



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:35 PM UTC

PDB ID : 8P7X / pdb_00008p7x
EMDB ID : EMD-17132
Title : Mycoplasma pneumoniae 70S ribosome in chloramphenicol-treated cells
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.
Deposited on : 2023-05-31
Resolution : 3.03 Å (reported)
Based on initial models : 7OOD, 7OOC

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:

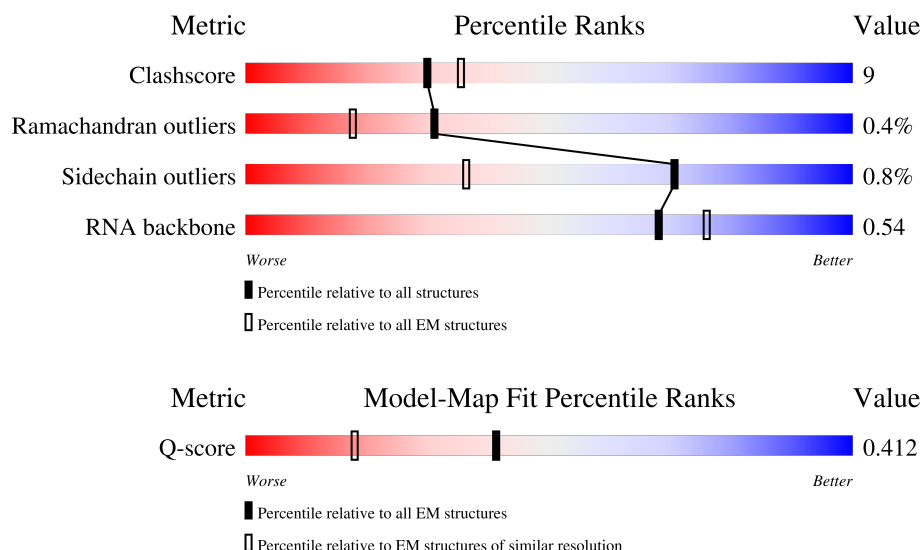
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.03 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	14081 (2.50 - 3.50)

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	0	48	8% 79% 21%
2	1	59	81% 19%
3	2	37	5% 92% 8%

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Mol	Chain	Length	Quality of chain
4	3	2907	
5	4	108	
6	5	1520	
7	6	76	
8	7	75	
9	8	76	
10	A	294	
11	B	273	
12	C	205	
13	D	219	
14	E	215	
15	F	155	
16	G	142	
17	H	132	
18	I	108	
19	J	121	
20	K	139	
21	L	124	
22	M	61	
23	N	86	
24	O	94	
25	P	85	
26	Q	104	
27	R	87	
28	S	87	

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Mol	Chain	Length	Quality of chain
29	T	60	
30	X	444	
31	Y	21	
32	Z	36	
33	a	287	
34	b	287	
35	c	212	
36	d	180	
37	e	184	
38	f	149	
39	g	161	
40	h	137	
41	i	146	
42	j	122	
43	k	151	
44	l	139	
45	m	124	
46	n	116	
47	o	119	
48	p	127	
49	q	100	
50	r	159	
51	s	237	
52	t	111	
53	u	104	

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Mol	Chain	Length	Quality of chain
54	v	65	17% 74% 25% .
55	w	111	29% 76% 23% .
56	x	97	93% 63% 33% ..
57	y	57	11% 75% 23% .
58	z	53	9% 77% 15% 6%

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 151591 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 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	48	Total	C	N	O	S	0	0
			392	242	85	63	2		

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			477	300	99	77	1		

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	37	Total	C	N	O	S	0	0
			304	189	65	46	4		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	2893	Total	C	N	O	P	0	0
			61995	27704	11293	20105	2893		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	108	Total	C	N	O	P	0	0
			2305	1030	415	752	108		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	1507	Total	C	N	O	P	0	0
			32258	14420	5847	10484	1507		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1003	A	G	conflict	GB 26117688

- Molecule 7 is a RNA chain called tRNA-Ala (E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	76	Total	C	N	O	P	0	0
			1620	723	287	534	76		

- Molecule 8 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	75	Total	C	N	O	P	0	0
			1599	712	279	533	75		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	17	G	-	insertion	GB 26117688
7	55	C	U	conflict	GB 26117688

- Molecule 9 is a RNA chain called tRNA-Lys (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	76	Total	C	N	O	P	0	0
			1615	722	284	533	76		

- Molecule 10 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	266	Total	C	N	O	S	0	0
			2138	1359	376	394	9		

- Molecule 11 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	232	Total	C	N	O	S	0	0
			1835	1158	343	329	5		

- Molecule 12 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	204	Total	C	N	O	S	0	0
			1669	1057	316	292	4		

- Molecule 13 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	155	Total	C	N	O	S	0	0
			1191	753	228	207	3		

- Molecule 14 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	184	Total	C	N	O	S	0	0
			1509	950	270	287	2		

- Molecule 15 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	155	Total	C	N	O	S	0	0
			1254	790	240	217	7		

- Molecule 16 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 17 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	129	Total	C	N	O	S	0	0
			1040	661	195	183	1		

- Molecule 18 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	104	Total	C	N	O	S	0	0
			832	536	147	148	1		

- Molecule 19 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 20 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	135	Total	C	N	O	S	0	0
			1071	677	212	180	2		

- Molecule 21 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	123	Total	C	N	O		0	0
			991	618	200	173			

- Molecule 22 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	60	Total	C	N	O	S	0	0
			474	302	96	72	4		

- Molecule 23 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	85	Total	C	N	O		0	0
			689	436	130	123			

- Molecule 24 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	87	Total	C	N	O	S	0	0
			705	453	130	118	4		

- Molecule 25 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	85	Total	C	N	O	S	0	0
			693	436	138	118	1		

- Molecule 26 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	71	Total	C	N	O	S	0	0
			590	378	115	93	4		

- Molecule 27 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	86	Total	C	N	O	S	0	0
			700	444	132	122	2		

- Molecule 28 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	79	Total	C	N	O		0	0
			643	391	138	114			

- Molecule 29 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	59	Total	C	N	O	S	0	0
			519	326	111	80	2		

- Molecule 30 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	30	Total	C	N	O	S	0	0
			242	155	43	43	1		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	21	Total	C	N	O	P	0	0
			446	200	80	145	21		

- Molecule 32 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Z	36	Total	C	N	O	0	0
			187	112	37	38		

- Molecule 33 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 34 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	231	Total	C	N	O	S	0	0
			1778	1129	320	322	7		

- Molecule 35 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	211	Total	C	N	O	S	0	0
			1654	1053	299	299	3		

- Molecule 36 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	179	Total	C	N	O	S	0	0
			1416	910	251	251	4		

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	e	176	Total	C	N	O	0	0
			1396	899	247	250		

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	149	Total	C	N	O	S	0	0
			1208	779	212	214	3		

- Molecule 39 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	125	Total	C	N	O	S	0	0
			951	606	165	177	3		

- Molecule 40 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 41 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 42 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 43 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	150	Total	C	N	O	S	0	0
			1170	741	228	200	1		

- Molecule 44 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 45 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 46 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	116	Total	C	N	O	S	0	0
			918	573	181	162	2		

- Molecule 47 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	118	Total	C	N	O	S	0	0
			966	609	186	170	1		

- Molecule 48 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	118	Total	C	N	O	S	0	0
			981	624	194	161	2		

- Molecule 49 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	142	Total	C	N	O	S	0	0
			1091	677	212	195	7		

- Molecule 51 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	95	Total	C	N	O	S	0	0
			740	486	125	128	1		

- Molecule 52 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	111	Total	C	N	O	S	0	0
			871	550	166	152	3		

- Molecule 53 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	88	Total	C	N	O	S	0	0
			670	416	132	121	1		

- Molecule 54 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	64	Total	C	N	O	S	0	0
			520	320	109	90	1		

- Molecule 55 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	110	Total	C	N	O		0	0
			906	576	168	162			

- Molecule 56 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	96	Total	C	N	O	S	0	0
			761	481	133	143	4		

- Molecule 57 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

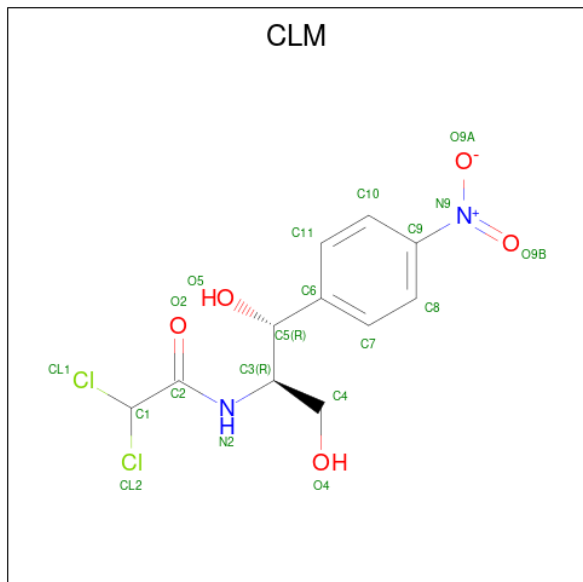
- Molecule 58 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	2	1	Total	Zn	0
			1	1	
59	M	1	Total	Zn	0
			1	1	
59	Q	1	Total	Zn	0
			1	1	
59	x	1	Total	Zn	0
			1	1	
59	y	1	Total	Zn	0
			1	1	
59	z	1	Total	Zn	0
			1	1	

