	2.57	0.40
54:4:18:LEU:HD22	55:5:29:LEU:HD12	2.01	0.40
55:5:77:TRP:O	55:5:80:LEU:N	2.54	0.40
1:A:66:PRO:HG2	1:A:67:TYR:CE2	2.57	0.40
1:A:227:ARG:NH2	45:u:3659:G:O2'	2.50	0.40
4:D:278:ASP:O	4:D:281:ALA:HB3	2.20	0.40
7:G:63:LEU:HD12	13:N:32:GLN:HB3	2.02	0.40
8:H:41:ILE:HG12	8:H:73:ILE:CG1	2.52	0.40
10:J:165:TRP:CH2	10:J:170:TYR:HE2	2.39	0.40
13:N:50:ARG:NH2	45:u:279:A:OP2	2.54	0.40
29:d:42:ALA:N	29:d:43:PRO:CD	2.85	0.40
30:e:43:ASN:O	30:e:44:ARG:C	2.63	0.40
40:o:23:VAL:HG13	40:o:68:LEU:HB3	2.04	0.40
45:u:35:U:H5'	45:u:36:U:OP2	2.21	0.40
45:u:482:G:H2'	45:u:483:G:N9	2.36	0.40
45:u:1203:G:C6	45:u:1204:C:C4	3.10	0.40
45:u:1383:G:C2	45:u:1384:C:C2	3.10	0.40
45:u:1732:C:O2	45:u:1798:G:C2	2.75	0.40
45:u:1806:G:C6	45:u:1807:C:C4	3.09	0.40
45:u:2301:G:C2	45:u:2302:C:C2	3.09	0.40
45:u:2463:G:C6	45:u:2464:C:C4	3.10	0.40
45:u:2481:G:N2	45:u:2498:C:C2	2.90	0.40
45:u:2688:G:N1	45:u:2689:C:C4	2.89	0.40
45:u:2882:A:H2'	45:u:2883:G:H5'	2.04	0.40
45:u:4116:C:O2	45:u:4116:C:O2'	2.36	0.40
45:u:4198:G:C5	45:u:4199:C:C5	3.09	0.40
45:u:4453:C:H2'	45:u:4454:G:O4'	2.21	0.40
45:u:4561:C:C2	45:u:4562:C:C5	3.10	0.40
45:u:4664:A:H2'	45:u:4665:A:O4'	2.21	0.40
45:u:4714:C:C5	45:u:4715:C:C5	3.09	0.40
47:w:31:G:C6	47:w:32:C:C4	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:103:A:C8	47:w:104:A:C8	3.09	0.40
47:w:112:G:C2	47:w:113:C:C2	3.10	0.40
48:x:88:GLY:HA2	48:x:116:GLN:NE2	2.36	0.40
55:5:392:TYR:CZ	55:5:413:VAL:HG22	2.57	0.40
1:A:27:ALA:O	1:A:128:ARG:NH2	2.54	0.40
5:E:41:SER:CB	45:u:978:G:H5'	2.51	0.40
5:E:124:HIS:CD2	45:u:1282:G:C5	3.09	0.40
5:E:225:GLU:CA	42:r:135:LYS:CE	2.98	0.40
8:H:172:ILE:HD12	38:m:90:ASN:HB3	2.02	0.40
12:M:64:PHE:HB2	12:M:65:PRO:HD2	2.03	0.40
23:X:147:LEU:HD23	49:y:20:ARG:NH2	2.35	0.40
25:Z:38:TYR:CD1	25:Z:76:ASN:OD1	2.74	0.40
44:t:30:PRO:O	44:t:33:GLY:N	2.49	0.40
45:u:211:G:N1	45:u:212:A:N7	2.70	0.40
45:u:471:A:N1	45:u:472:C:N1	2.69	0.40
45:u:518:G:C6	45:u:519:C:C4	3.09	0.40
45:u:674:G:C6	45:u:675:C:C4	3.10	0.40
45:u:680:G:C2	45:u:681:G:C4	3.09	0.40
45:u:941:C:H2'	45:u:942:G:O4'	2.21	0.40
45:u:1349:G:C2	45:u:1350:C:C2	3.10	0.40
45:u:1385:G:C6	45:u:1386:C:C4	3.09	0.40
45:u:1550:G:N1	45:u:1551:C:C2	2.89	0.40
45:u:1981:G:O2'	45:u:1982:G:C8	2.75	0.40
45:u:2058:G:C6	45:u:2059:C:C4	3.09	0.40
45:u:2408:U:H1'	45:u:2409:U:C5	2.56	0.40
45:u:3706:C:H2'	45:u:3707:U:O4'	2.22	0.40
45:u:4472:G:H2'	45:u:4473:A:H5'	2.04	0.40
47:w:106:G:N1	47:w:107:C:C4	2.90	0.40
48:x:184:ALA:N	49:y:47:MET:HG3	2.17	0.40
48:x:297:LEU:HD13	48:x:297:LEU:HA	1.90	0.40
48:x:458:PHE:CZ	49:y:36:ILE:HG22	2.56	0.40
48:x:462:VAL:O	48:x:463:LYS:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/244 (99%)	209 (86%)	28 (12%)	5 (2%)	5	30
2	B	392/394 (100%)	345 (88%)	42 (11%)	5 (1%)	9	42
3	C	360/362 (99%)	322 (89%)	27 (8%)	11 (3%)	3	22
4	D	290/292 (99%)	262 (90%)	25 (9%)	3 (1%)	12	49
5	E	232/248 (94%)	179 (77%)	36 (16%)	17 (7%)	1	10
6	F	223/225 (99%)	204 (92%)	17 (8%)	2 (1%)	14	51
7	G	239/241 (99%)	203 (85%)	31 (13%)	5 (2%)	5	30
8	H	188/190 (99%)	166 (88%)	19 (10%)	3 (2%)	7	38
9	I	200/213 (94%)	181 (90%)	15 (8%)	4 (2%)	6	31
10	J	167/169 (99%)	147 (88%)	13 (8%)	7 (4%)	2	17
11	L	208/210 (99%)	180 (86%)	16 (8%)	12 (6%)	1	14
12	M	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	18	56
13	N	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
14	O	197/199 (99%)	184 (93%)	12 (6%)	1 (0%)	24	63
15	P	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
16	Q	185/187 (99%)	169 (91%)	14 (8%)	2 (1%)	11	46
17	R	178/180 (99%)	166 (93%)	9 (5%)	3 (2%)	7	36
18	S	173/175 (99%)	157 (91%)	12 (7%)	4 (2%)	5	28
19	T	157/159 (99%)	139 (88%)	15 (10%)	3 (2%)	6	32
20	U	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	2	18
21	V	129/131 (98%)	115 (89%)	13 (10%)	1 (1%)	16	54
22	W	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	7	38
23	X	117/119 (98%)	109 (93%)	6 (5%)	2 (2%)	7	36
24	Y	132/134 (98%)	114 (86%)	17 (13%)	1 (1%)	16	54
25	Z	133/135 (98%)	113 (85%)	13 (10%)	7 (5%)	1	15
26	a	145/147 (99%)	122 (84%)	19 (13%)	4 (3%)	4	24
27	b	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	9	40
28	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	d	105/107 (98%)	91 (87%)	13 (12%)	1 (1%)	12	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	e	126/128 (98%)	115 (91%)	6 (5%)	5 (4%)	2	18
31	f	107/109 (98%)	94 (88%)	8 (8%)	5 (5%)	2	16
32	g	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	14	51
33	h	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3	21
34	i	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	6	31
35	j	84/86 (98%)	71 (84%)	8 (10%)	5 (6%)	1	13
36	k	67/69 (97%)	56 (84%)	7 (10%)	4 (6%)	1	13
37	l	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	5	30
38	m	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
39	n	21/23 (91%)	21 (100%)	0	0	100	100
40	o	102/104 (98%)	92 (90%)	7 (7%)	3 (3%)	3	23
41	p	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	11	46
42	r	132/136 (97%)	113 (86%)	12 (9%)	7 (5%)	1	15
43	s	196/198 (99%)	164 (84%)	22 (11%)	10 (5%)	1	15
44	t	161/163 (99%)	102 (63%)	33 (20%)	26 (16%)	0	2
48	x	418/461 (91%)	372 (89%)	45 (11%)	1 (0%)	43	78
49	y	60/62 (97%)	52 (87%)	8 (13%)	0	100	100
50	z	27/29 (93%)	25 (93%)	1 (4%)	1 (4%)	2	20
51	1	21/162 (13%)	21 (100%)	0	0	100	100
53	3	118/120 (98%)	99 (84%)	18 (15%)	1 (1%)	16	54
54	4	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
55	5	632/705 (90%)	538 (85%)	88 (14%)	6 (1%)	14	51
All	All	8026/8406 (96%)	7041 (88%)	792 (10%)	193 (2%)	7	27

All (193) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	TRP
3	C	273	LEU
5	E	91	PRO
5	E	95	ASP
5	E	118	PRO
5	E	175	LEU
5	E	221	PRO

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Mol	Chain	Res	Type
7	G	45	ILE
7	G	128	VAL
8	H	40	HIS
8	H	110	SER
9	I	47	PRO
11	L	64	VAL
11	L	67	HIS
17	R	36	ASN
18	S	165	PRO
20	U	47	ILE
25	Z	84	ARG
26	a	90	ALA
29	d	94	GLU
30	e	92	ASN
31	f	80	ASN
33	h	7	ARG
36	k	61	PRO
40	o	32	SER
42	r	86	ALA
43	s	62	ARG
43	s	201	PRO
44	t	29	ALA
44	t	30	PRO
44	t	31	LYS
44	t	53	TRP
44	t	89	PRO
44	t	144	ASP
44	t	148	PRO
44	t	149	HIS
48	x	445	THR
55	5	84	ILE
55	5	89	TYR
1	A	217	GLN
2	B	38	SER
2	B	302	ASN
3	C	73	VAL
3	C	155	GLU
3	C	275	SER
4	D	187	SER
5	E	85	LEU
5	E	92	VAL
5	E	174	PRO

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Mol	Chain	Res	Type
5	E	234	GLU
10	J	116	GLY
10	J	155	HIS
11	L	63	THR
11	L	143	GLU
11	L	172	GLU
17	R	130	ASN
18	S	88	SER
19	T	81	LYS
20	U	98	ASP
23	X	131	ASP
25	Z	34	SER
26	a	76	ASP
30	e	44	ARG
34	i	11	LEU
35	j	36	LYS
35	j	39	TYR
42	r	67	ARG
42	r	71	ARG
43	s	70	GLU
43	s	106	LYS
43	s	109	ALA
44	t	5	PHE
44	t	26	SER
44	t	39	PRO
44	t	58	ILE
44	t	106	PHE
55	5	360	TYR
55	5	361	TYR
2	B	18	PRO
3	C	16	GLU
3	C	132	ALA
3	C	248	ARG
5	E	96	LYS
5	E	179	ARG
5	E	232	GLU
6	F	239	GLU
9	I	205	PRO
10	J	11	PRO
10	J	146	ARG
16	Q	14	ARG
17	R	19	LYS

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Mol	Chain	Res	Type
21	V	14	PHE
25	Z	55	ALA
25	Z	124	THR
26	a	92	LYS
30	e	125	PRO
30	e	126	ASN
31	f	37	ASP
31	f	79	GLY
33	h	97	LYS
34	i	3	LEU
36	k	32	VAL
37	l	47	THR
42	r	19	LYS
42	r	85	ASN
43	s	69	LEU
43	s	108	PRO
43	s	142	GLY
44	t	54	LYS
44	t	67	ARG
44	t	105	THR
44	t	137	GLN
53	3	64	ASP
55	5	661	ASP
1	A	180	LEU
2	B	54	THR
5	E	129	PHE
5	E	224	GLN
8	H	101	ILE
11	L	5	ARG
11	L	52	SER
19	T	29	THR
24	Y	83	GLU
25	Z	31	ASP
26	a	98	ALA
30	e	89	LEU
32	g	65	MET
33	h	89	ARG
36	k	29	LYS
41	p	41	PHE
44	t	2	PRO
44	t	18	THR
1	A	130	SER

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Mol	Chain	Res	Type
2	B	309	LEU
4	D	20	PHE
5	E	218	LEU
5	E	229	PHE
7	G	123	ALA
7	G	125	LYS
10	J	153	ALA
11	L	6	ASN
11	L	103	ARG
16	Q	148	VAL
20	U	27	HIS
25	Z	91	LEU
31	f	107	PRO
33	h	40	ALA
35	j	34	CYS
35	j	61	THR
36	k	21	LYS
40	o	77	CYS
42	r	11	ARG
43	s	34	ASN
44	t	7	PRO
55	5	616	ASP
1	A	67	TYR
3	C	222	ARG
3	C	309	ILE
10	J	124	GLY
11	L	100	PRO
11	L	169	ILE
14	O	49	ARG
18	S	5	GLY
20	U	67	LYS
22	W	15	PRO
31	f	106	TYR
35	j	60	GLY
40	o	33	LEU
44	t	10	ILE
44	t	19	GLY
44	t	22	VAL
3	C	133	LEU
9	I	99	ILE
27	b	21	ILE
43	s	73	PRO