- Molecule 60 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
60	3	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
61	3	1	Total	K	0
			1	1	

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

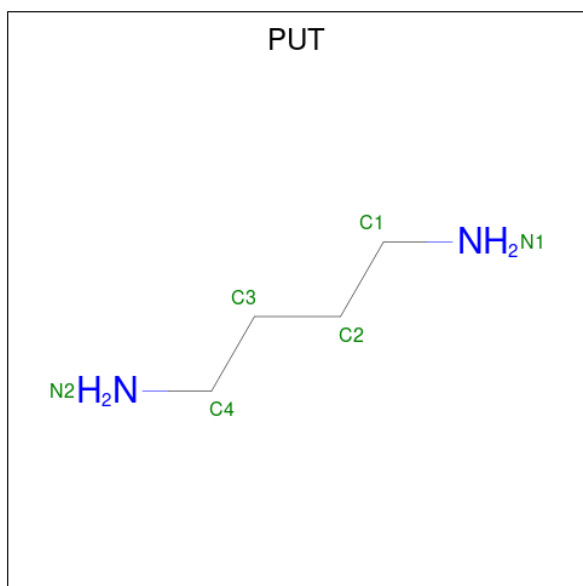
Mol	Chain	Residues	Atoms		AltConf
62	3	218	Total	Mg	0
			218	218	
62	4	1	Total	Mg	0
			1	1	
62	5	89	Total	Mg	0
			89	89	
62	6	1	Total	Mg	0
			1	1	
62	7	2	Total	Mg	0
			2	2	
62	8	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
62	K	1	Total	Mg	0
			1	1	
62	P	1	Total	Mg	0
			1	1	
62	S	1	Total	Mg	0
			1	1	
62	Y	2	Total	Mg	0
			2	2	
62	a	1	Total	Mg	0
			1	1	
62	b	2	Total	Mg	0
			2	2	
62	i	1	Total	Mg	0
			1	1	
62	y	2	Total	Mg	0
			2	2	

- Molecule 63 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



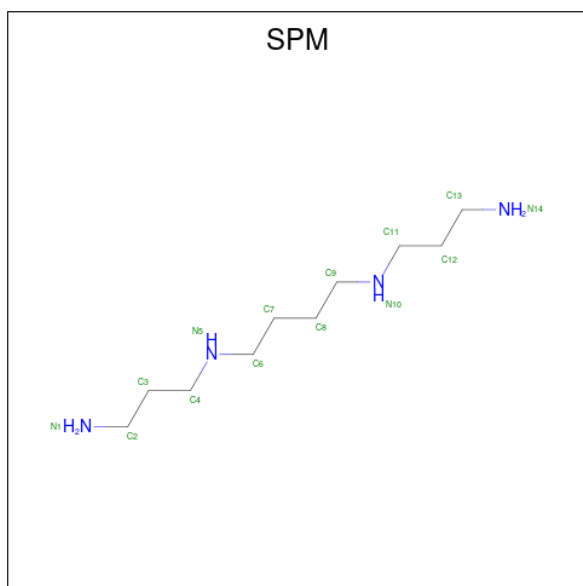
Mol	Chain	Residues	Atoms			AltConf
63	3	1	Total	C	N	0
			6	4	2	
63	3	1	Total	C	N	0
			6	4	2	
63	3	1	Total	C	N	0
			6	4	2	

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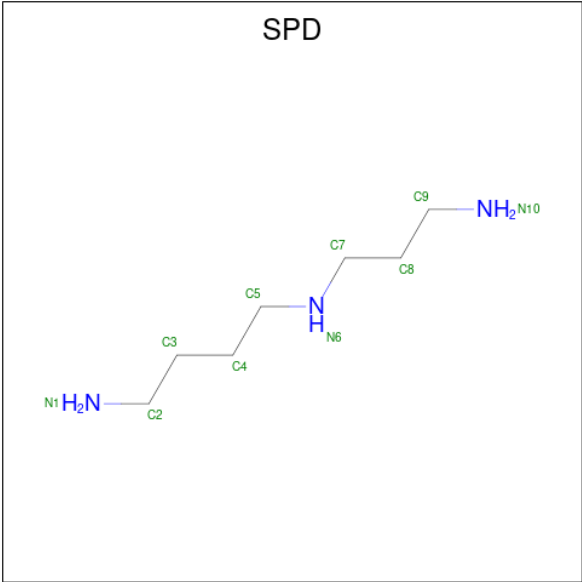
Mol	Chain	Residues	Atoms			AltConf
63	3	1	Total	C	N	0
			6	4	2	
63	3	1	Total	C	N	0
			6	4	2	
63	3	1	Total	C	N	0
			6	4	2	
63	3	1	Total	C	N	0
			6	4	2	
63	5	1	Total	C	N	0
			6	4	2	

- Molecule 64 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
64	3	1	Total	C	N	0
			14	10	4	
64	3	1	Total	C	N	0
			14	10	4	
64	3	1	Total	C	N	0
			14	10	4	
64	b	1	Total	C	N	0
			14	10	4	

- Molecule 65 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



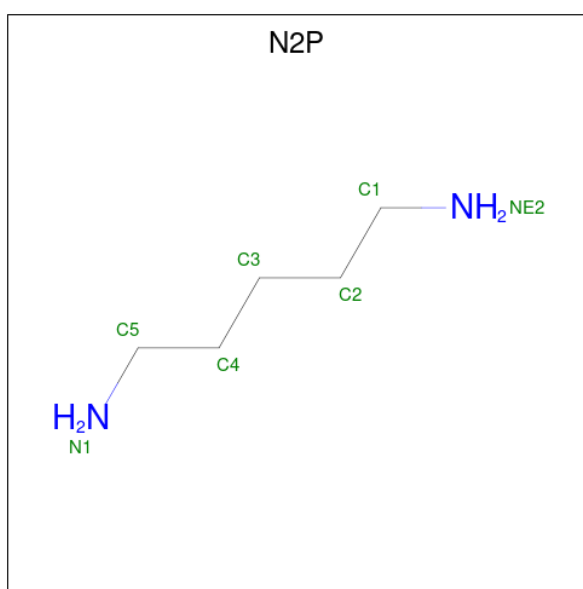
Mol	Chain	Residues	Atoms			AltConf
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	

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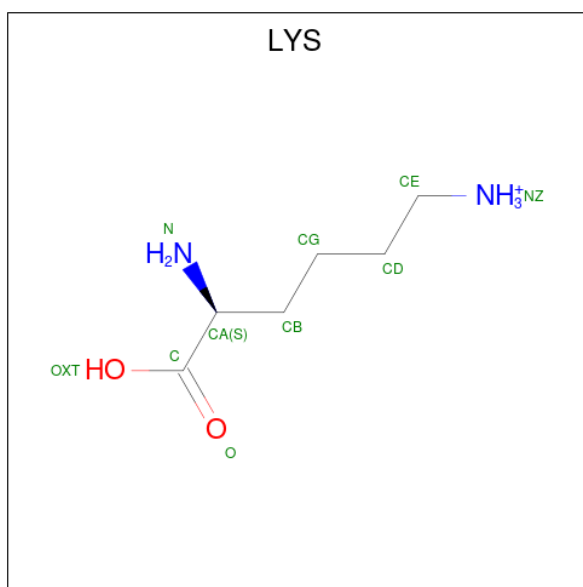
Mol	Chain	Residues	Atoms			AltConf
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	5	1	Total	C	N	0
			10	7	3	
65	5	1	Total	C	N	0
			10	7	3	

- Molecule 66 is PENTANE-1,5-DIAMINE (CCD ID: N2P) (formula: $C_5H_{14}N_2$).



Mol	Chain	Residues	Atoms			AltConf
66	3	1	Total	C	N	0
			7	5	2	
66	3	1	Total	C	N	0
			7	5	2	
66	3	1	Total	C	N	0
			7	5	2	
66	5	1	Total	C	N	0
			7	5	2	

- Molecule 67 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).

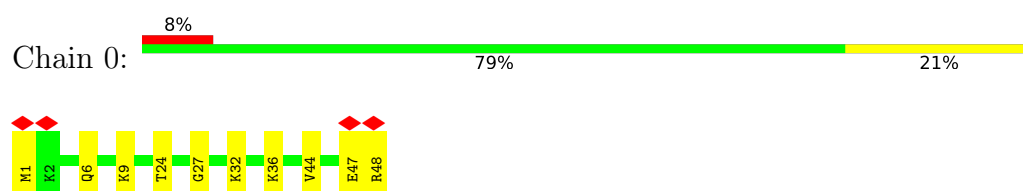


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
67	8	1	9	6	2	1	0

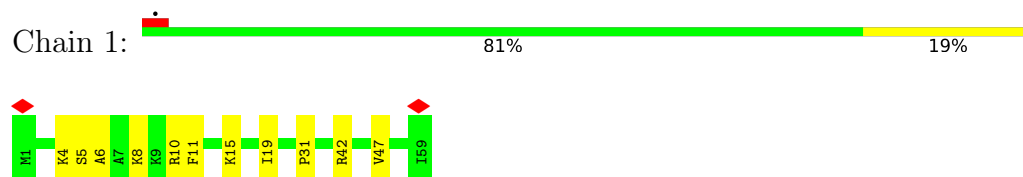
3 Residue-property plots [i](#)