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Mol	Chain	Res	Type
4	D	125	VAL
11	L	134	PRO
25	Z	90	PRO
3	C	265	GLY
5	E	103	VAL
6	F	230	VAL
7	G	238	GLY
9	I	201	PRO
19	T	44	GLY
10	J	174	ILE
12	M	7	VAL
18	S	155	PRO
44	t	3	PRO
44	t	98	ILE
23	X	119	ILE
42	r	69	GLY
44	t	23	GLY
50	z	71	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/187 (100%)	158 (84%)	29 (16%)	2	12
2	B	336/342 (98%)	282 (84%)	54 (16%)	2	11
3	C	302/302 (100%)	261 (86%)	41 (14%)	3	14
4	D	247/247 (100%)	218 (88%)	29 (12%)	5	18
5	E	208/221 (94%)	183 (88%)	25 (12%)	5	17
6	F	194/195 (100%)	167 (86%)	27 (14%)	3	14
7	G	206/206 (100%)	181 (88%)	25 (12%)	5	17
8	H	169/169 (100%)	147 (87%)	22 (13%)	4	15
9	I	174/180 (97%)	151 (87%)	23 (13%)	4	15
10	J	142/142 (100%)	125 (88%)	17 (12%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	176/176 (100%)	142 (81%)	34 (19%)	1	7
12	M	117/117 (100%)	101 (86%)	16 (14%)	3	14
13	N	171/171 (100%)	148 (86%)	23 (14%)	4	14
14	O	171/171 (100%)	144 (84%)	27 (16%)	2	11
15	P	134/134 (100%)	121 (90%)	13 (10%)	8	24
16	Q	163/163 (100%)	142 (87%)	21 (13%)	4	15
17	R	159/159 (100%)	141 (89%)	18 (11%)	5	19
18	S	156/156 (100%)	133 (85%)	23 (15%)	3	13
19	T	139/139 (100%)	120 (86%)	19 (14%)	3	14
20	U	89/89 (100%)	83 (93%)	6 (7%)	15	36
21	V	101/101 (100%)	82 (81%)	19 (19%)	1	8
22	W	55/55 (100%)	48 (87%)	7 (13%)	4	16
23	X	107/107 (100%)	94 (88%)	13 (12%)	5	17
24	Y	124/124 (100%)	109 (88%)	15 (12%)	5	17
25	Z	117/117 (100%)	107 (92%)	10 (8%)	10	29
26	a	119/119 (100%)	108 (91%)	11 (9%)	8	27
27	b	62/62 (100%)	56 (90%)	6 (10%)	8	24
28	c	79/79 (100%)	66 (84%)	13 (16%)	2	10
29	d	98/98 (100%)	79 (81%)	19 (19%)	1	7
30	e	114/114 (100%)	94 (82%)	20 (18%)	2	9
31	f	88/88 (100%)	74 (84%)	14 (16%)	2	11
32	g	98/98 (100%)	84 (86%)	14 (14%)	3	13
33	h	109/109 (100%)	99 (91%)	10 (9%)	8	27
34	i	86/86 (100%)	79 (92%)	7 (8%)	11	31
35	j	73/73 (100%)	63 (86%)	10 (14%)	3	14
36	k	64/64 (100%)	57 (89%)	7 (11%)	6	21
37	l	47/47 (100%)	40 (85%)	7 (15%)	3	12
38	m	48/48 (100%)	40 (83%)	8 (17%)	2	10
39	n	22/22 (100%)	19 (86%)	3 (14%)	3	14
40	o	92/92 (100%)	78 (85%)	14 (15%)	3	12
41	p	74/74 (100%)	66 (89%)	8 (11%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	r	120/120 (100%)	96 (80%)	24 (20%)	1	7
43	s	166/166 (100%)	156 (94%)	10 (6%)	17	39
44	t	136/136 (100%)	127 (93%)	9 (7%)	15	37
48	x	360/388 (93%)	344 (96%)	16 (4%)	25	47
49	y	53/53 (100%)	51 (96%)	2 (4%)	29	50
50	z	26/26 (100%)	20 (77%)	6 (23%)	1	5
51	1	20/20 (100%)	20 (100%)	0	100	100
53	3	61/101 (60%)	58 (95%)	3 (5%)	22	43
54	4	30/30 (100%)	29 (97%)	1 (3%)	33	55
55	5	528/615 (86%)	512 (97%)	16 (3%)	36	57
All	All	6917/7098 (97%)	6103 (88%)	814 (12%)	7	18

All (814) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	44	ILE
1	A	49	ILE
1	A	64	ARG
1	A	77	ILE
1	A	82	ILE
1	A	96	LEU
1	A	97	ASN
1	A	101	VAL
1	A	102	LEU
1	A	123	ARG
1	A	128	ARG
1	A	142	GLU
1	A	149	LYS
1	A	158	ILE
1	A	163	ARG
1	A	165	VAL
1	A	175	ILE
1	A	180	LEU
1	A	193	ARG
1	A	200	ARG
1	A	207	VAL
1	A	218	HIS

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Mol	Chain	Res	Type
1	A	221	LYS
1	A	226	ARG
1	A	227	ARG
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
2	B	4	ARG
2	B	10	ARG
2	B	19	ARG
2	B	21	ARG
2	B	31	SER
2	B	39	LYS
2	B	43	LEU
2	B	56	ILE
2	B	61	ASP
2	B	66	LYS
2	B	67	VAL
2	B	73	VAL
2	B	74	GLU
2	B	90	VAL
2	B	94	GLU
2	B	99	LEU
2	B	101	THR
2	B	103	LYS
2	B	116	ARG
2	B	135	LYS
2	B	138	GLN
2	B	146	LEU
2	B	154	LYS
2	B	158	GLN
2	B	162	VAL
2	B	167	GLN
2	B	173	LEU
2	B	201	LEU
2	B	203	GLN
2	B	213	GLN
2	B	214	ASP
2	B	232	THR
2	B	240	LEU
2	B	244	THR
2	B	249	ARG
2	B	258	HIS

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Mol	Chain	Res	Type
2	B	261	ARG
2	B	262	VAL
2	B	268	ARG
2	B	279	GLU
2	B	294	LYS
2	B	312	LYS
2	B	314	ILE
2	B	329	ASP
2	B	333	LEU
2	B	340	THR
2	B	352	LEU
2	B	354	GLN
2	B	356	LYS
2	B	357	ARG
2	B	366	LYS
2	B	368	ILE
2	B	381	THR
2	B	383	GLU
3	C	14	LYS
3	C	20	LYS
3	C	44	LEU
3	C	54	VAL
3	C	55	SER
3	C	57	LEU
3	C	66	SER
3	C	71	ARG
3	C	80	ARG
3	C	95	MET
3	C	101	MET
3	C	113	ARG
3	C	114	ARG
3	C	120	LYS
3	C	124	ILE
3	C	144	ILE
3	C	147	VAL
3	C	150	LEU
3	C	155	GLU
3	C	159	GLU
3	C	165	LYS
3	C	175	LYS
3	C	179	ASP
3	C	188	ARG

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Mol	Chain	Res	Type
3	C	193	LYS
3	C	195	LYS
3	C	204	ARG
3	C	208	CYS
3	C	219	LYS
3	C	232	VAL
3	C	237	ILE
3	C	246	VAL
3	C	281	MET
3	C	284	MET
3	C	287	THR
3	C	307	LYS
3	C	312	ARG
3	C	333	LYS
3	C	342	ARG
3	C	345	ARG
3	C	348	LYS
4	D	4	VAL
4	D	22	ARG
4	D	23	ARG
4	D	33	ARG
4	D	37	VAL
4	D	50	ARG
4	D	89	LYS
4	D	94	ASN
4	D	104	LEU
4	D	110	LEU
4	D	111	ASN
4	D	124	GLU
4	D	129	GLU
4	D	179	ARG
4	D	189	GLU
4	D	196	ARG
4	D	202	GLN
4	D	208	MET
4	D	221	LYS
4	D	225	GLN
4	D	239	MET
4	D	248	ARG
4	D	249	GLU
4	D	256	LYS
4	D	264	LYS

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Mol	Chain	Res	Type
4	D	268	ARG
4	D	279	ARG
4	D	284	LYS
4	D	293	ARG
5	E	43	ASN
5	E	46	LEU
5	E	52	ARG
5	E	101	ARG
5	E	105	LEU
5	E	124	HIS
5	E	126	ARG
5	E	136	LEU
5	E	137	ARG
5	E	148	ILE
5	E	158	VAL
5	E	162	LYS
5	E	171	VAL
5	E	190	VAL
5	E	197	ILE
5	E	206	LYS
5	E	208	LEU
5	E	212	TYR
5	E	218	LEU
5	E	219	ARG
5	E	233	LYS
5	E	250	ASP
5	E	254	LEU
5	E	282	LEU
5	E	284	PHE
6	F	33	LYS
6	F	38	LYS
6	F	41	GLN
6	F	44	LEU
6	F	49	ARG
6	F	68	ARG
6	F	70	GLU
6	F	72	ARG
6	F	76	MET
6	F	82	ASN
6	F	90	LYS
6	F	91	LEU
6	F	100	ILE

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Mol	Chain	Res	Type
6	F	127	LEU
6	F	137	ILE
6	F	154	GLU
6	F	179	ARG
6	F	181	LEU
6	F	189	MET
6	F	190	GLU
6	F	192	LEU
6	F	201	LYS
6	F	202	ARG
6	F	214	LYS
6	F	216	SER
6	F	239	GLU
6	F	248	ARG
7	G	28	VAL
7	G	55	VAL
7	G	75	LYS
7	G	95	LEU
7	G	106	THR
7	G	110	LYS
7	G	112	GLN
7	G	131	LYS
7	G	148	GLU
7	G	150	LYS
7	G	151	LYS
7	G	154	LEU
7	G	170	LEU
7	G	173	LEU
7	G	175	ARG
7	G	176	LYS
7	G	177	MET
7	G	189	ARG
7	G	202	VAL
7	G	210	GLU
7	G	217	LYS
7	G	220	GLU
7	G	229	ARG
7	G	240	ASN
7	G	259	LYS
8	H	1	MET
8	H	20	LEU
8	H	26	ILE

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Mol	Chain	Res	Type
8	H	41	ILE
8	H	52	LYS
8	H	57	VAL
8	H	59	LYS
8	H	65	LYS
8	H	66	GLU
8	H	74	CYS
8	H	78	GLN
8	H	104	VAL
8	H	111	LEU
8	H	123	ILE
8	H	125	ARG
8	H	128	MET
8	H	129	ARG
8	H	141	LYS
8	H	162	GLN
8	H	173	ARG
8	H	177	ASP
8	H	183	GLU
9	I	8	CYS
9	I	13	LYS
9	I	35	ASP
9	I	36	LEU
9	I	39	LYS
9	I	43	VAL
9	I	48	LEU
9	I	76	MET
9	I	97	ILE
9	I	116	ARG
9	I	125	THR
9	I	129	VAL
9	I	136	MET
9	I	144	ASN
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	180	GLU
9	I	195	CYS
9	I	198	LYS
9	I	202	ASN
9	I	208	LYS
9	I	212	LEU

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Mol	Chain	Res	Type
10	J	15	LEU
10	J	16	ARG
10	J	33	LEU
10	J	34	THR
10	J	49	VAL
10	J	68	ILE
10	J	72	CYS
10	J	83	LEU
10	J	90	ARG
10	J	91	GLU
10	J	96	LYS
10	J	110	GLN
10	J	111	GLU
10	J	113	ILE
10	J	146	ARG
10	J	151	ILE
10	J	168	GLN
11	L	10	LEU
11	L	11	LYS
11	L	28	GLN
11	L	35	ARG
11	L	46	ILE
11	L	49	ARG
11	L	59	VAL
11	L	61	CYS
11	L	64	VAL
11	L	65	ARG
11	L	67	HIS
11	L	77	SER
11	L	80	GLU
11	L	92	ARG
11	L	94	ILE
11	L	99	ASP
11	L	107	THR
11	L	111	GLN
11	L	113	ASN
11	L	115	GLN
11	L	121	ARG
11	L	123	LYS
11	L	130	LYS
11	L	143	GLU
11	L	145	LYS

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Mol	Chain	Res	Type
11	L	158	ARG
11	L	162	LYS
11	L	165	LYS
11	L	186	ARG
11	L	190	ARG
11	L	194	ILE
11	L	195	ARG
11	L	198	ARG
11	L	201	GLU
12	M	4	ARG
12	M	8	GLU
12	M	25	VAL
12	M	33	GLN
12	M	37	LEU
12	M	38	VAL
12	M	46	ARG
12	M	48	GLN
12	M	53	LYS
12	M	57	LEU
12	M	61	ILE
12	M	70	GLN
12	M	96	GLU
12	M	105	THR
12	M	119	ARG
12	M	130	LEU
13	N	9	GLU
13	N	17	ASP
13	N	26	ARG
13	N	32	GLN
13	N	44	ARG
13	N	47	LYS
13	N	61	ILE
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	80	THR
13	N	87	HIS
13	N	89	VAL
13	N	92	LEU
13	N	104	GLU
13	N	108	ARG
13	N	131	GLU

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Mol	Chain	Res	Type
13	N	151	ILE
13	N	174	LEU
13	N	197	THR
13	N	198	LEU
13	N	199	GLN
13	N	202	ARG
14	O	5	GLN
14	O	16	LEU
14	O	27	VAL
14	O	31	ARG
14	O	36	VAL
14	O	37	ARG
14	O	38	CYS
14	O	42	ASN
14	O	49	ARG
14	O	52	LEU
14	O	60	LYS
14	O	62	MET
14	O	67	SER
14	O	82	ARG
14	O	85	ARG
14	O	103	LYS
14	O	119	VAL
14	O	128	ARG
14	O	145	VAL
14	O	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	185	VAL
14	O	187	LYS
14	O	195	VAL
14	O	201	PHE
14	O	202	LEU
15	P	5	SER
15	P	24	VAL
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	92	LEU
15	P	99	GLU
15	P	100	SER
15	P	105	LYS

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Mol	Chain	Res	Type
15	P	118	GLN
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	9	LYS
16	Q	13	VAL
16	Q	31	LEU
16	Q	37	ARG
16	Q	54	SER
16	Q	58	ARG
16	Q	63	LEU
16	Q	85	THR
16	Q	89	ASP
16	Q	91	ARG
16	Q	93	GLN
16	Q	95	VAL
16	Q	108	ARG
16	Q	112	ARG
16	Q	115	LYS
16	Q	126	LEU
16	Q	132	LYS
16	Q	143	ARG
16	Q	144	LYS
16	Q	187	LYS
17	R	10	LEU
17	R	15	LEU
17	R	39	GLN
17	R	40	GLN
17	R	41	ILE
17	R	43	LYS
17	R	50	ILE
17	R	52	ARG
17	R	75	HIS
17	R	89	MET
17	R	99	MET
17	R	103	ARG
17	R	106	LEU
17	R	107	ARG
17	R	113	LYS
17	R	123	LEU
17	R	138	LEU

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Mol	Chain	Res	Type
17	R	178	GLN
18	S	2	LYS
18	S	9	GLU
18	S	13	VAL
18	S	17	LEU
18	S	39	VAL
18	S	48	VAL
18	S	67	VAL
18	S	70	LYS
18	S	82	LEU
18	S	83	ARG
18	S	84	TYR
18	S	86	SER
18	S	95	ARG
18	S	100	LEU
18	S	102	THR
18	S	125	GLN
18	S	127	MET
18	S	128	LYS
18	S	129	VAL
18	S	132	ILE
18	S	147	ASP
18	S	149	LYS
18	S	159	LEU
19	T	5	LYS
19	T	9	ARG
19	T	14	MET
19	T	17	ARG
19	T	31	MET
19	T	33	ILE
19	T	52	MET
19	T	60	LYS
19	T	81	LYS
19	T	96	ILE
19	T	99	SER
19	T	118	GLU
19	T	131	GLN
19	T	142	ARG
19	T	144	ASN
19	T	146	LYS
19	T	152	GLU
19	T	157	GLU

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Mol	Chain	Res	Type
19	T	159	MET
20	U	33	ILE
20	U	45	GLU
20	U	65	ARG
20	U	67	LYS
20	U	97	ARG
20	U	99	TRP
21	V	15	ARG
21	V	18	LEU
21	V	31	ASN
21	V	35	LYS
21	V	45	ILE
21	V	46	LYS
21	V	51	ARG
21	V	57	VAL
21	V	60	MET
21	V	61	VAL
21	V	69	LYS
21	V	82	ILE
21	V	91	LYS
21	V	97	TYR
21	V	99	GLU
21	V	106	VAL
21	V	109	LYS
21	V	113	LYS
21	V	123	LYS
22	W	4	GLU
22	W	27	LYS
22	W	41	LEU
22	W	43	LYS
22	W	44	ARG
22	W	54	LEU
22	W	57	ARG
23	X	39	LYS
23	X	41	ARG
23	X	42	THR
23	X	50	LYS
23	X	52	LEU
23	X	59	LYS
23	X	62	ARG
23	X	63	LYS
23	X	94	ASN

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Mol	Chain	Res	Type
23	X	111	GLN
23	X	129	ARG
23	X	145	ASP
23	X	152	LYS
24	Y	2	LYS
24	Y	7	VAL
24	Y	8	THR
24	Y	28	LYS
24	Y	34	LEU
24	Y	52	ASP
24	Y	55	VAL
24	Y	59	ARG
24	Y	65	GLN
24	Y	72	GLN
24	Y	79	VAL
24	Y	87	ARG
24	Y	104	VAL
24	Y	115	ARG
24	Y	126	ARG
25	Z	3	LYS
25	Z	11	VAL
25	Z	57	MET
25	Z	59	LYS
25	Z	60	LYS
25	Z	67	LYS
25	Z	68	ILE
25	Z	93	LYS
25	Z	100	VAL
25	Z	121	ARG
26	a	12	ARG
26	a	14	HIS
26	a	39	HIS
26	a	40	HIS
26	a	47	LYS
26	a	59	ARG
26	a	82	VAL
26	a	84	GLU
26	a	116	LYS
26	a	122	VAL
26	a	140	VAL
27	b	21	ILE
27	b	22	LYS

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Mol	Chain	Res	Type
27	b	27	GLN
27	b	28	ARG
27	b	43	MET
27	b	51	LYS
28	c	28	VAL
28	c	37	MET
28	c	40	GLN
28	c	50	ASN
28	c	59	GLU
28	c	61	GLU
28	c	77	ASN
28	c	78	ASN
28	c	81	LEU
28	c	87	LYS
28	c	91	VAL
28	c	94	LEU
28	c	98	ASP
29	d	19	GLU
29	d	23	ARG
29	d	26	THR
29	d	33	ILE
29	d	36	VAL
29	d	44	ARG
29	d	48	GLU
29	d	56	GLU
29	d	75	LYS
29	d	78	ARG
29	d	79	ASN
29	d	85	ARG
29	d	86	VAL
29	d	90	ARG
29	d	94	GLU
29	d	102	LEU
29	d	105	LEU
29	d	107	THR
29	d	116	ASN
30	e	8	VAL
30	e	9	LYS
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	24	GLN

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Mol	Chain	Res	Type
30	e	30	LYS
30	e	36	ARG
30	e	46	ARG
30	e	48	ARG
30	e	64	LYS
30	e	76	LYS
30	e	78	LEU
30	e	80	HIS
30	e	91	CYS
30	e	104	SER
30	e	106	LYS
30	e	107	ASN
30	e	109	LYS
30	e	113	GLU
31	f	33	VAL
31	f	36	ARG
31	f	38	GLU
31	f	40	GLU
31	f	46	ARG
31	f	52	LYS
31	f	56	ASN
31	f	64	PRO
31	f	69	VAL
31	f	84	VAL
31	f	100	ARG
31	f	101	ILE
31	f	103	VAL
31	f	110	ILE
32	g	5	LEU
32	g	6	THR
32	g	11	LEU
32	g	14	ASN
32	g	15	THR
32	g	43	LYS
32	g	54	ARG
32	g	60	ARG
32	g	64	LEU
32	g	66	ARG
32	g	74	VAL
32	g	90	ARG
32	g	100	GLN
32	g	115	LYS

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Mol	Chain	Res	Type
33	h	14	LYS
33	h	28	LEU
33	h	65	GLN
33	h	67	GLU
33	h	88	THR
33	h	97	LYS
33	h	104	THR
33	h	117	ARG
33	h	121	VAL
33	h	122	LYS
34	i	33	LEU
34	i	44	ILE
34	i	71	LYS
34	i	86	LYS
34	i	87	ARG
34	i	89	GLU
34	i	103	LYS
35	j	2	THR
35	j	3	LYS
35	j	15	THR
35	j	20	ARG
35	j	25	LYS
35	j	29	LEU
35	j	33	THR
35	j	61	THR
35	j	63	ARG
35	j	79	ARG
36	k	31	ASN
36	k	39	SER
36	k	44	THR
36	k	57	LYS
36	k	66	VAL
36	k	69	LEU
36	k	70	LYS
37	l	8	ARG
37	l	16	LYS
37	l	17	GLN
37	l	28	ARG
37	l	36	ARG
37	l	46	ARG
37	l	49	LEU
38	m	79	GLU

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Mol	Chain	Res	Type
38	m	82	LEU
38	m	85	LEU
38	m	97	ARG
38	m	98	LYS
38	m	106	ARG
38	m	111	ARG
38	m	119	ASN
39	n	2	ARG
39	n	9	ARG
39	n	13	LEU
40	o	14	LYS
40	o	17	LYS
40	o	19	GLN
40	o	24	THR
40	o	26	TYR
40	o	28	LYS
40	o	33	LEU
40	o	36	GLN
40	o	55	ILE
40	o	61	LYS
40	o	69	ARG
40	o	82	MET
40	o	89	LYS
40	o	102	GLN
41	p	3	LYS
41	p	16	THR
41	p	24	LYS
41	p	52	VAL
41	p	54	ILE
41	p	60	CYS
41	p	74	THR
41	p	84	ARG
42	r	10	VAL
42	r	17	LEU
42	r	18	ILE
42	r	20	ARG
42	r	21	ASN
42	r	24	THR
42	r	26	SER
42	r	28	GLU
42	r	32	LEU
42	r	37	SER

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Mol	Chain	Res	Type
42	r	39	ARG
42	r	41	ASN
42	r	60	VAL
42	r	67	ARG
42	r	70	GLN
42	r	71	ARG
42	r	78	VAL
42	r	80	THR
42	r	103	HIS
42	r	107	ARG
42	r	108	MET
42	r	118	LEU
42	r	122	LYS
42	r	124	VAL
43	s	38	LYS
43	s	50	LYS
43	s	62	ARG
43	s	77	LYS
43	s	94	ASP
43	s	107	VAL
43	s	146	LYS
43	s	149	ARG
43	s	174	LEU
43	s	191	GLN
44	t	1	MET
44	t	14	TYR
44	t	16	ARG
44	t	40	LYS
44	t	104	ILE
44	t	106	PHE
44	t	114	ARG
44	t	123	ARG
44	t	124	GLU
48	x	45	CYS
48	x	64	TRP
48	x	65	MET
48	x	66	ARG
48	x	68	ILE
48	x	187	ILE
48	x	192	VAL
48	x	249	ILE
48	x	251	VAL

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Mol	Chain	Res	Type
48	x	355	LEU
48	x	406	GLU
48	x	436	ASP
48	x	438	LEU
48	x	441	ILE
48	x	458	PHE
48	x	462	VAL
49	y	40	THR
49	y	59	ILE
50	z	73	VAL
50	z	76	MET
50	z	78	LEU
50	z	79	LEU
50	z	81	ILE
50	z	87	LEU
53	3	88	LEU
53	3	90	SER
53	3	93	LEU
54	4	21	LEU
55	5	4	LEU
55	5	82	ARG
55	5	122	LEU
55	5	123	PHE
55	5	173	ILE
55	5	175	CYS
55	5	178	LEU
55	5	285	TYR
55	5	286	LEU
55	5	366	LEU
55	5	367	LEU
55	5	524	SER
55	5	562	THR
55	5	597	LEU
55	5	601	ARG
55	5	602	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	140	ASN
1	A	215	ASN

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Mol	Chain	Res	Type
2	B	42	HIS
3	C	21	ASN
3	C	38	ASN
3	C	41	HIS
3	C	43	ASN
3	C	329	ASN
4	D	9	ASN
4	D	131	ASN
4	D	225	GLN
5	E	178	ASN
5	E	217	GLN
5	E	246	GLN
5	E	275	ASN
6	F	58	HIS
6	F	82	ASN
7	G	29	ASN
7	G	85	GLN
7	G	90	GLN
7	G	149	ASN
7	G	153	GLN
7	G	159	HIS
8	H	15	ASN
8	H	39	ASN
8	H	162	GLN
9	I	59	GLN
9	I	73	ASN
9	I	100	ASN
9	I	123	GLN
13	N	15	GLN
13	N	32	GLN
14	O	96	GLN
15	P	34	GLN
15	P	56	GLN
16	Q	44	ASN
16	Q	93	GLN
16	Q	125	GLN
18	S	108	GLN
18	S	122	HIS
19	T	79	GLN
19	T	144	ASN
21	V	27	ASN
22	W	45	ASN

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Mol	Chain	Res	Type
23	X	57	GLN
23	X	69	ASN
23	X	94	ASN
24	Y	18	HIS
24	Y	56	GLN
26	a	44	ASN
26	a	62	HIS
26	a	120	GLN
27	b	60	ASN
28	c	50	ASN
29	d	93	ASN
29	d	116	ASN
30	e	102	ASN
30	e	117	GLN
31	f	56	ASN
31	f	78	HIS
33	h	30	GLN
34	i	20	ASN
35	j	48	ASN
35	j	76	HIS
37	l	33	ASN
38	m	119	ASN
40	o	19	GLN
41	p	72	ASN
42	r	21	ASN
42	r	121	GLN
43	s	41	GLN
43	s	176	ASN
43	s	200	ASN
44	t	70	GLN
44	t	156	ASN
48	x	202	ASN
48	x	218	HIS
48	x	241	ASN
48	x	244	ASN
48	x	300	ASN
48	x	343	HIS
48	x	393	GLN
48	x	414	ASN
49	y	62	ASN
54	4	12	ASN
55	5	46	HIS

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Mol	Chain	Res	Type
55	5	168	ASN
55	5	217	ASN
55	5	222	HIS
55	5	352	HIS
55	5	515	ASN
55	5	531	GLN
55	5	537	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	u	3647/3662 (99%)	1211 (33%)	0
46	v	119/120 (99%)	20 (16%)	0
47	w	155/156 (99%)	52 (33%)	0
All	All	3921/3938 (99%)	1283 (32%)	0

All (1283) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	u	2	G
45	u	8	U
45	u	9	C
45	u	10	A
45	u	12	A
45	u	13	U
45	u	21	G
45	u	25	A
45	u	30	C
45	u	39	A
45	u	42	A
45	u	43	U
45	u	44	A
45	u	48	G
45	u	49	U
45	u	56	A
45	u	58	G
45	u	59	A
45	u	64	A
45	u	65	A
45	u	69	A
45	u	71	C

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Mol	Chain	Res	Type
45	u	72	C
45	u	73	A
45	u	74	G
45	u	91	G
45	u	93	G
45	u	94	A
45	u	95	G
45	u	108	A
45	u	109	G
45	u	110	C
45	u	116	G
45	u	118	C
45	u	119	G
45	u	120	A
45	u	121	A
45	u	125	C
45	u	126	C
45	u	128	C
45	u	129	C
45	u	134	G
45	u	135	G
45	u	136	C
45	u	143	C
45	u	144	G
45	u	146	G
45	u	157	U
45	u	158	A
45	u	159	C
45	u	160	G
45	u	161	G
45	u	164	G
45	u	166	C
45	u	167	C
45	u	170	C
45	u	171	U
45	u	172	C
45	u	173	C
45	u	174	C
45	u	175	C
45	u	177	G
45	u	183	C
45	u	184	U

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Mol	Chain	Res	Type
45	u	185	C
45	u	186	G
45	u	187	U
45	u	188	G
45	u	189	G
45	u	197	A
45	u	200	U
45	u	201	C
45	u	202	C
45	u	203	U
45	u	205	C
45	u	206	U
45	u	210	C
45	u	211	G
45	u	216	C
45	u	217	C
45	u	218	A
45	u	219	G
45	u	220	C
45	u	221	C
45	u	224	U
45	u	225	G
45	u	226	G
45	u	227	A
45	u	233	U
45	u	234	G
45	u	246	G
45	u	253	G
45	u	255	C
45	u	257	C
45	u	265	C
45	u	266	C
45	u	267	G
45	u	272	U
45	u	275	C
45	u	276	C
45	u	277	G
45	u	278	G
45	u	280	G
45	u	286	U
45	u	296	A
45	u	297	U