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

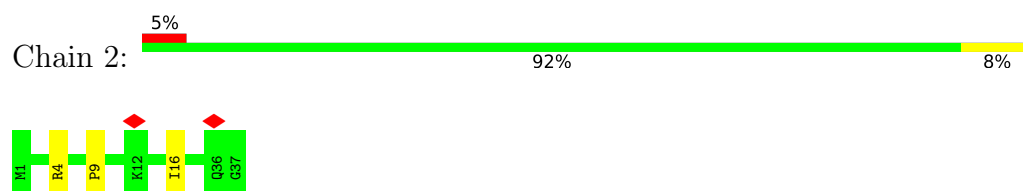
- Molecule 1: 50S ribosomal protein L34



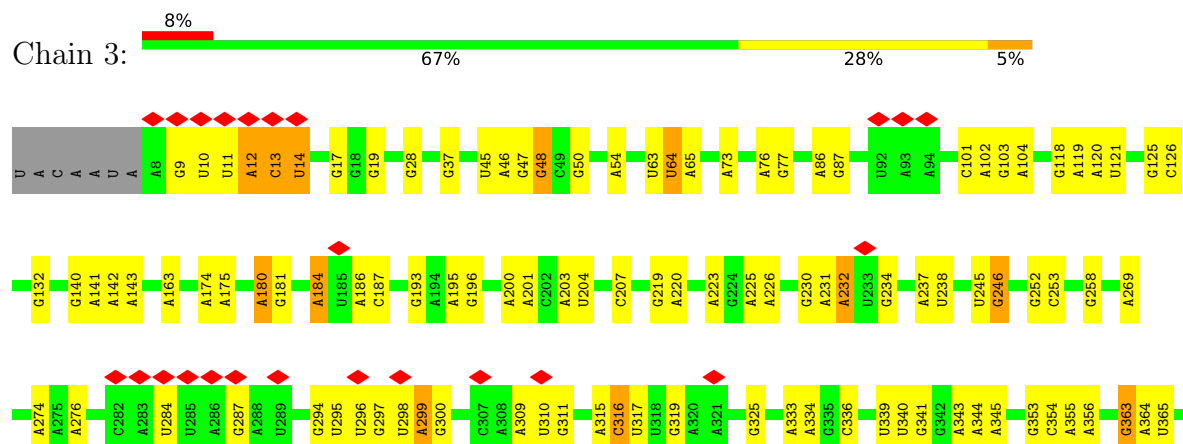
- Molecule 2: 50S ribosomal protein L35

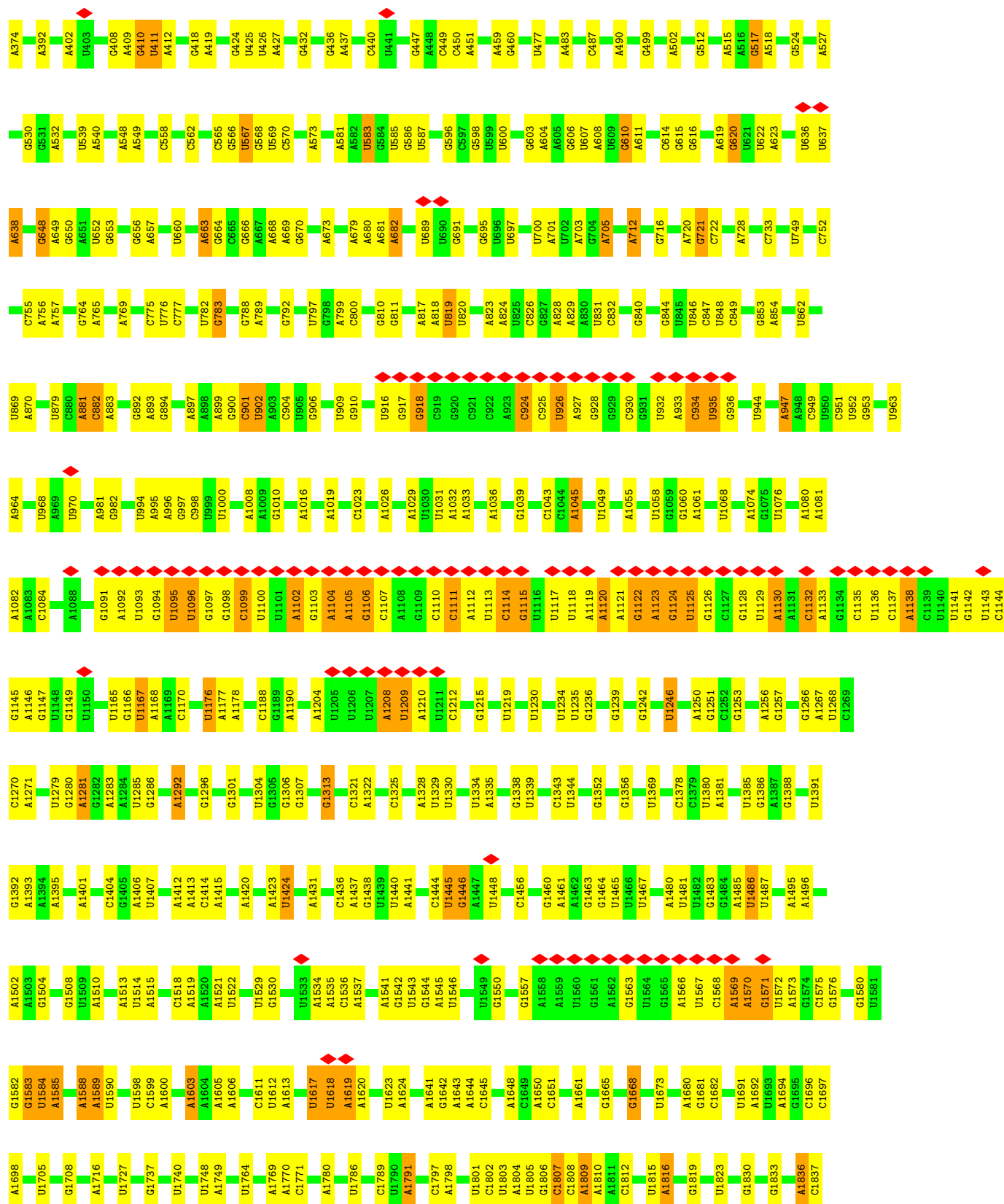


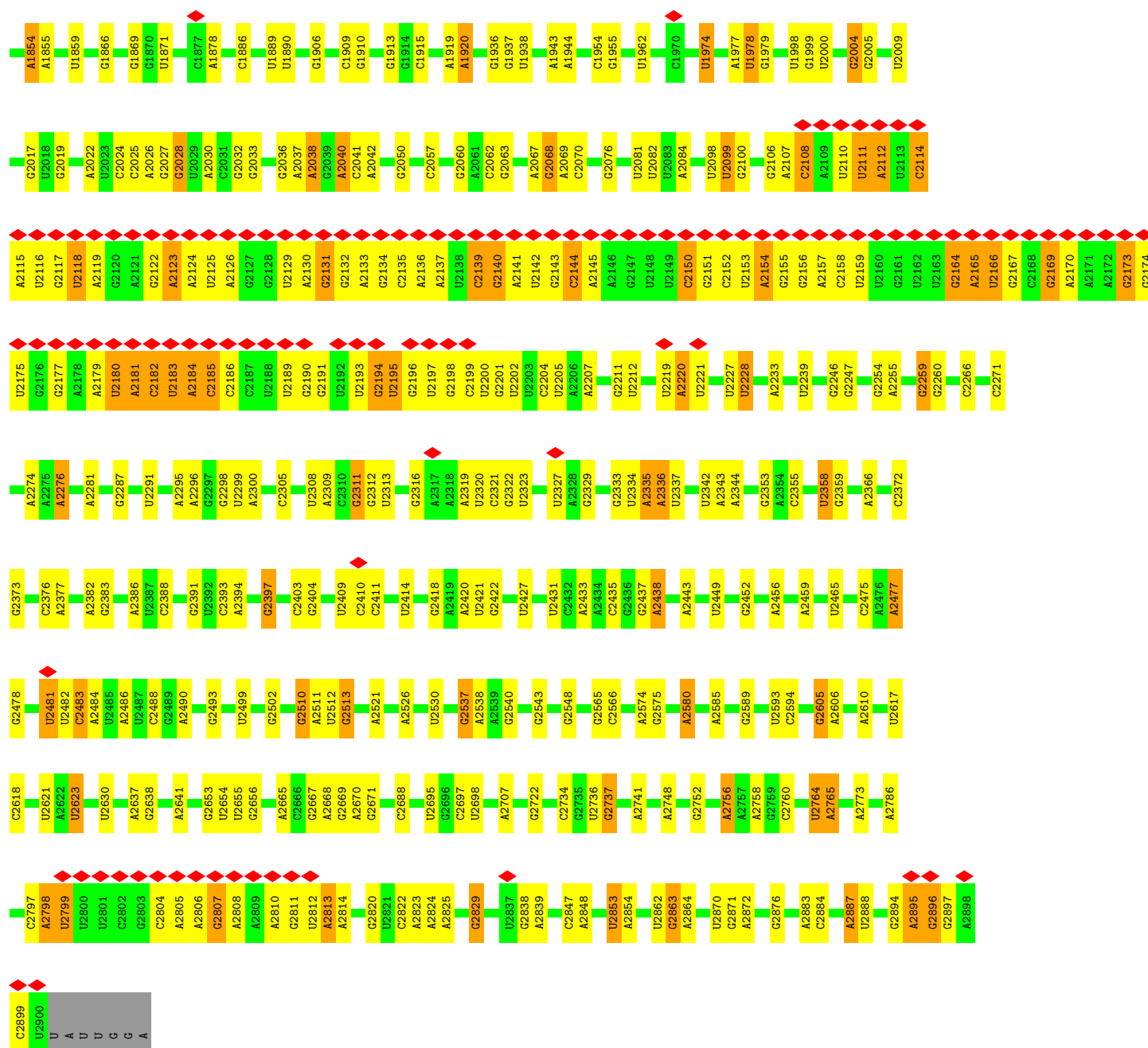
- Molecule 3: 50S ribosomal protein L36



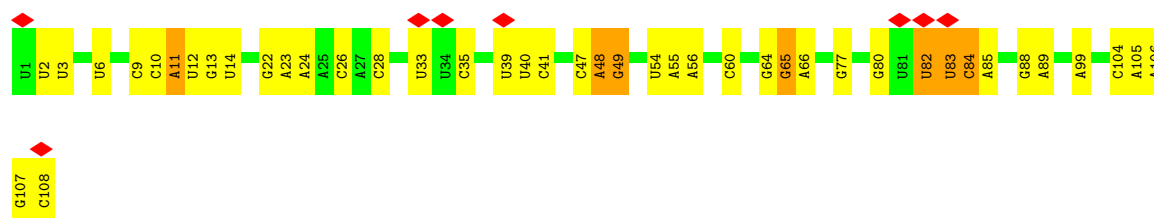
- Molecule 4: 23S ribosomal RNA



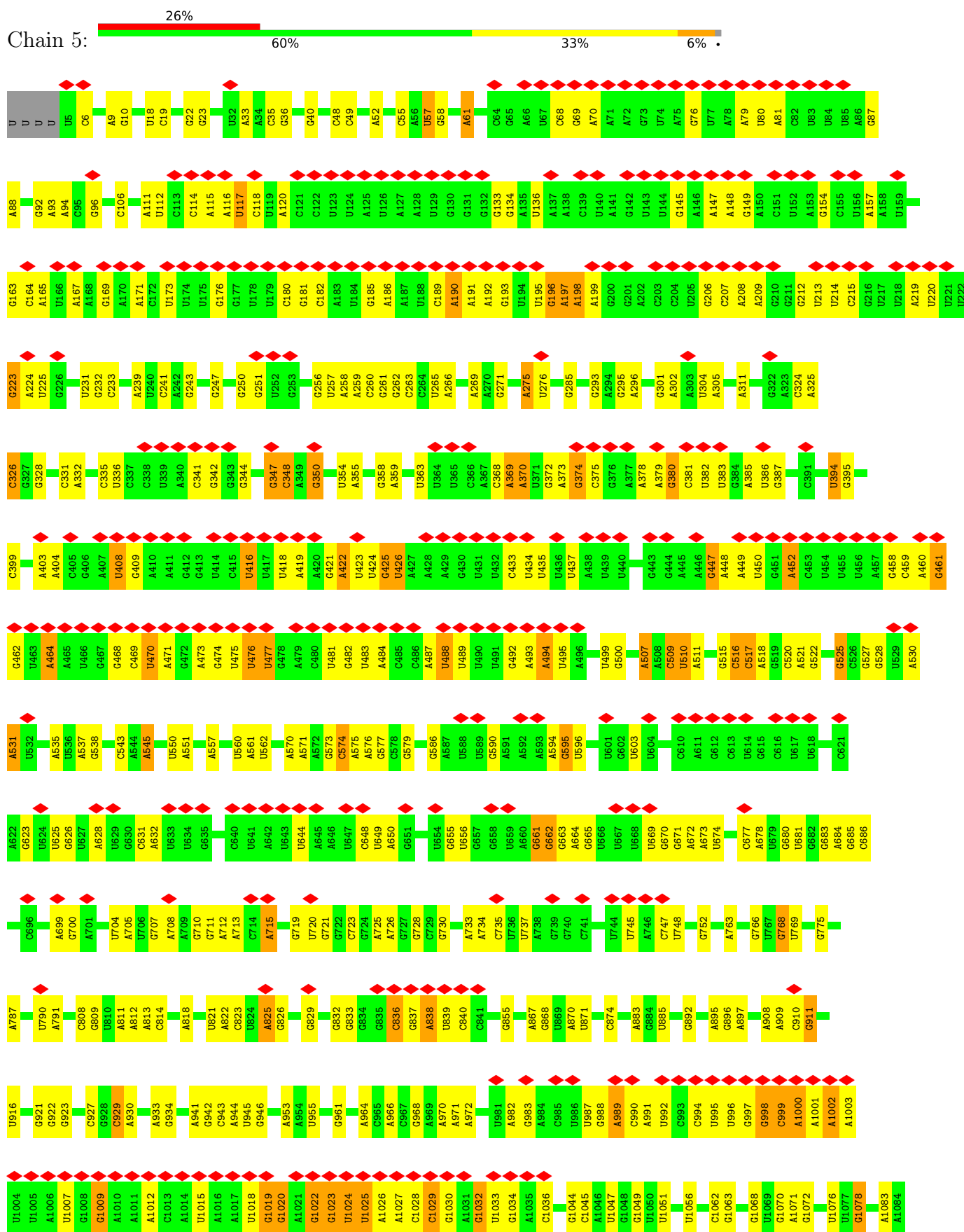


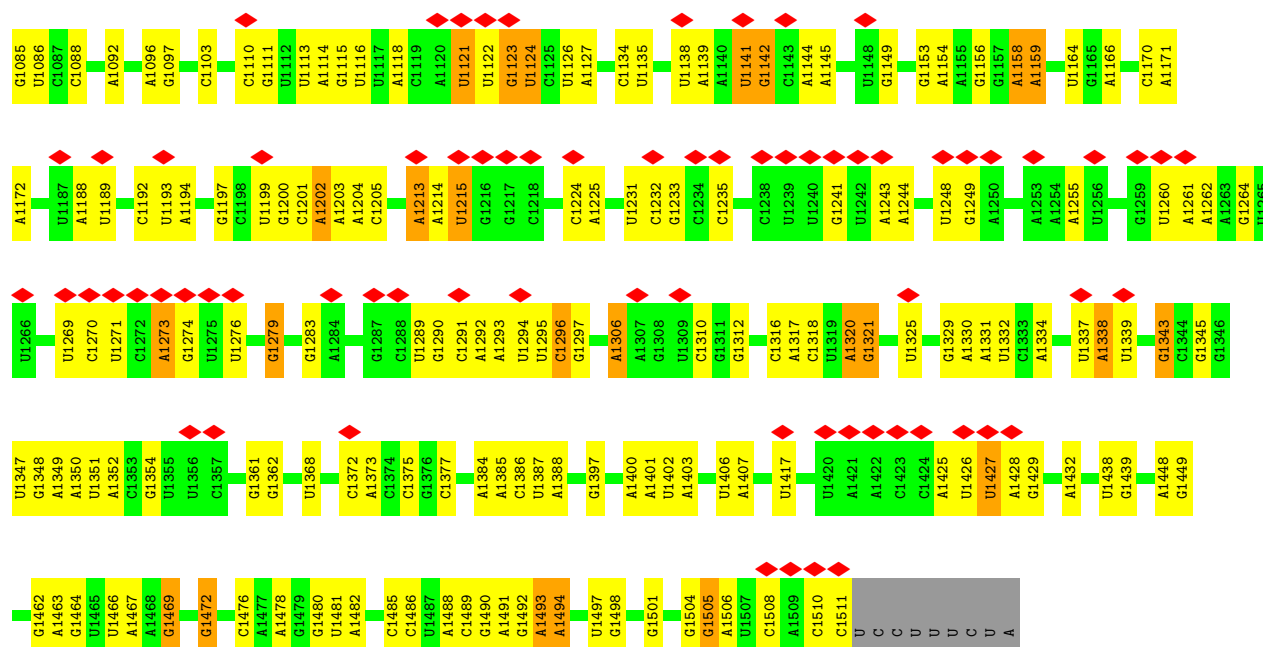


- Molecule 5: 5S ribosomal RNA

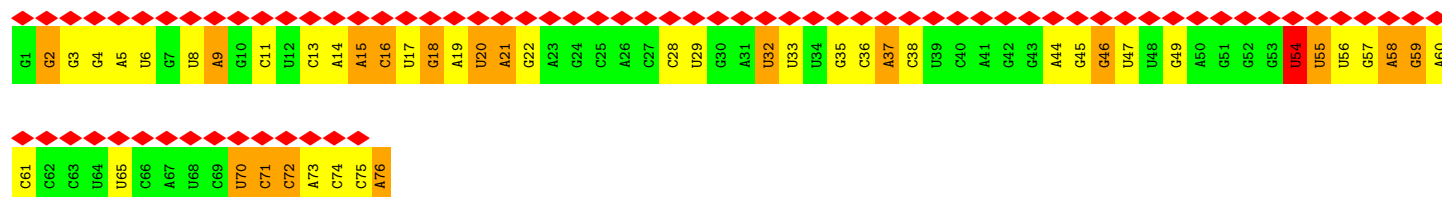


- Molecule 6: 16S ribosomal RNA

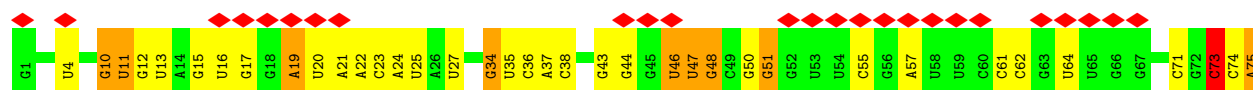




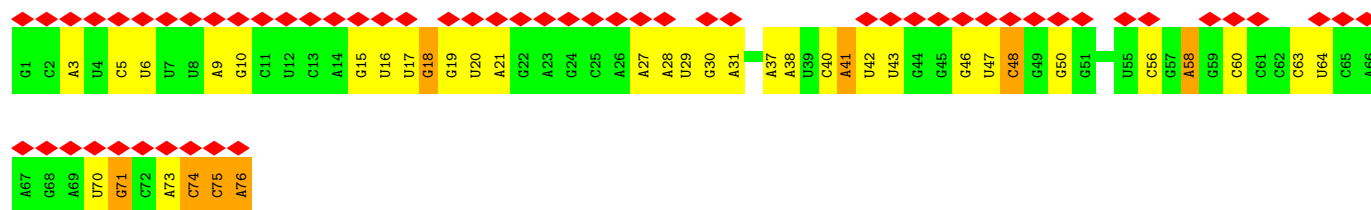
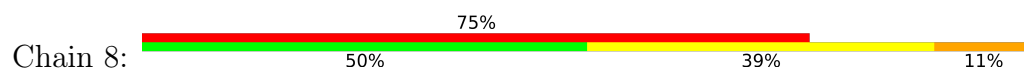
- Molecule 7: tRNA-Ala (E-site)



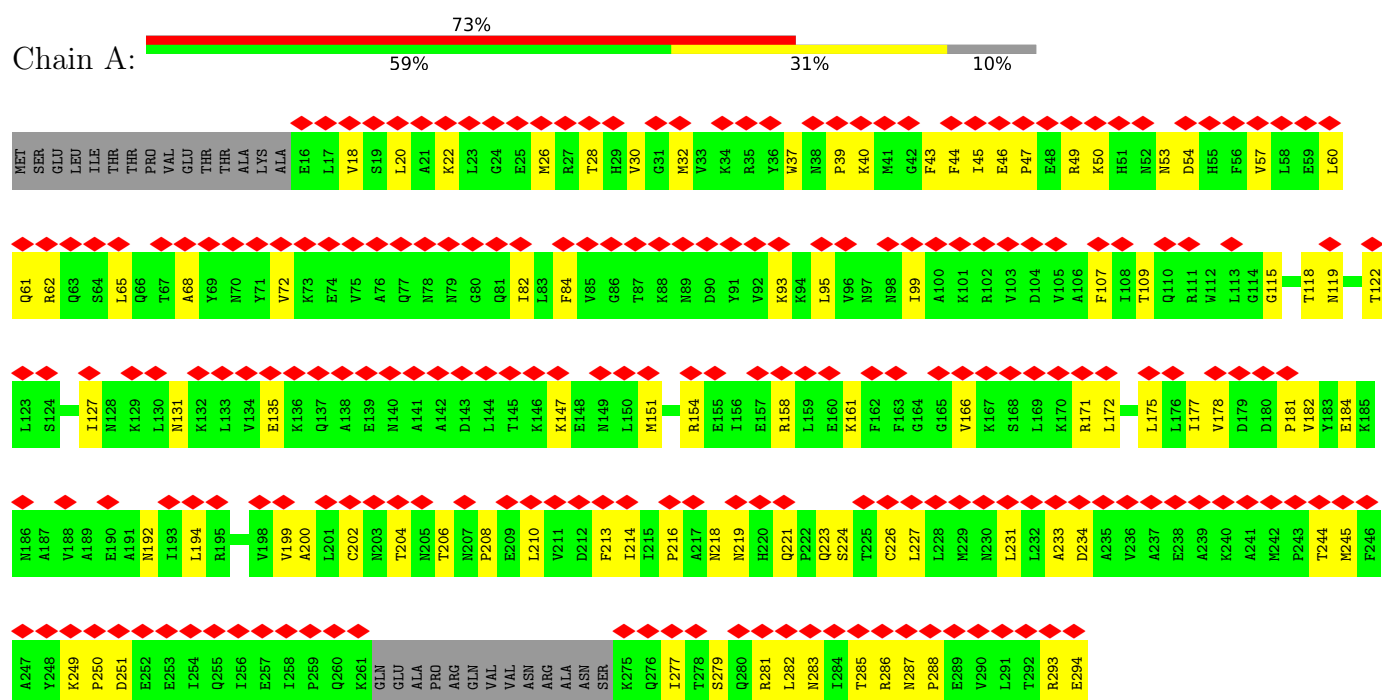
- Molecule 8: tRNA-Asp (P-site)

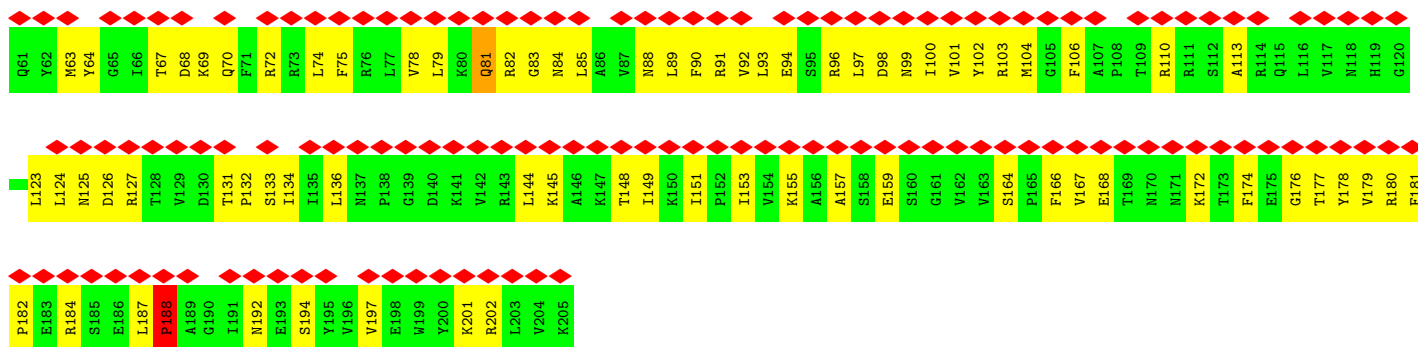


- Molecule 9: tRNA-Lys (A-site)

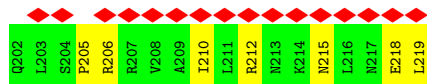
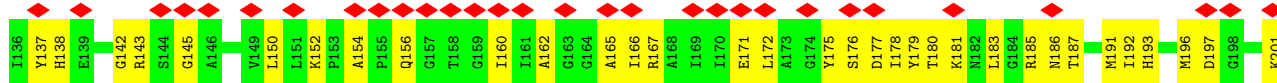
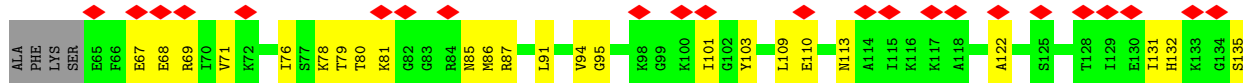
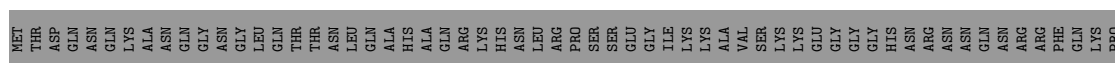