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Mol	Chain	Res	Type
45	u	300	A
45	u	306	A
45	u	309	C
45	u	315	G
45	u	316	U
45	u	319	A
45	u	321	U
45	u	322	C
45	u	326	C
45	u	328	A
45	u	334	A
45	u	337	U
45	u	340	C
45	u	347	A
45	u	349	A
45	u	350	C
45	u	353	A
45	u	357	U
45	u	361	C
45	u	362	A
45	u	363	A
45	u	385	A
45	u	386	A
45	u	387	G
45	u	399	G
45	u	405	U
45	u	406	C
45	u	407	A
45	u	409	G
45	u	410	A
45	u	412	G
45	u	413	G
45	u	424	U
45	u	429	A
45	u	431	G
45	u	432	U
45	u	434	A
45	u	446	C
45	u	448	G
45	u	449	C
45	u	451	C
45	u	452	A

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Mol	Chain	Res	Type
45	u	453	G
45	u	454	U
45	u	455	C
45	u	458	C
45	u	466	A
45	u	467	U
45	u	468	U
45	u	469	C
45	u	470	A
45	u	471	A
45	u	473	C
45	u	485	C
45	u	486	C
45	u	487	G
45	u	498	C
45	u	499	G
45	u	500	G
45	u	501	C
45	u	502	C
45	u	503	C
45	u	504	G
45	u	506	C
45	u	509	A
45	u	510	U
45	u	513	U
45	u	514	U
45	u	515	C
45	u	519	C
45	u	649	A
45	u	654	C
45	u	655	C
45	u	663	G
45	u	664	G
45	u	665	C
45	u	666	G
45	u	667	A
45	u	668	C
45	u	681	G
45	u	682	G
45	u	683	C
45	u	684	G
45	u	685	C

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Mol	Chain	Res	Type
45	u	686	A
45	u	687	U
45	u	689	U
45	u	690	C
45	u	692	A
45	u	694	C
45	u	695	G
45	u	696	C
45	u	697	G
45	u	701	G
45	u	703	G
45	u	707	C
45	u	718	C
45	u	721	G
45	u	722	G
45	u	724	C
45	u	728	U
45	u	729	G
45	u	730	G
45	u	737	C
45	u	742	G
45	u	745	G
45	u	746	A
45	u	747	A
45	u	748	G
45	u	749	G
45	u	756	G
45	u	911	U
45	u	914	U
45	u	915	A
45	u	917	A
45	u	918	G
45	u	919	C
45	u	920	C
45	u	925	C
45	u	927	G
45	u	928	C
45	u	929	A
45	u	930	G
45	u	931	C
45	u	932	A
45	u	933	G

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Mol	Chain	Res	Type
45	u	934	C
45	u	935	A
45	u	936	C
45	u	937	U
45	u	938	C
45	u	939	G
45	u	940	C
45	u	942	G
45	u	943	A
45	u	944	A
45	u	945	U
45	u	946	C
45	u	947	C
45	u	957	G
45	u	958	G
45	u	960	A
45	u	961	G
45	u	962	C
45	u	963	G
45	u	964	A
45	u	965	G
45	u	966	A
45	u	967	C
45	u	968	C
45	u	969	C
45	u	970	G
45	u	971	U
45	u	972	C
45	u	973	G
45	u	976	G
45	u	977	C
45	u	978	G
45	u	979	C
45	u	982	U
45	u	983	C
45	u	984	C
45	u	989	U
45	u	990	C
45	u	992	C
45	u	1051	G
45	u	1070	G
45	u	1072	C

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Mol	Chain	Res	Type
45	u	1073	G
45	u	1075	G
45	u	1076	C
45	u	1083	U
45	u	1097	C
45	u	1175	A
45	u	1176	C
45	u	1177	U
45	u	1181	C
45	u	1182	C
45	u	1183	C
45	u	1193	C
45	u	1204	C
45	u	1209	U
45	u	1211	G
45	u	1212	G
45	u	1214	C
45	u	1215	C
45	u	1219	G
45	u	1221	G
45	u	1222	A
45	u	1233	G
45	u	1234	G
45	u	1235	G
45	u	1236	C
45	u	1237	C
45	u	1238	A
45	u	1239	C
45	u	1240	G
45	u	1241	C
45	u	1242	G
45	u	1243	C
45	u	1244	G
45	u	1245	C
45	u	1255	A
45	u	1256	G
45	u	1259	G
45	u	1266	G
45	u	1267	C
45	u	1268	G
45	u	1269	G
45	u	1270	A

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Mol	Chain	Res	Type
45	u	1272	C
45	u	1273	G
45	u	1274	A
45	u	1275	G
45	u	1279	A
45	u	1280	C
45	u	1281	G
45	u	1285	U
45	u	1286	C
45	u	1287	G
45	u	1288	G
45	u	1289	C
45	u	1293	G
45	u	1294	A
45	u	1295	C
45	u	1296	G
45	u	1297	U
45	u	1301	C
45	u	1303	A
45	u	1304	C
45	u	1313	C
45	u	1326	A
45	u	1329	G
45	u	1330	A
45	u	1337	A
45	u	1344	C
45	u	1354	A
45	u	1358	G
45	u	1364	U
45	u	1365	C
45	u	1366	G
45	u	1367	C
45	u	1368	A
45	u	1369	C
45	u	1370	G
45	u	1371	A
45	u	1372	A
45	u	1376	C
45	u	1377	G
45	u	1378	C
45	u	1379	C
45	u	1380	G

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Mol	Chain	Res	Type
45	u	1381	U
45	u	1387	A
45	u	1390	G
45	u	1391	A
45	u	1394	G
45	u	1397	A
45	u	1398	A
45	u	1399	G
45	u	1407	C
45	u	1408	G
45	u	1409	C
45	u	1410	U
45	u	1411	C
45	u	1413	C
45	u	1414	C
45	u	1416	G
45	u	1418	C
45	u	1420	A
45	u	1421	G
45	u	1429	C
45	u	1432	G
45	u	1435	G
45	u	1436	C
45	u	1439	C
45	u	1440	U
45	u	1441	C
45	u	1442	C
45	u	1445	U
45	u	1446	C
45	u	1448	G
45	u	1449	C
45	u	1455	G
45	u	1456	C
45	u	1457	G
45	u	1475	G
45	u	1477	C
45	u	1478	C
45	u	1481	C
45	u	1482	G
45	u	1483	C
45	u	1484	G
45	u	1485	C

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Mol	Chain	Res	Type
45	u	1486	C
45	u	1489	G
45	u	1497	A
45	u	1498	G
45	u	1501	C
45	u	1502	G
45	u	1504	G
45	u	1514	U
45	u	1516	G
45	u	1518	A
45	u	1523	A
45	u	1524	A
45	u	1533	A
45	u	1534	A
45	u	1547	A
45	u	1563	A
45	u	1564	A
45	u	1566	C
45	u	1568	C
45	u	1578	U
45	u	1582	U
45	u	1586	G
45	u	1591	U
45	u	1592	G
45	u	1596	U
45	u	1602	U
45	u	1612	G
45	u	1613	A
45	u	1614	C
45	u	1624	G
45	u	1625	G
45	u	1631	A
45	u	1633	G
45	u	1634	A
45	u	1636	U
45	u	1638	A
45	u	1641	G
45	u	1654	G
45	u	1655	C
45	u	1656	U
45	u	1661	C
45	u	1670	G

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Mol	Chain	Res	Type
45	u	1676	C
45	u	1677	U
45	u	1678	C
45	u	1679	A
45	u	1691	G
45	u	1692	C
45	u	1696	C
45	u	1697	G
45	u	1698	C
45	u	1699	A
45	u	1719	A
45	u	1720	C
45	u	1721	G
45	u	1722	C
45	u	1724	G
45	u	1725	U
45	u	1733	G
45	u	1734	G
45	u	1735	U
45	u	1742	A
45	u	1746	A
45	u	1750	G
45	u	1753	G
45	u	1754	U
45	u	1755	C
45	u	1756	U
45	u	1757	U
45	u	1758	G
45	u	1760	G
45	u	1761	G
45	u	1764	G
45	u	1767	A
45	u	1768	C
45	u	1772	C
45	u	1776	A
45	u	1777	C
45	u	1781	U
45	u	1787	A
45	u	1799	G
45	u	1800	U
45	u	1803	G
45	u	1804	A

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Mol	Chain	Res	Type
45	u	1805	A
45	u	1812	C
45	u	1815	G
45	u	1818	G
45	u	1819	G
45	u	1820	C
45	u	1821	G
45	u	1822	U
45	u	1828	C
45	u	1830	G
45	u	1832	C
45	u	1833	G
45	u	1834	U
45	u	1835	G
45	u	1836	G
45	u	1842	G
45	u	1847	C
45	u	1848	C
45	u	1855	G
45	u	1867	A
45	u	1869	G
45	u	1882	U
45	u	1885	G
45	u	1886	G
45	u	1889	U
45	u	1892	A
45	u	1897	A
45	u	1899	G
45	u	1900	C
45	u	1910	G
45	u	1918	U
45	u	1919	G
45	u	1920	C
45	u	1921	C
45	u	1922	G
45	u	1923	A
45	u	1931	C
45	u	1947	U
45	u	1952	G
45	u	1955	G
45	u	1956	A
45	u	1957	U

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Mol	Chain	Res	Type
45	u	1958	A
45	u	1959	U
45	u	1960	A
45	u	1961	G
45	u	1962	A
45	u	1964	A
45	u	1968	G
45	u	1969	G
45	u	1970	A
45	u	1975	G
45	u	1976	G
45	u	1977	C
45	u	1979	A
45	u	1980	U
45	u	1981	G
45	u	1983	A
45	u	1984	A
45	u	1985	G
45	u	1986	U
45	u	1987	C
45	u	1988	G
45	u	1990	A
45	u	1991	A
45	u	1992	U
45	u	1993	C
45	u	1997	U
45	u	1998	A
45	u	2001	G
45	u	2002	A
45	u	2003	G
45	u	2004	U
45	u	2005	G
45	u	2008	U
45	u	2010	A
45	u	2011	C
45	u	2019	C
45	u	2020	U
45	u	2021	G
45	u	2024	G
45	u	2025	A
45	u	2026	A
45	u	2027	U

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Mol	Chain	Res	Type
45	u	2028	C
45	u	2044	U
45	u	2046	G
45	u	2047	A
45	u	2048	U
45	u	2052	G
45	u	2055	G
45	u	2056	G
45	u	2062	C
45	u	2064	G
45	u	2068	C
45	u	2069	A
45	u	2070	U
45	u	2071	A
45	u	2079	G
45	u	2084	C
45	u	2085	G
45	u	2089	G
45	u	2090	U
45	u	2091	C
45	u	2092	G
45	u	2093	A
45	u	2094	G
45	u	2095	A
45	u	2097	U
45	u	2100	A
45	u	2101	C
45	u	2103	G
45	u	2107	C
45	u	2108	G
45	u	2109	G
45	u	2110	C
45	u	2111	G
45	u	2112	G
45	u	2113	G
45	u	2114	G
45	u	2115	G
45	u	2116	C
45	u	2117	G
45	u	2118	G
45	u	2119	C
45	u	2120	G

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Mol	Chain	Res	Type
45	u	2122	G
45	u	2123	C
45	u	2124	G
45	u	2125	C
45	u	2126	G
45	u	2127	C
45	u	2129	C
45	u	2130	G
45	u	2131	C
45	u	2247	C
45	u	2248	C
45	u	2250	C
45	u	2251	G
45	u	2252	G
45	u	2253	A
45	u	2254	G
45	u	2255	C
45	u	2256	C
45	u	2257	C
45	u	2258	C
45	u	2259	G
45	u	2260	C
45	u	2261	G
45	u	2263	A
45	u	2264	C
45	u	2265	G
45	u	2266	C
45	u	2267	U
45	u	2268	A
45	u	2269	C
45	u	2270	G
45	u	2274	C
45	u	2275	G
45	u	2279	A
45	u	2288	G
45	u	2289	C
45	u	2299	G
45	u	2300	A
45	u	2301	G
45	u	2312	U
45	u	2313	A
45	u	2314	G

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Mol	Chain	Res	Type
45	u	2324	C
45	u	2331	G
45	u	2332	A
45	u	2333	G
45	u	2335	C
45	u	2337	C
45	u	2348	G
45	u	2351	C
45	u	2360	A
45	u	2364	G
45	u	2370	A
45	u	2371	U
45	u	2382	A
45	u	2383	C
45	u	2395	A
45	u	2396	A
45	u	2397	G
45	u	2398	U
45	u	2399	G
45	u	2417	A
45	u	2422	C
45	u	2424	G
45	u	2425	U
45	u	2428	A
45	u	2429	A
45	u	2433	G
45	u	2434	G
45	u	2440	U
45	u	2441	C
45	u	2447	U
45	u	2450	G
45	u	2458	C
45	u	2469	C
45	u	2471	G
45	u	2473	A
45	u	2474	G
45	u	2475	G
45	u	2485	U
45	u	2488	C
45	u	2489	C
45	u	2490	U
45	u	2491	C

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Mol	Chain	Res	Type
45	u	2493	G
45	u	2495	U
45	u	2499	C
45	u	2503	G
45	u	2504	C
45	u	2505	C
45	u	2506	G
45	u	2507	A
45	u	2512	A
45	u	2513	A
45	u	2514	G
45	u	2519	U
45	u	2521	G
45	u	2527	A
45	u	2530	U
45	u	2536	A
45	u	2537	A
45	u	2544	G
45	u	2546	G
45	u	2547	G
45	u	2553	A
45	u	2554	U
45	u	2555	G
45	u	2564	G
45	u	2566	G
45	u	2568	C
45	u	2571	C
45	u	2575	U
45	u	2577	C
45	u	2583	C
45	u	2587	A
45	u	2588	C
45	u	2589	C
45	u	2591	A
45	u	2601	A
45	u	2602	G
45	u	2611	A
45	u	2620	G
45	u	2623	A
45	u	2624	G
45	u	2627	C
45	u	2638	G

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Mol	Chain	Res	Type
45	u	2640	G
45	u	2647	A
45	u	2653	C
45	u	2661	U
45	u	2662	G
45	u	2663	G
45	u	2669	C
45	u	2673	G
45	u	2676	A
45	u	2679	G
45	u	2681	G
45	u	2686	G
45	u	2687	U
45	u	2688	G
45	u	2695	A
45	u	2696	A
45	u	2704	C
45	u	2708	U
45	u	2710	C
45	u	2711	G
45	u	2712	G
45	u	2714	G
45	u	2716	C
45	u	2721	G
45	u	2724	G
45	u	2725	A
45	u	2726	G
45	u	2733	C
45	u	2740	U
45	u	2743	A
45	u	2754	G
45	u	2755	A
45	u	2756	G
45	u	2760	G
45	u	2761	U
45	u	2762	G
45	u	2767	U
45	u	2768	C
45	u	2769	U
45	u	2770	C
45	u	2772	C
45	u	2787	A

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Mol	Chain	Res	Type
45	u	2788	U
45	u	2789	A
45	u	2790	U
45	u	2794	C
45	u	2795	A
45	u	2796	G
45	u	2798	A
45	u	2806	A
45	u	2807	A
45	u	2814	C
45	u	2824	C
45	u	2825	A
45	u	2826	U
45	u	2827	G
45	u	2828	U
45	u	2829	U
45	u	2835	A
45	u	2838	G
45	u	2839	U
45	u	2842	G
45	u	2855	G
45	u	2858	A
45	u	2859	G
45	u	2862	G
45	u	2869	U
45	u	2896	G
45	u	2897	G
45	u	2898	G
45	u	2904	U
45	u	2905	C
45	u	2910	G
45	u	3594	C
45	u	3595	U
45	u	3596	A
45	u	3597	G
45	u	3598	C
45	u	3605	C
45	u	3606	U
45	u	3615	G
45	u	3617	G
45	u	3625	G
45	u	3626	G

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Mol	Chain	Res	Type
45	u	3630	A
45	u	3635	A
45	u	3644	U
45	u	3653	A
45	u	3662	A
45	u	3668	C
45	u	3670	C
45	u	3671	G
45	u	3673	C
45	u	3674	G
45	u	3680	U
45	u	3682	A
45	u	3689	G
45	u	3692	A
45	u	3696	C
45	u	3698	G
45	u	3702	A
45	u	3709	U
45	u	3710	G
45	u	3711	A
45	u	3712	A
45	u	3715	U
45	u	3716	C
45	u	3717	A
45	u	3718	A
45	u	3722	G
45	u	3728	A
45	u	3729	U
45	u	3737	A
45	u	3740	G
45	u	3748	A
45	u	3750	G
45	u	3752	C
45	u	3753	G
45	u	3755	G
45	u	3756	A
45	u	3759	A
45	u	3760	A
45	u	3764	U
45	u	3773	U
45	u	3774	A
45	u	3775	A

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Mol	Chain	Res	Type
45	u	3776	G
45	u	3777	G
45	u	3778	U
45	u	3780	G
45	u	3783	A
45	u	3784	A
45	u	3786	U
45	u	3788	C
45	u	3798	U
45	u	3799	A
45	u	3802	U
45	u	3810	C
45	u	3811	G
45	u	3812	C
45	u	3813	A
45	u	3814	U
45	u	3817	A
45	u	3819	G
45	u	3822	U
45	u	3831	U
45	u	3836	A
45	u	3838	U
45	u	3839	G
45	u	3840	U
45	u	3859	G
45	u	3867	A
45	u	3877	A
45	u	3878	C
45	u	3879	G
45	u	3889	G
45	u	3897	G
45	u	3900	G
45	u	3901	A
45	u	3905	A
45	u	3906	A
45	u	3907	G
45	u	3912	U
45	u	3915	U
45	u	3916	G
45	u	3917	A
45	u	3924	C
45	u	3925	U

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Mol	Chain	Res	Type
45	u	3926	C
45	u	3927	U
45	u	3938	G
45	u	3939	G
45	u	3943	A
45	u	3946	G
45	u	4069	U
45	u	4070	U
45	u	4076	G
45	u	4084	G
45	u	4085	A
45	u	4086	G
45	u	4087	G
45	u	4088	C
45	u	4091	G
45	u	4092	G
45	u	4093	G
45	u	4094	G
45	u	4097	G
45	u	4104	G
45	u	4105	A
45	u	4107	G
45	u	4112	C
45	u	4114	C
45	u	4115	G
45	u	4116	C
45	u	4117	U
45	u	4118	U
45	u	4119	C
45	u	4120	U
45	u	4121	G
45	u	4122	G
45	u	4125	C
45	u	4127	A
45	u	4134	C
45	u	4143	G
45	u	4144	C
45	u	4145	C
45	u	4155	C
45	u	4161	G
45	u	4162	C
45	u	4163	U

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Mol	Chain	Res	Type
45	u	4165	C
45	u	4166	G
45	u	4168	G
45	u	4170	A
45	u	4171	C
45	u	4182	G
45	u	4183	G
45	u	4184	G
45	u	4191	G
45	u	4203	A
45	u	4208	U
45	u	4212	A
45	u	4213	A
45	u	4216	G
45	u	4217	G
45	u	4218	U
45	u	4219	A
45	u	4225	G
45	u	4226	G
45	u	4229	U
45	u	4232	U
45	u	4233	A
45	u	4238	G
45	u	4241	C
45	u	4251	A
45	u	4254	G
45	u	4255	A
45	u	4258	C
45	u	4265	U
45	u	4266	G
45	u	4267	G
45	u	4268	A
45	u	4271	A
45	u	4273	A
45	u	4282	A
45	u	4291	G
45	u	4297	G
45	u	4302	U
45	u	4303	C
45	u	4304	A
45	u	4305	G
45	u	4306	U

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Mol	Chain	Res	Type
45	u	4307	A
45	u	4311	A
45	u	4312	U
45	u	4313	A
45	u	4314	C
45	u	4317	A
45	u	4318	C
45	u	4319	C
45	u	4329	G
45	u	4330	G
45	u	4331	G
45	u	4332	C
45	u	4335	C
45	u	4336	A
45	u	4349	C
45	u	4350	C
45	u	4354	U
45	u	4355	G
45	u	4360	U
45	u	4367	G
45	u	4368	G
45	u	4372	U
45	u	4373	G
45	u	4377	G
45	u	4378	A
45	u	4379	A
45	u	4380	A
45	u	4387	C
45	u	4391	G
45	u	4394	A
45	u	4395	U
45	u	4396	A
45	u	4398	C
45	u	4405	G
45	u	4419	U
45	u	4420	U
45	u	4421	C
45	u	4422	A
45	u	4424	A
45	u	4426	C
45	u	4430	G
45	u	4432	C

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Mol	Chain	Res	Type
45	u	4433	G
45	u	4438	U
45	u	4439	U
45	u	4441	A
45	u	4444	C
45	u	4448	G
45	u	4449	A
45	u	4450	U
45	u	4453	C
45	u	4454	G
45	u	4463	U
45	u	4464	A
45	u	4471	U
45	u	4472	G
45	u	4473	A
45	u	4475	G
45	u	4476	C
45	u	4481	U
45	u	4482	U
45	u	4484	A
45	u	4488	A
45	u	4491	G
45	u	4495	G
45	u	4500	U
45	u	4510	A
45	u	4511	A
45	u	4512	U
45	u	4513	A
45	u	4515	G
45	u	4519	C
45	u	4520	G
45	u	4522	G
45	u	4524	G
45	u	4527	G
45	u	4528	G
45	u	4529	G
45	u	4535	A
45	u	4548	A
45	u	4549	G
45	u	4550	G
45	u	4557	U
45	u	4567	G

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Mol	Chain	Res	Type
45	u	4570	G
45	u	4573	G
45	u	4575	G
45	u	4577	U
45	u	4583	C
45	u	4584	A
45	u	4585	U
45	u	4586	G
45	u	4590	A
45	u	4591	U
45	u	4606	G
45	u	4618	G
45	u	4636	U
45	u	4637	G
45	u	4641	U
45	u	4647	G
45	u	4648	A
45	u	4656	A
45	u	4657	U
45	u	4661	G
45	u	4670	C
45	u	4672	A
45	u	4677	U
45	u	4687	A
45	u	4694	G
45	u	4695	C
45	u	4699	U
45	u	4700	A
45	u	4701	A
45	u	4702	G
45	u	4709	U
45	u	4719	G
45	u	4720	C
45	u	4721	G
45	u	4730	C
45	u	4731	G
45	u	4732	G
45	u	4733	C
45	u	4734	A
45	u	4737	G
45	u	4741	C
45	u	4745	G

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Mol	Chain	Res	Type
45	u	4746	C
45	u	4749	C
45	u	4750	G
45	u	4753	U
45	u	4754	G
45	u	4756	C
45	u	4758	U
45	u	4760	G
45	u	4764	A
45	u	4768	G
45	u	4770	U
45	u	4771	C
45	u	4774	C
45	u	4869	U
45	u	4871	C
45	u	4872	G
45	u	4873	G
45	u	4874	A
45	u	4875	G
45	u	4876	U
45	u	4877	G
45	u	4878	C
45	u	4883	C
45	u	4884	G
45	u	4885	U
45	u	4886	C
45	u	4889	G
45	u	4890	G
45	u	4893	A
45	u	4895	C
45	u	4896	G
45	u	4898	G
45	u	4900	C
45	u	4901	G
45	u	4904	G
45	u	4906	C
45	u	4910	G
45	u	4911	A
45	u	4912	G
45	u	4913	G
45	u	4924	C
45	u	4926	C

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Mol	Chain	Res	Type
45	u	4927	G
45	u	4930	C
45	u	4931	G
45	u	4932	U
45	u	4934	A
45	u	4935	C
45	u	4936	G
45	u	4939	C
45	u	4941	G
45	u	4942	C
45	u	4944	C
45	u	4945	G
45	u	4948	C
45	u	4949	G
45	u	4950	U
45	u	4951	G
45	u	4952	G
45	u	4959	U
45	u	4964	C
45	u	4965	U
45	u	4966	A
45	u	4967	A
45	u	4975	G
45	u	4976	U
45	u	4985	U
45	u	4988	U
45	u	4989	U
45	u	4990	C
45	u	4991	U
45	u	5007	A
45	u	5013	C
45	u	5014	A
45	u	5017	G
45	u	5018	C
45	u	5022	U
45	u	5023	C
45	u	5024	C
45	u	5025	C
45	u	5026	U
45	u	5027	C
45	u	5028	G
45	u	5031	G

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Mol	Chain	Res	Type
45	u	5033	G
45	u	5041	G
45	u	5047	C
45	u	5050	C
45	u	5052	C
45	u	5053	U
45	u	5054	C
45	u	5056	A
45	u	5058	A
45	u	5060	A
45	u	5061	A
45	u	5062	G
45	u	5066	U
46	v	7	G
46	v	11	A
46	v	21	G
46	v	25	G
46	v	33	U
46	v	40	U
46	v	51	G
46	v	53	U
46	v	54	A
46	v	64	G
46	v	74	A
46	v	76	U
46	v	97	G
46	v	99	G
46	v	100	A
46	v	106	G
46	v	109	U
46	v	110	G
46	v	111	C
46	v	120	U
47	w	2	G
47	w	3	A
47	w	34	U
47	w	35	C
47	w	38	U
47	w	39	G
47	w	49	G
47	w	51	U
47	w	52	A

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Mol	Chain	Res	Type
47	w	55	U
47	w	57	C
47	w	59	A
47	w	62	A
47	w	63	U
47	w	74	U
47	w	75	G
47	w	79	G
47	w	80	A
47	w	81	C
47	w	82	A
47	w	83	C
47	w	84	A
47	w	85	U
47	w	86	U
47	w	87	G
47	w	94	G
47	w	95	A
47	w	99	U
47	w	101	C
47	w	103	A
47	w	104	A
47	w	105	C
47	w	107	C
47	w	109	C
47	w	110	U
47	w	111	U
47	w	112	G
47	w	113	C
47	w	114	G
47	w	115	G
47	w	117	C
47	w	121	G
47	w	122	G
47	w	123	U
47	w	124	U
47	w	125	C
47	w	126	C
47	w	127	U
47	w	137	A
47	w	143	G
47	w	150	C

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Mol	Chain	Res	Type
47	w	156	U

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

8 monosaccharides 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	$\# Z > 2$
59	NAG	K	1	55,59	14,14,15	0.47	0	17,19,21	0.64	0
59	NAG	K	2	59	14,14,15	0.26	0	17,19,21	0.55	0
59	BMA	K	3	59	11,11,12	0.65	0	15,15,17	0.85	1 (6%)
59	MAN	K	4	59	11,11,12	0.83	0	15,15,17	1.62	2 (13%)
59	MAN	K	5	59	11,11,12	0.70	0	15,15,17	1.21	2 (13%)
59	MAN	K	6	59	11,11,12	0.89	0	15,15,17	0.95	2 (13%)
59	MAN	K	7	59	11,11,12	1.23	1 (9%)	15,15,17	1.24	2 (13%)
59	MAN	K	8	59	11,11,12	0.66	0	15,15,17	1.02	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	NAG	K	1	55,59	-	2/6/23/26	0/1/1/1
59	NAG	K	2	59	-	1/6/23/26	0/1/1/1
59	BMA	K	3	59	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	MAN	K	4	59	-	0/2/19/22	0/1/1/1
59	MAN	K	5	59	-	1/2/19/22	0/1/1/1
59	MAN	K	6	59	-	0/2/19/22	0/1/1/1
59	MAN	K	7	59	-	0/2/19/22	0/1/1/1
59	MAN	K	8	59	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	K	7	MAN	C2-C3	2.39	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	K	4	MAN	C1-O5-C5	4.47	118.18	112.19
59	K	4	MAN	O2-C2-C3	-3.64	102.62	110.15
59	K	7	MAN	C1-O5-C5	3.21	116.49	112.19
59	K	5	MAN	C1-O5-C5	3.03	116.25	112.19
59	K	5	MAN	O2-C2-C3	-2.95	104.04	110.15
59	K	8	MAN	C1-O5-C5	2.83	115.98	112.19
59	K	6	MAN	O2-C2-C3	-2.41	105.15	110.15
59	K	7	MAN	O3-C3-C2	2.35	114.85	110.05
59	K	8	MAN	O2-C2-C3	-2.13	105.74	110.15
59	K	3	BMA	C1-O5-C5	2.11	115.02	112.19
59	K	6	MAN	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