- Molecule 10: 30S ribosomal protein S2

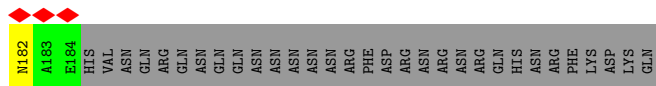
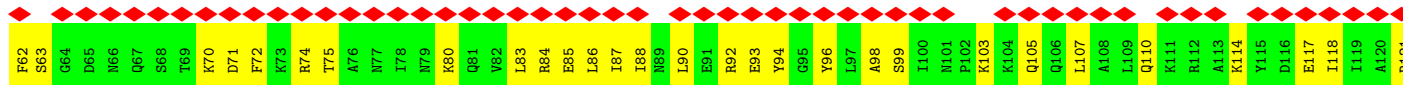
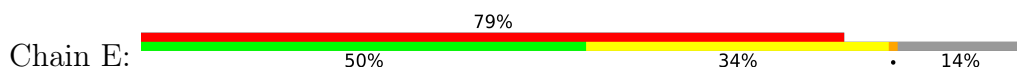




• Molecule 13: 30S ribosomal protein S5

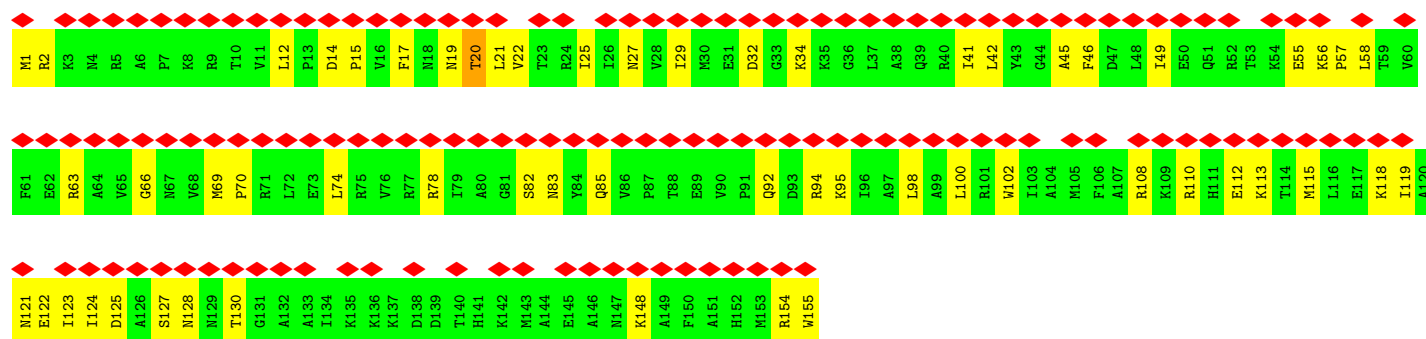


• Molecule 14: 30S ribosomal protein S6



• Molecule 15: 30S ribosomal protein S7

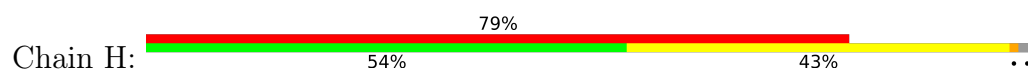




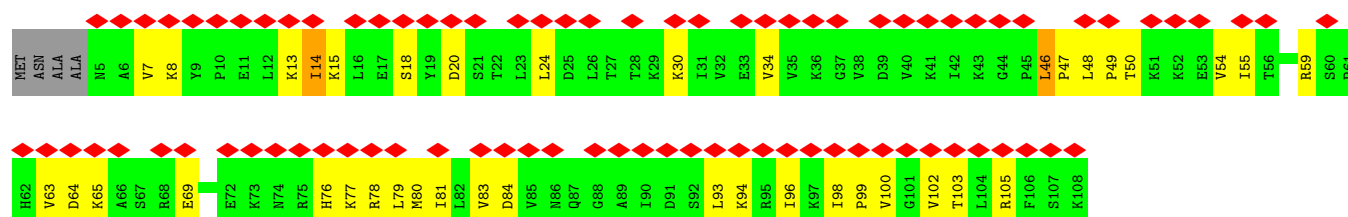
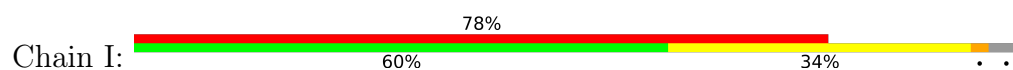
• Molecule 16: 30S ribosomal protein S8



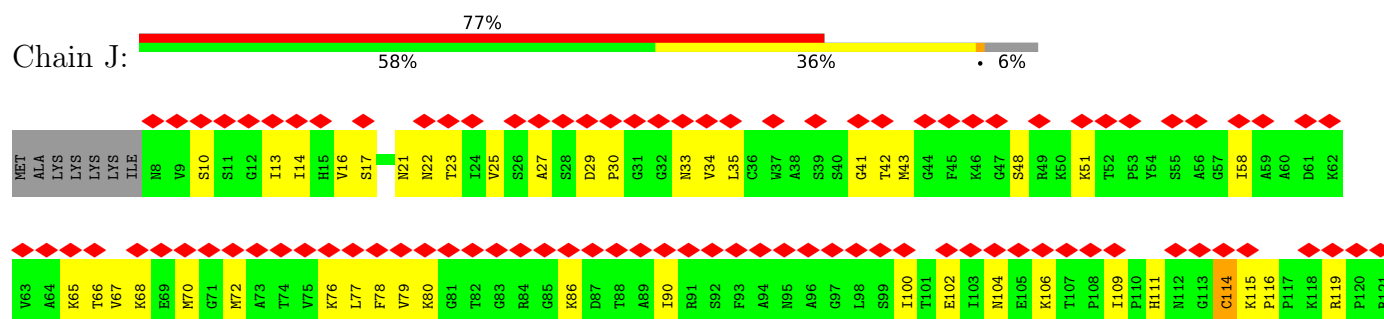
• Molecule 17: 30S ribosomal protein S9



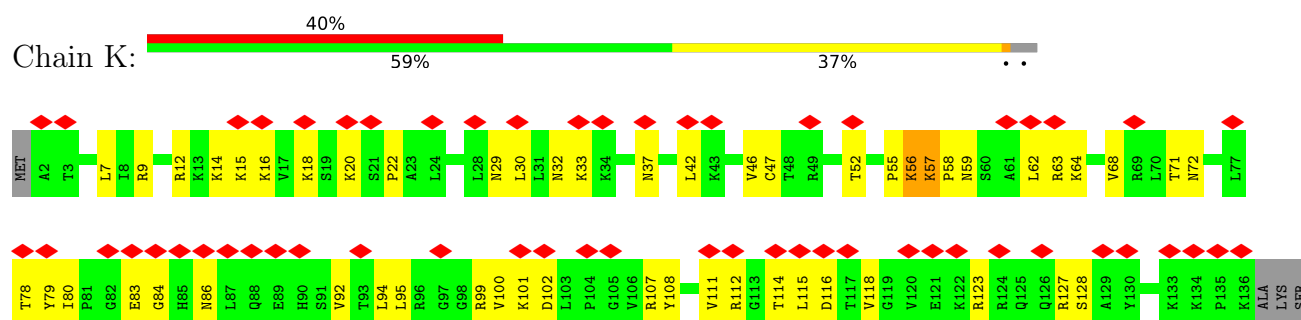
• Molecule 18: 30S ribosomal protein S10