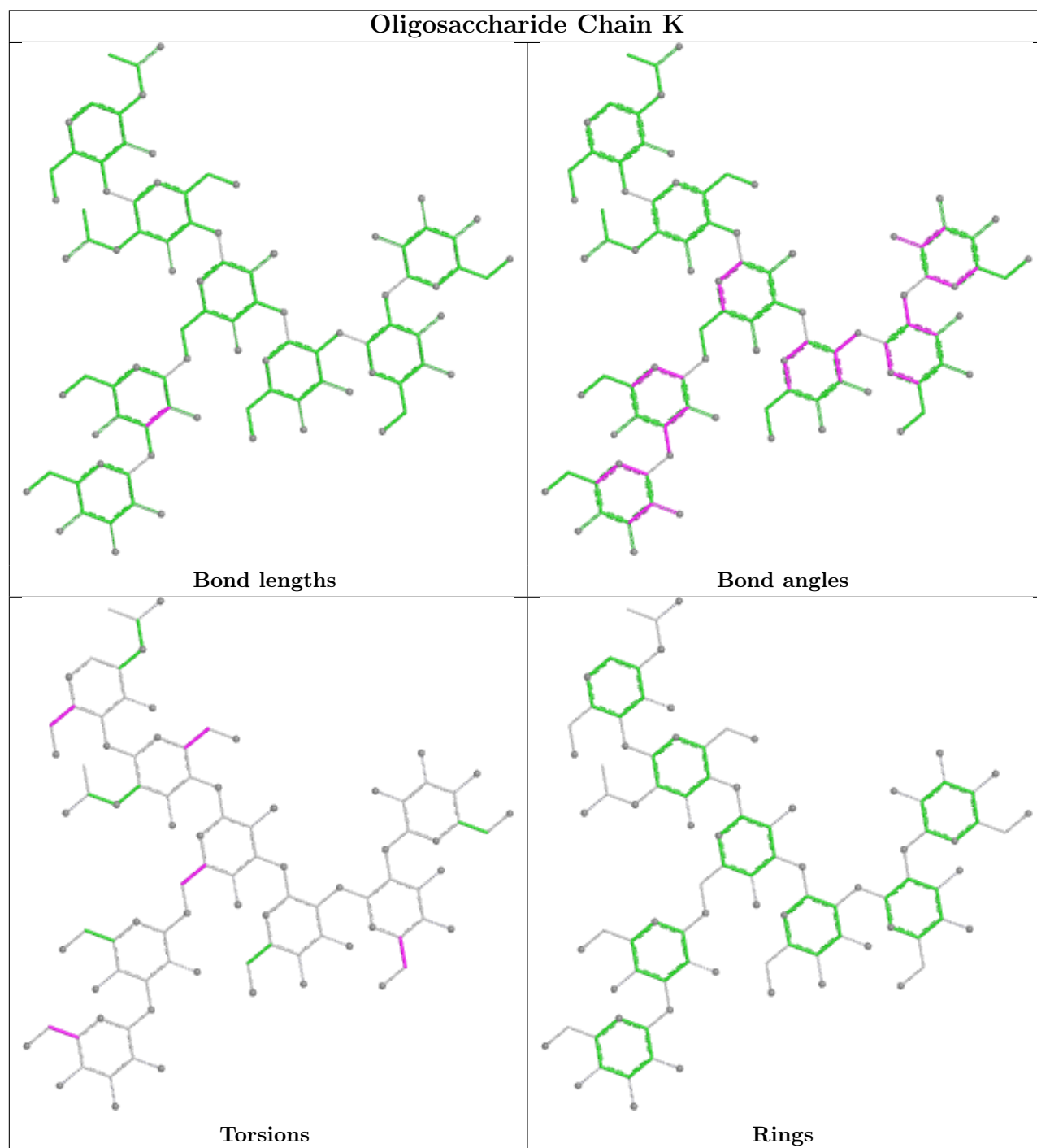
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	K	3	BMA	C4-C5-C6-O6
59	K	3	BMA	O5-C5-C6-O6
59	K	8	MAN	O5-C5-C6-O6
59	K	8	MAN	C4-C5-C6-O6
59	K	1	NAG	C4-C5-C6-O6
59	K	1	NAG	O5-C5-C6-O6
59	K	5	MAN	O5-C5-C6-O6
59	K	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 165 ligands modelled in this entry, 164 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
62	9UB	5	801	-	43,43,43	2.55	10 (23%)	48,59,59	1.64	13 (27%)

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
62	9UB	5	801	-	-	3/39/62/62	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	5	801	9UB	P26-O25	8.08	1.67	1.58
62	5	801	9UB	P22-O25	7.87	1.68	1.59
62	5	801	9UB	P26-C29	6.76	1.91	1.80
62	5	801	9UB	C37-C39	-3.75	1.46	1.53
62	5	801	9UB	C41-N40	3.60	1.46	1.34
62	5	801	9UB	C06-C07	3.01	1.57	1.51
62	5	801	9UB	C11-C12	2.68	1.56	1.51
62	5	801	9UB	C18-C17	2.49	1.56	1.50
62	5	801	9UB	C16-C17	2.36	1.56	1.51
62	5	801	9UB	C20-C19	2.14	1.55	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	5	801	9UB	C18-C17-C16	4.12	122.39	115.23
62	5	801	9UB	C20-C19-C17	-3.80	119.96	126.20
62	5	801	9UB	C39-N40-C41	-2.69	116.81	123.11
62	5	801	9UB	C01-C02-C03	2.61	120.59	114.59
62	5	801	9UB	C32-O31-C30	2.57	117.68	113.19
62	5	801	9UB	O31-C32-C35	2.50	114.20	109.70
62	5	801	9UB	C15-C14-C12	-2.41	122.11	127.62
62	5	801	9UB	O27-P26-C29	2.40	111.08	105.69
62	5	801	9UB	C10-C09-C07	-2.37	122.20	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	5	801	9UB	C08-C07-C06	2.32	119.25	115.23
62	5	801	9UB	C18-C17-C19	-2.23	117.89	123.63
62	5	801	9UB	C13-C12-C11	2.17	119.00	115.23
62	5	801	9UB	C33-C32-C35	-2.10	107.87	113.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

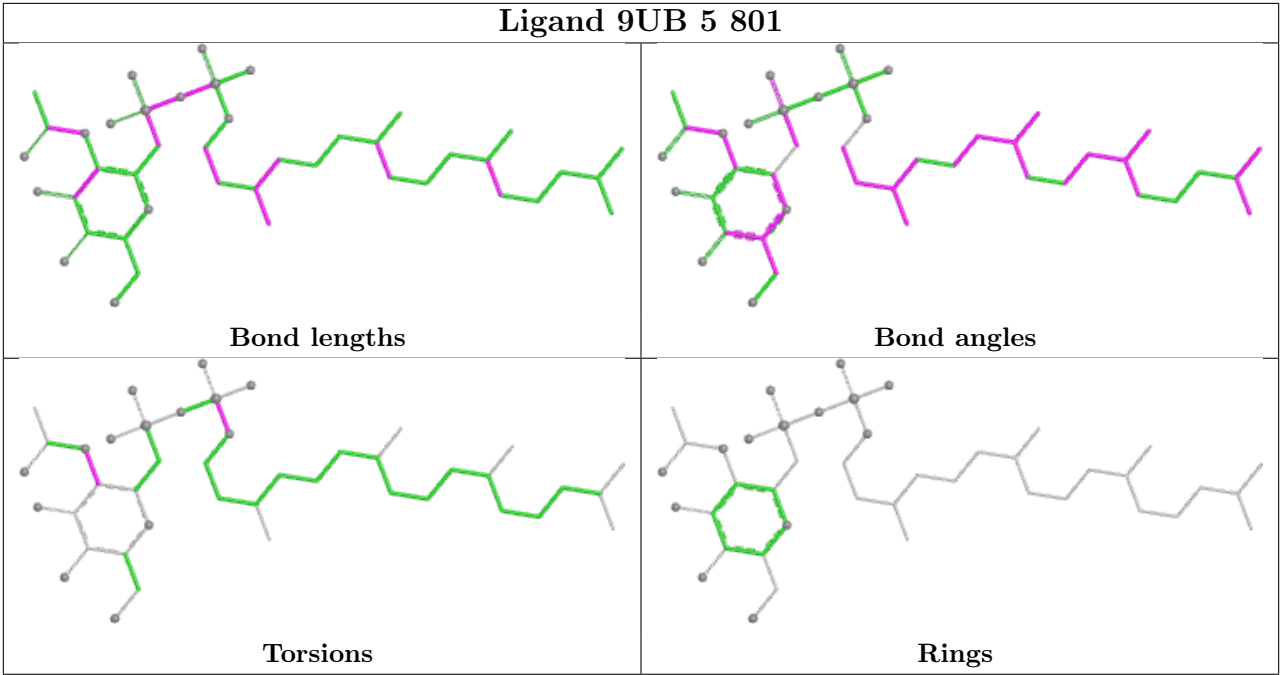
Mol	Chain	Res	Type	Atoms
62	5	801	9UB	C20-O21-P22-O25
62	5	801	9UB	C20-O21-P22-O23
62	5	801	9UB	C30-C39-N40-C41

There are no ring outliers.

1 monomer is involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	5	801	9UB	24	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
45	u	21
55	5	4
58	8	2
56	6	2
51	1	1
52	2	1
48	x	1
42	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	u	4776:G	O3'	4859:C	P	17.95
1	u	757:G	O3'	906:C	P	17.49
1	u	519:C	O3'	642:G	P	16.73
1	u	2910:G	O3'	3583:U	P	16.46

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	8	566:UNK	C	577:UNK	N	15.56
1	1	573:UNK	C	582:UNK	N	15.25
1	u	2131:C	O3'	2243:C	P	14.50
1	u	3950:U	O3'	4065:G	P	14.39
1	u	997:C	O3'	1047:C	P	13.95
1	6	46:UNK	C	53:UNK	N	13.30
1	2	42:UNK	C	50:UNK	N	12.34
1	8	598:UNK	C	600:UNK	N	11.54
1	6	82:UNK	C	88:UNK	N	10.20
1	u	1051:G	O3'	1064:G	P	8.98
1	x	202:ASN	C	203:THR	N	7.63
1	u	1222:A	O3'	1232:G	P	5.15
1	u	2016:C	O3'	2017:A	P	4.53
1	u	1100:U	O3'	1167:C	P	4.42
1	u	1699:A	O3'	1718:C	P	4.00
1	r	121:GLN	C	122:LYS	N	2.97
1	u	1840:G	O3'	1842:G	P	2.91
1	u	4939:C	O3'	4941:G	P	2.80
1	5	502:PHE	C	503:ASP	N	2.78
1	u	4942:C	O3'	4944:C	P	2.73
1	u	1823:G	O3'	1825:A	P	2.56
1	5	590:SER	C	591:ASP	N	2.33
1	u	692:A	O3'	693:C	P	2.00
1	u	197:A	O3'	198:A	P	1.77
1	u	472:C	O3'	473:C	P	1.37
1	u	1965:G	O3'	1966:C	P	1.33
1	u	680:G	O3'	681:G	P	1.20
1	5	550:THR	C	551:HIS	N	0.96
1	5	545:ASN	C	546:THR	N	0.91

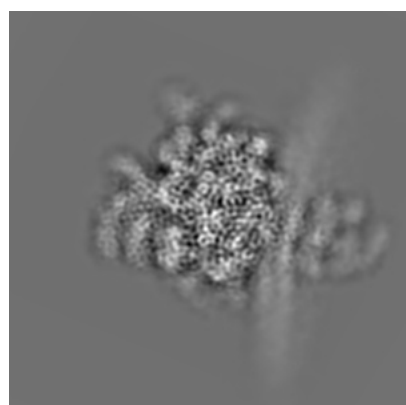
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4315. These allow visual inspection of the internal detail of the map and identification of artifacts.

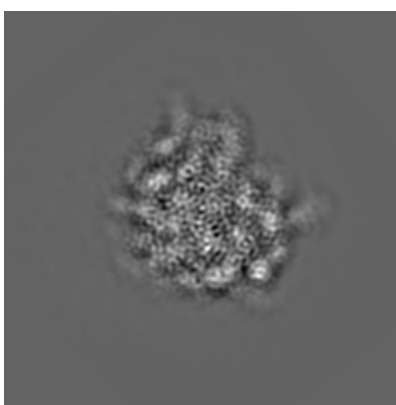
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

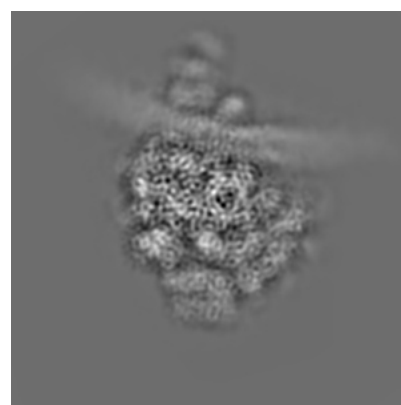
6.1.1 Primary map



X



Y

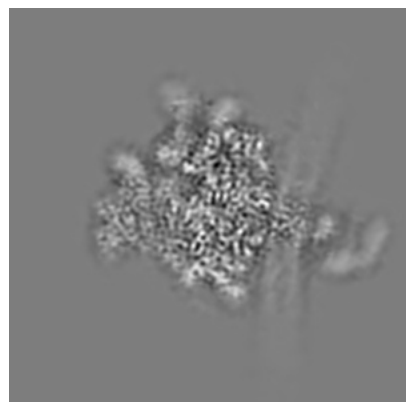


Z

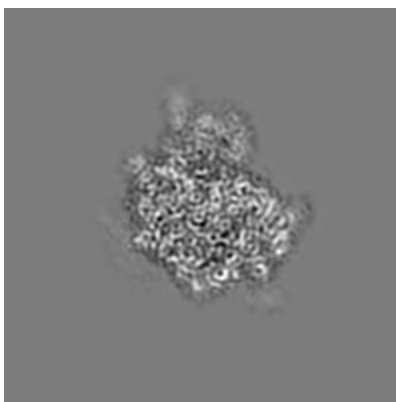
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

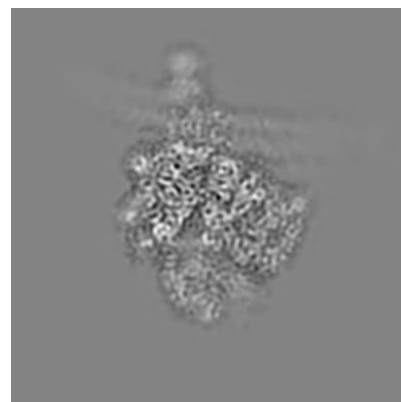
6.2.1 Primary map



X Index: 114



Y Index: 114

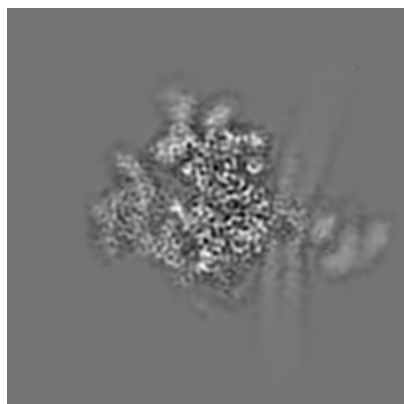


Z Index: 114

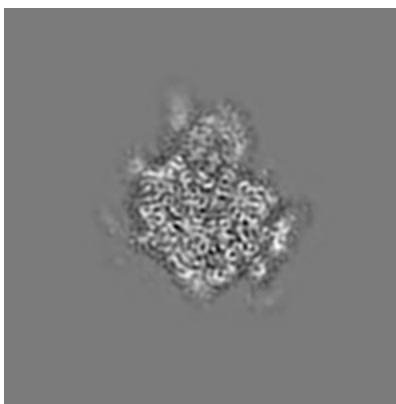
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

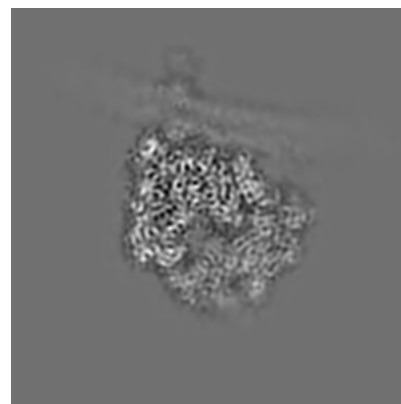
6.3.1 Primary map



X Index: 110



Y Index: 112

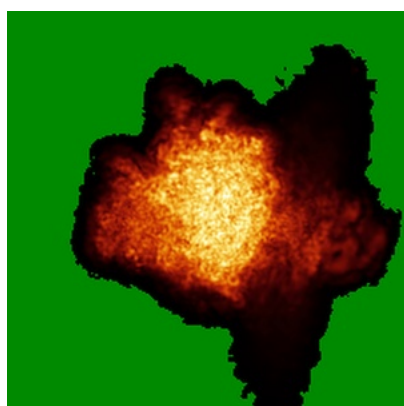


Z Index: 122

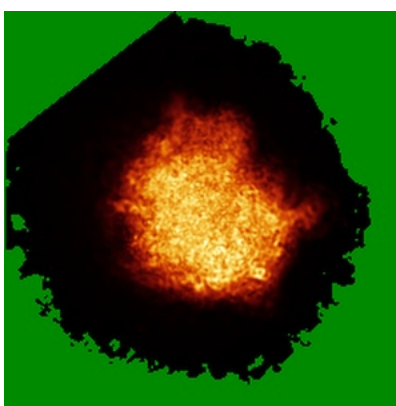
The images above show the largest variance slices of the map in three orthogonal directions.

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

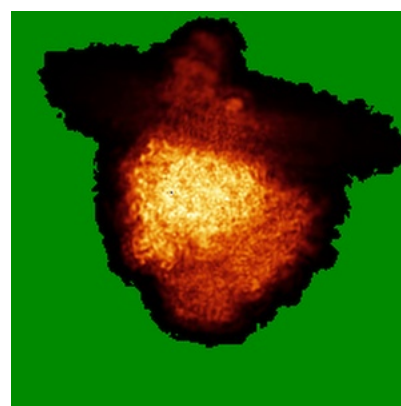
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

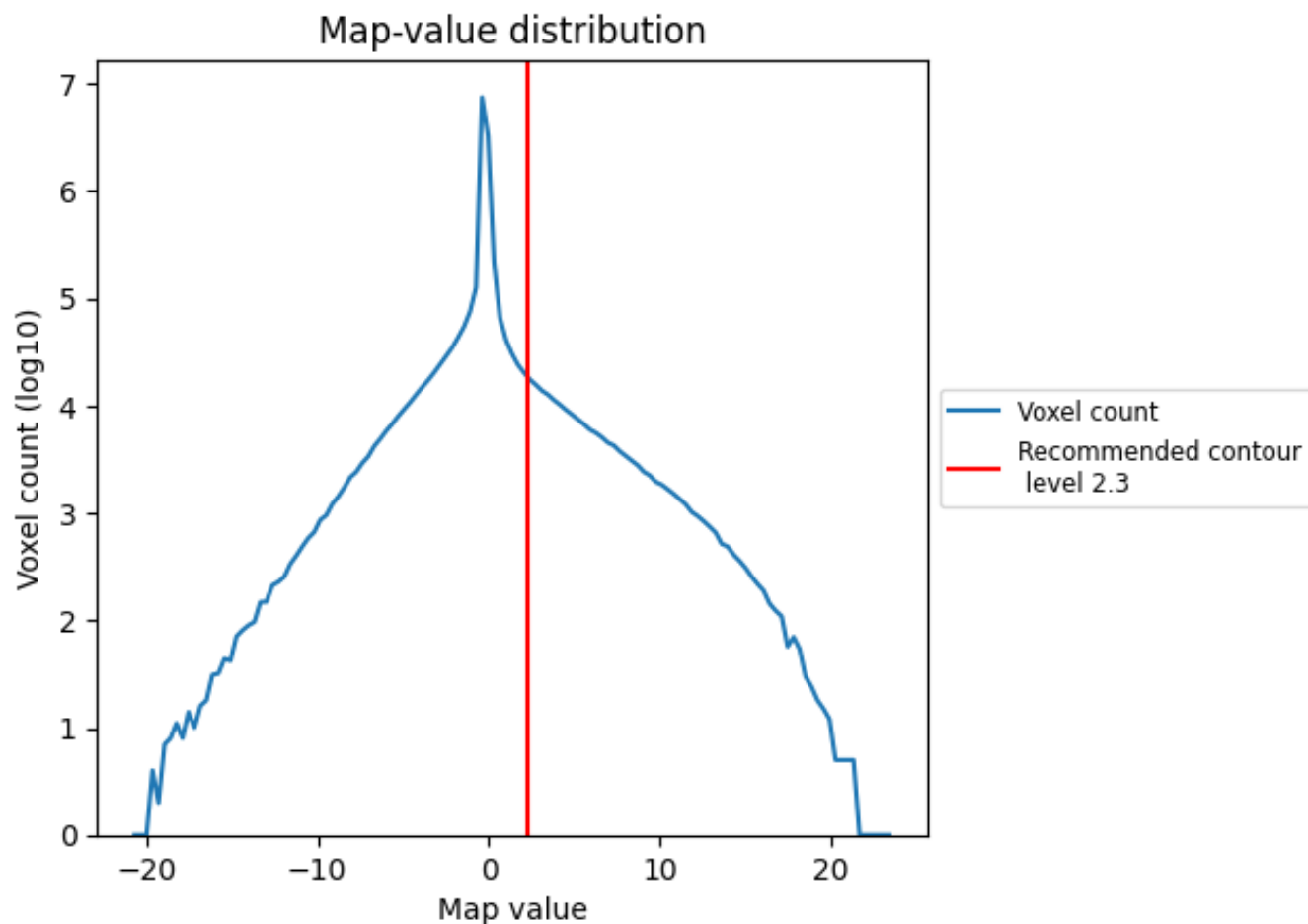
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

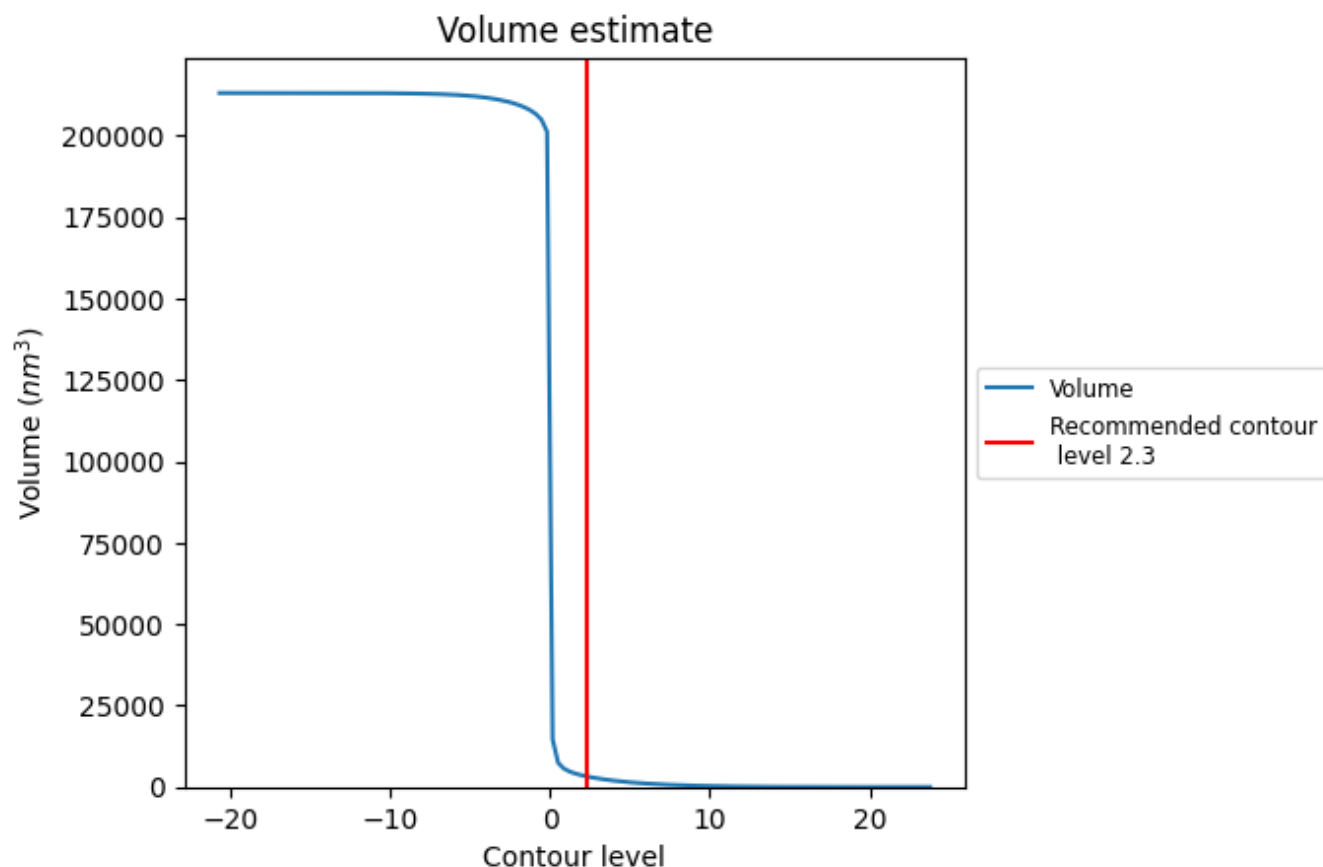
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