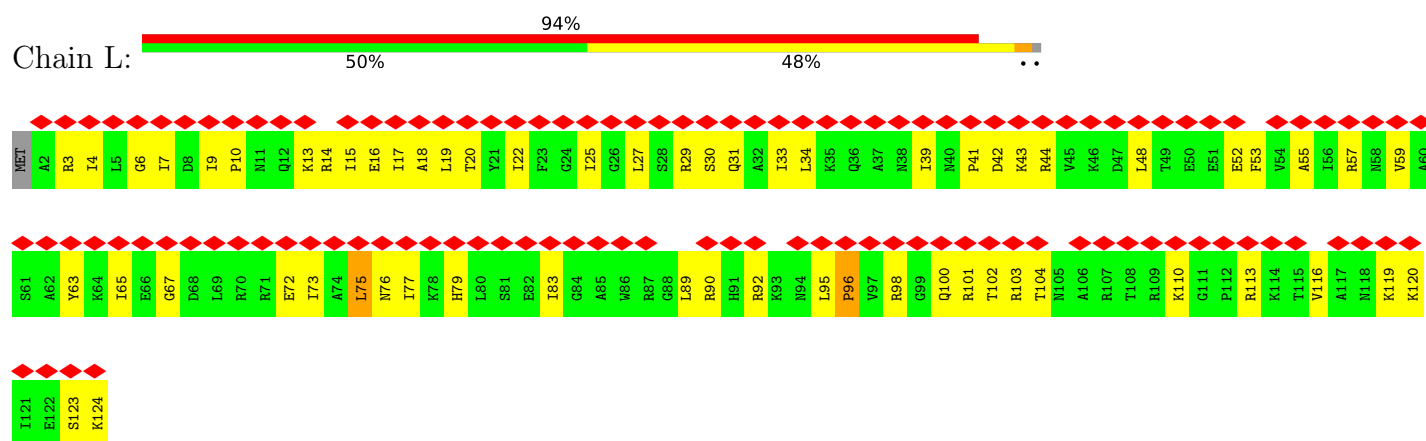
- Molecule 19: 30S ribosomal protein S11



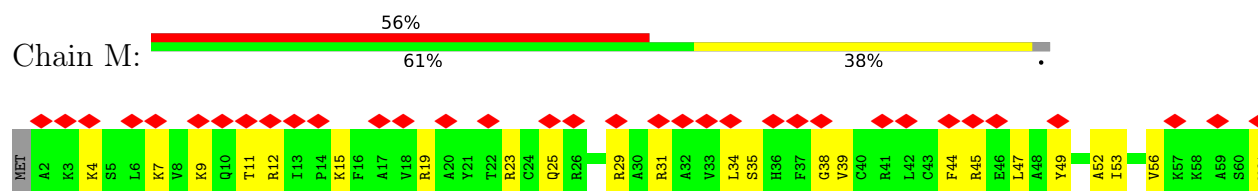
- Molecule 20: 30S ribosomal protein S12



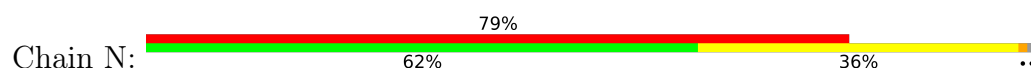
- Molecule 21: 30S ribosomal protein S13

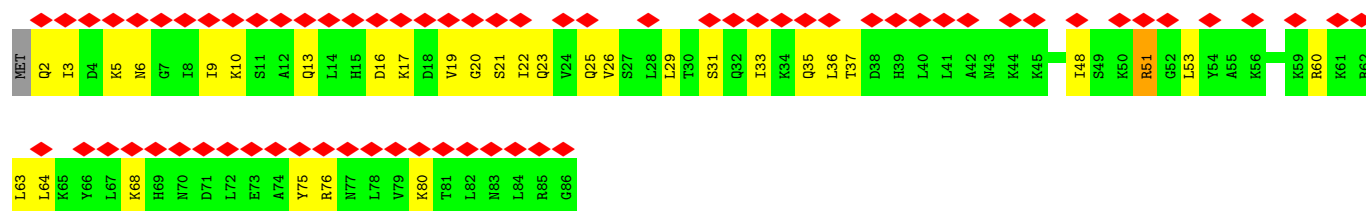


- Molecule 22: 30S ribosomal protein S14 type Z

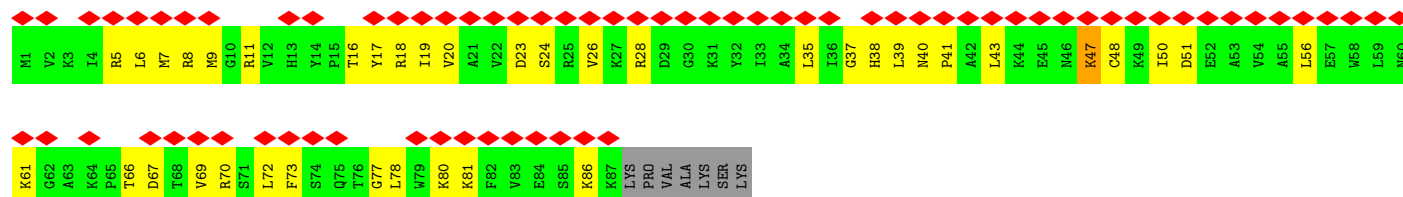
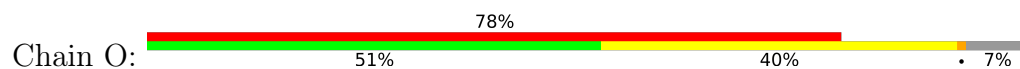


- Molecule 23: 30S ribosomal protein S15

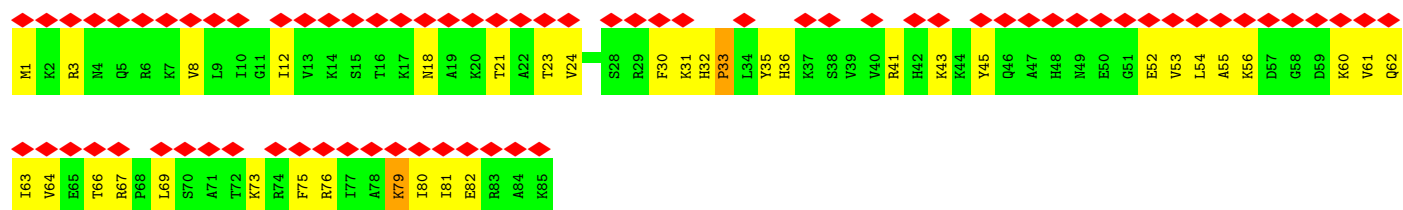
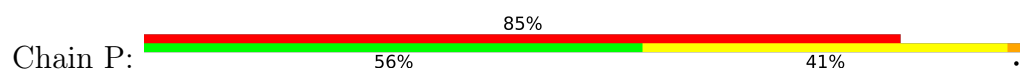




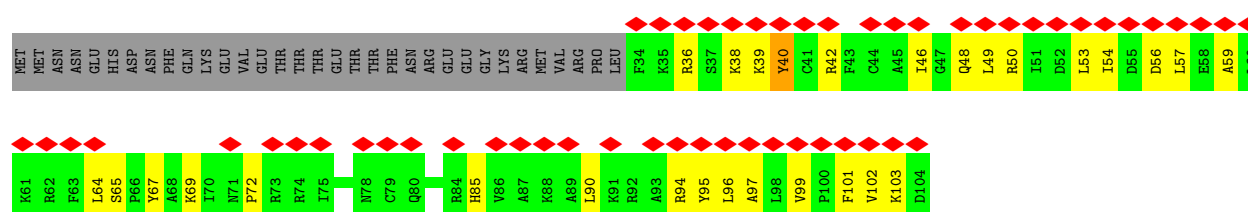
• Molecule 24: 30S ribosomal protein S16



• Molecule 25: 30S ribosomal protein S17



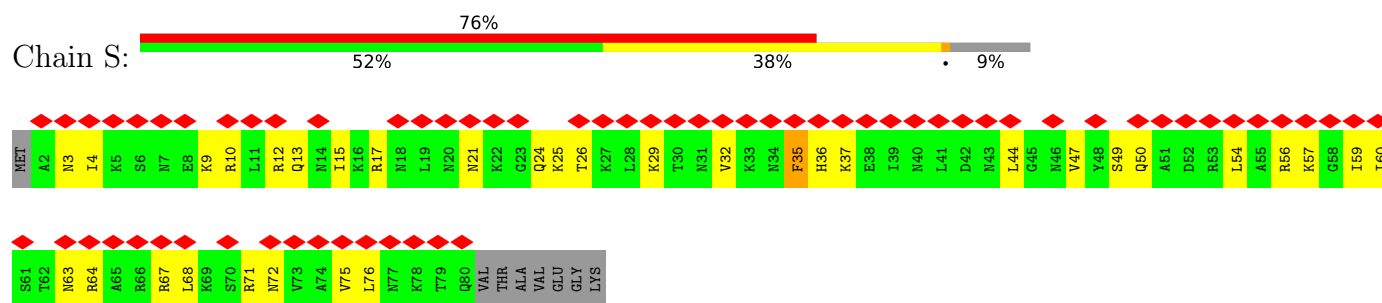
• Molecule 26: 30S ribosomal protein S18



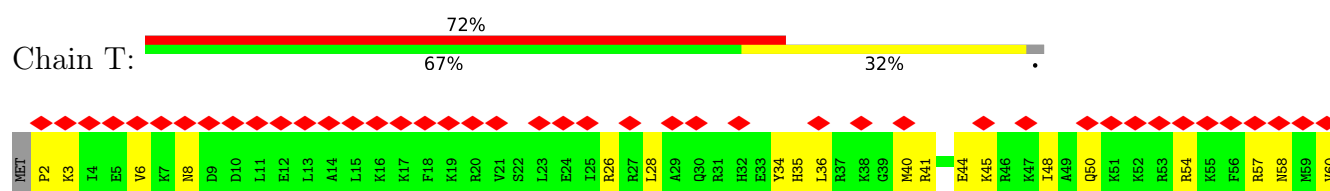
• Molecule 27: 30S ribosomal protein S19