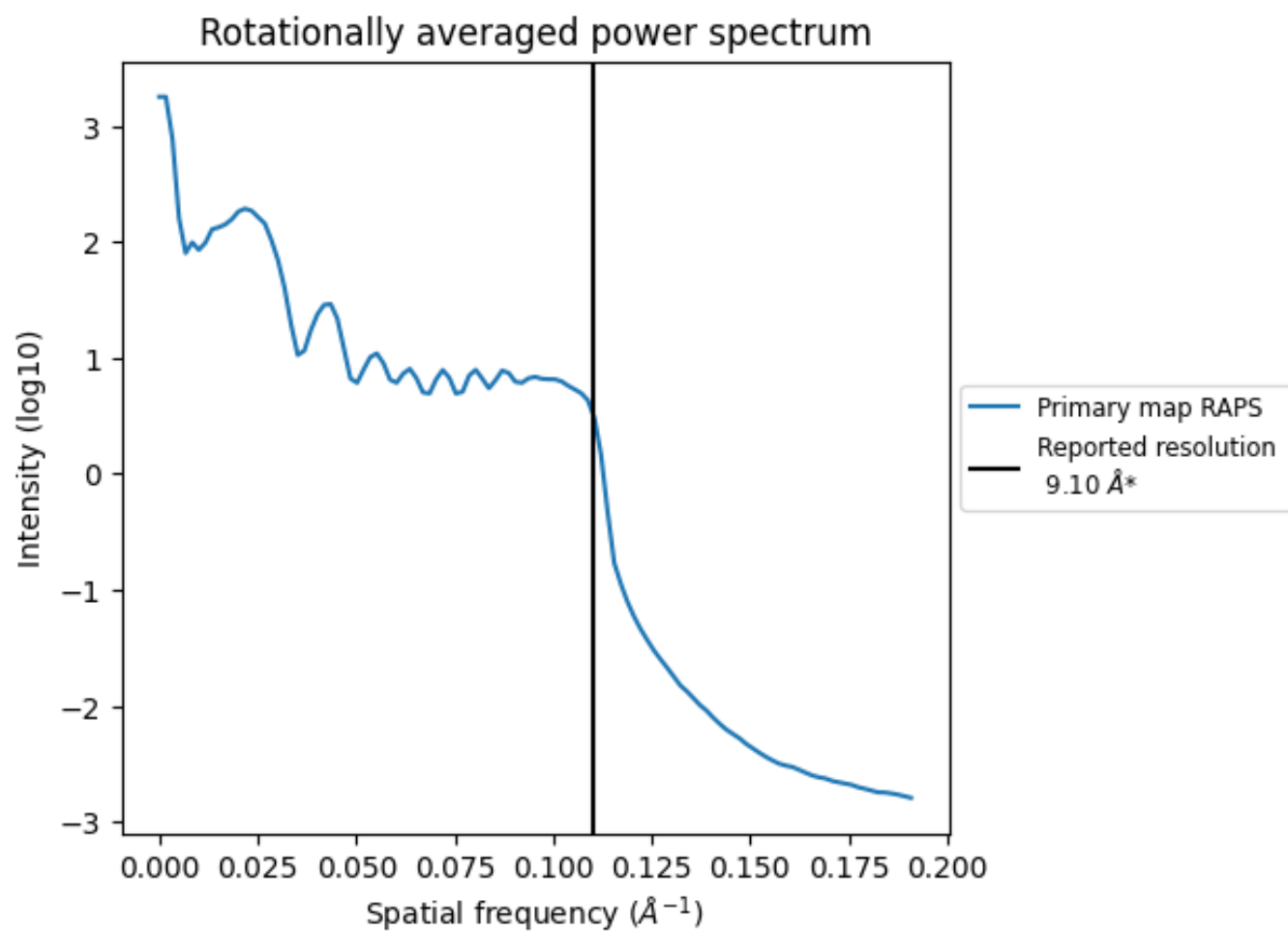
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3241 nm^3 ; this corresponds to an approximate mass of 2927 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 0.110 Å⁻¹

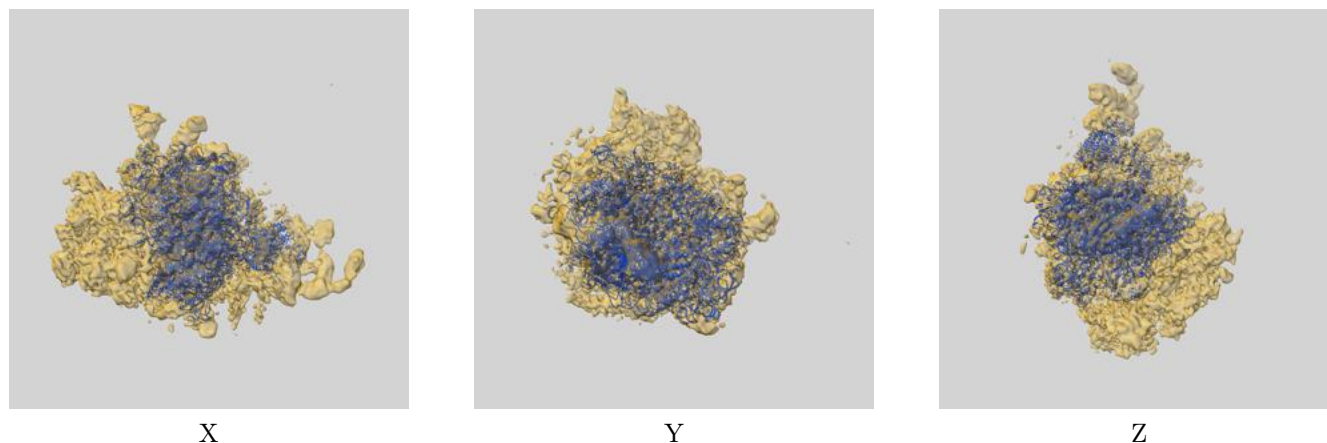
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

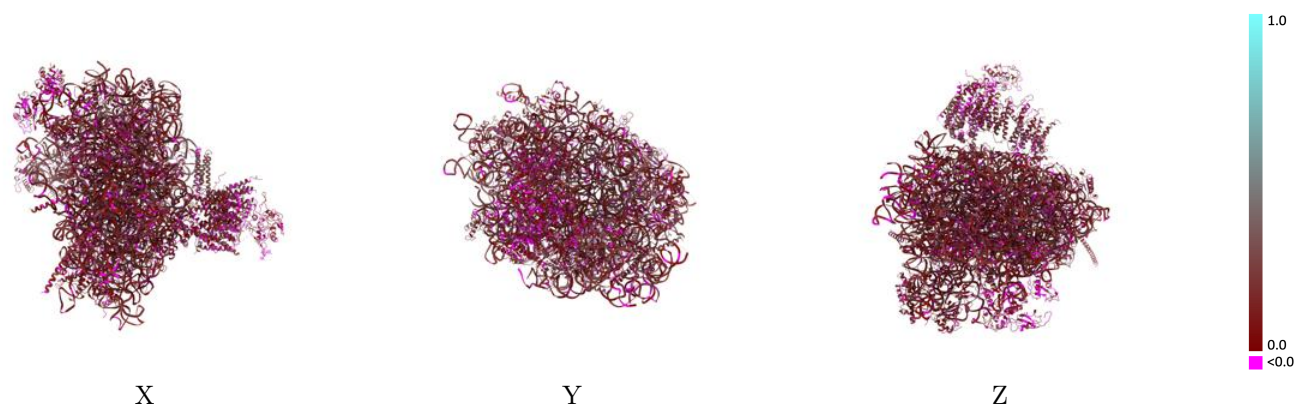
This section contains information regarding the fit between EMDB map EMD-4315 and PDB model 6FTG. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



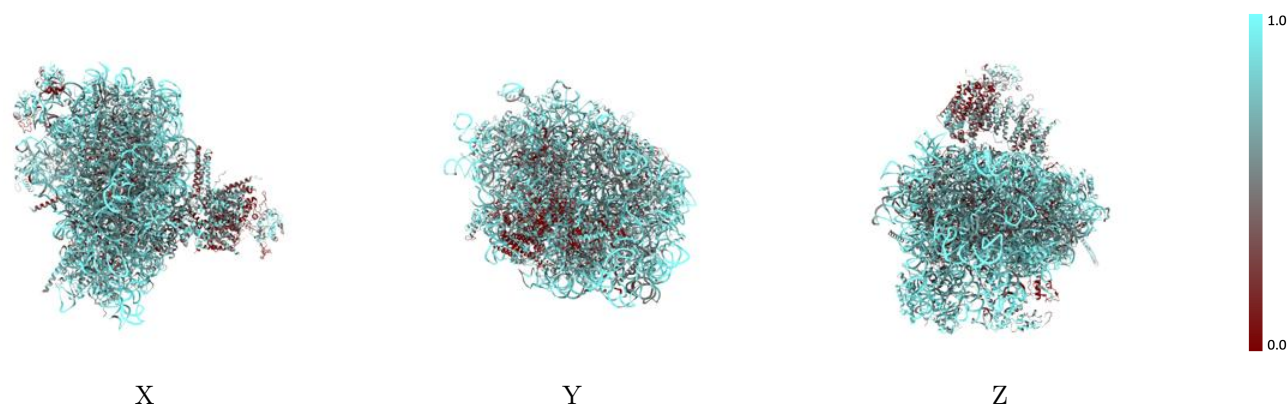
The images above show the 3D surface view of the map at the recommended contour level 2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



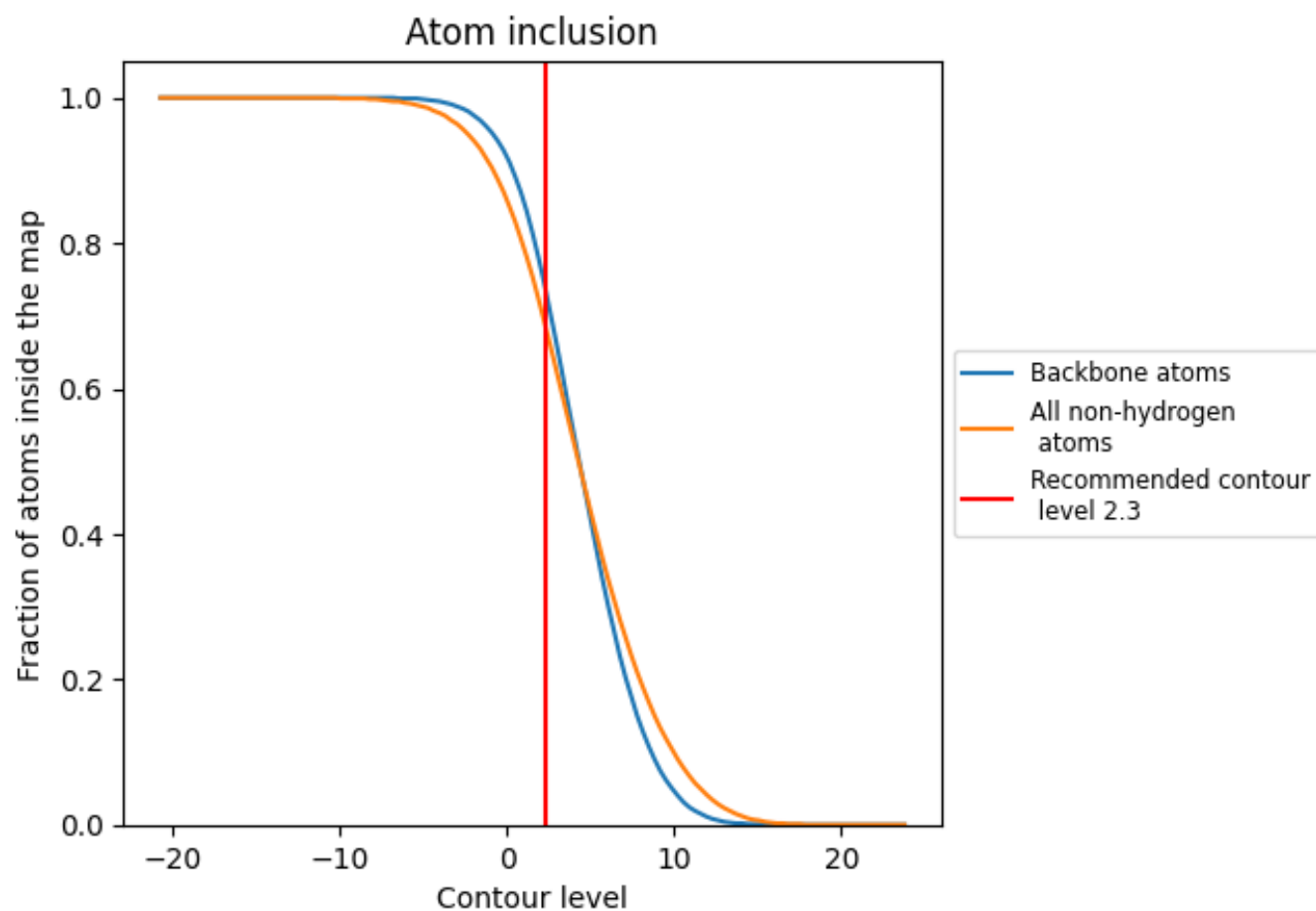
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 69% 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 (2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.1260
1	 0.4260	 0.1340
2	 0.3670	 0.1040
3	 0.5360	 0.1190
4	 0.3420	 0.0980
5	 0.4250	 0.0830
6	 0.3070	 0.0690
7	 0.3760	 0.0480
8	 0.4450	 0.1290
A	 0.4670	 0.0800
B	 0.5720	 0.0950
C	 0.5070	 0.0900
D	 0.7280	 0.1090
E	 0.6930	 0.1170
F	 0.5270	 0.1120
G	 0.6650	 0.1160
H	 0.7190	 0.1170
I	 0.6370	 0.1010
J	 0.7490	 0.1080
K	 0.1700	 -0.0520
L	 0.5790	 0.1080
M	 0.6900	 0.1160
N	 0.3460	 0.0720
O	 0.5480	 0.0990
P	 0.5280	 0.0830
Q	 0.5160	 0.1030
R	 0.6430	 0.1160
S	 0.5640	 0.0940
T	 0.4820	 0.1020
U	 0.7440	 0.1190
V	 0.5560	 0.0910
W	 0.5320	 0.0920
X	 0.5220	 0.1190
Y	 0.5540	 0.0980
Z	 0.6670	 0.1120



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Chain	Atom inclusion	Q-score
a	 0.4690	 0.0840
b	 0.5410	 0.1300
c	 0.7260	 0.1210
d	 0.5690	 0.1050
e	 0.3760	 0.0940
f	 0.5070	 0.0840
g	 0.4730	 0.0900
h	 0.6150	 0.1280
i	 0.6510	 0.1150
j	 0.4930	 0.0750
k	 0.6460	 0.1220
l	 0.4660	 0.1150
m	 0.5220	 0.0990
n	 0.3330	 0.0670
o	 0.5790	 0.0950
p	 0.4980	 0.0980
r	 0.5540	 0.1120
s	 0.6300	 0.0610
t	 0.5950	 0.0470
u	 0.7900	 0.1470
v	 0.8930	 0.1650
w	 0.7670	 0.1470
x	 0.5360	 0.1240
y	 0.4980	 0.0860
z	 0.5820	 0.1430