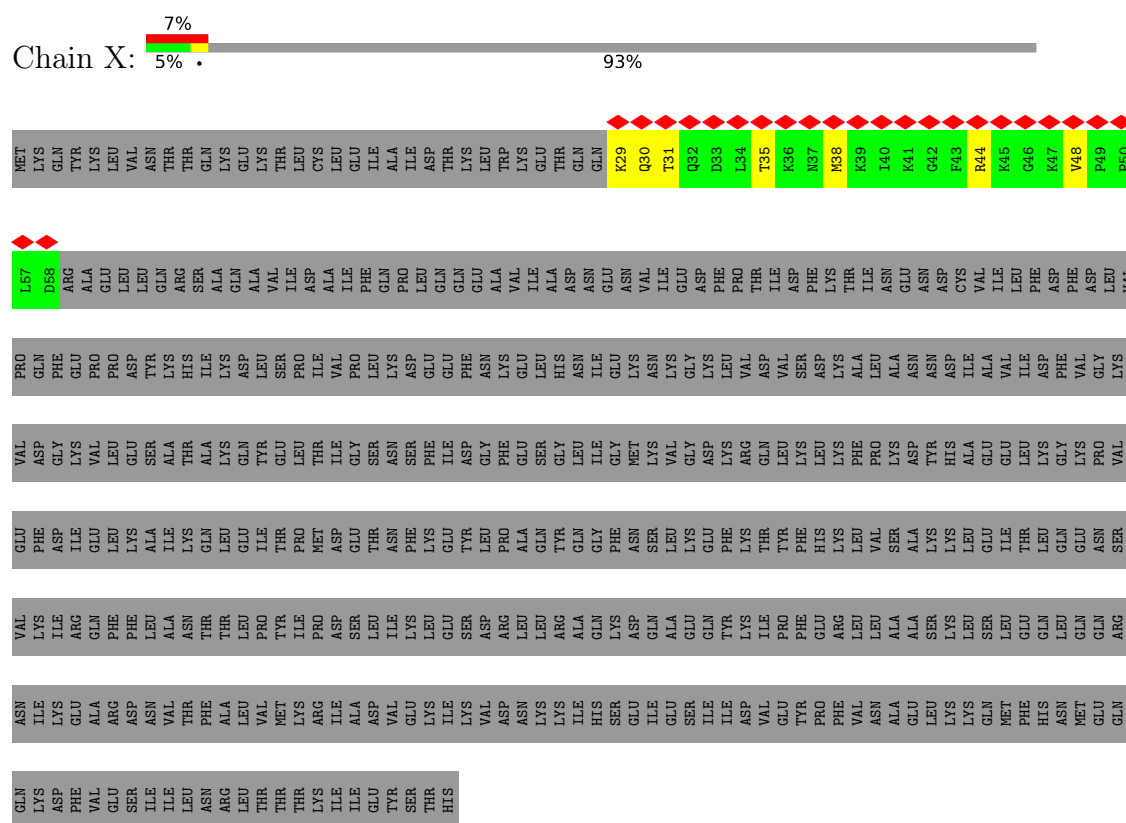
- Molecule 28: 30S ribosomal protein S20



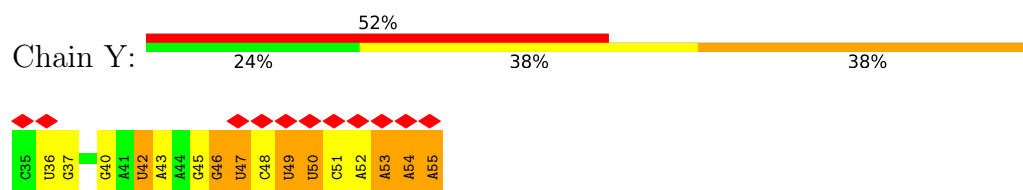
- Molecule 29: 30S ribosomal protein S21



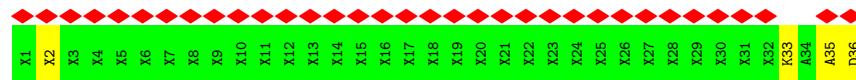
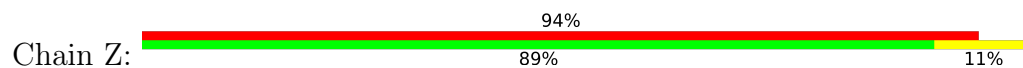
- Molecule 30: Trigger factor



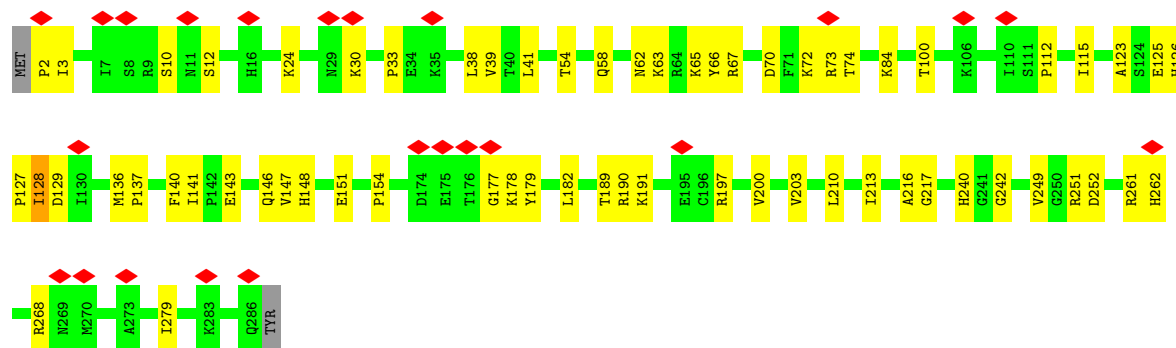
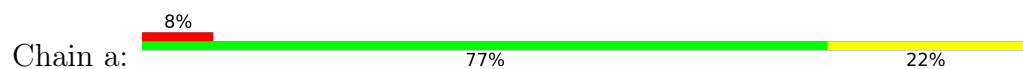
- Molecule 31: mRNA



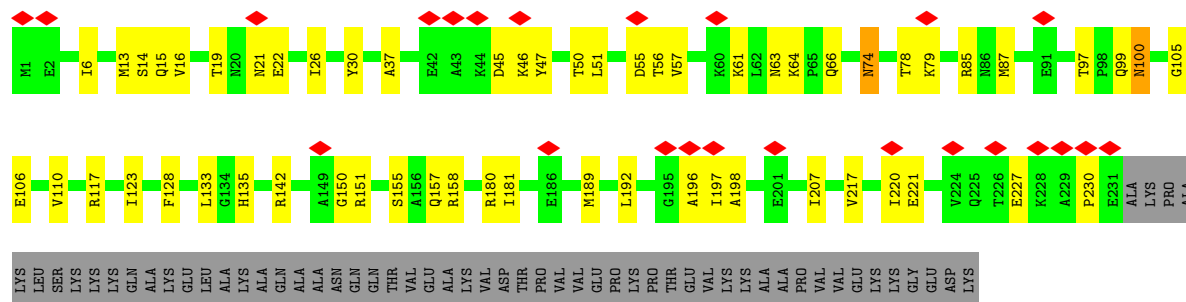
- Molecule 32: Nascent chain



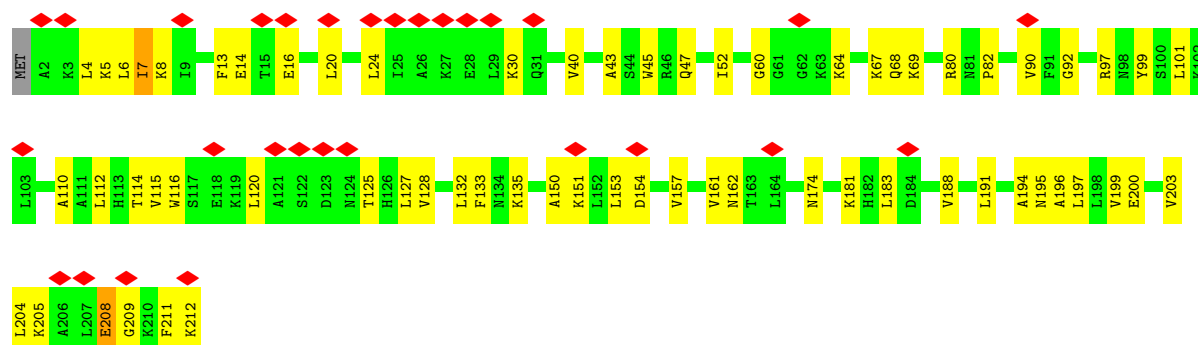
- Molecule 33: 50S ribosomal protein L2



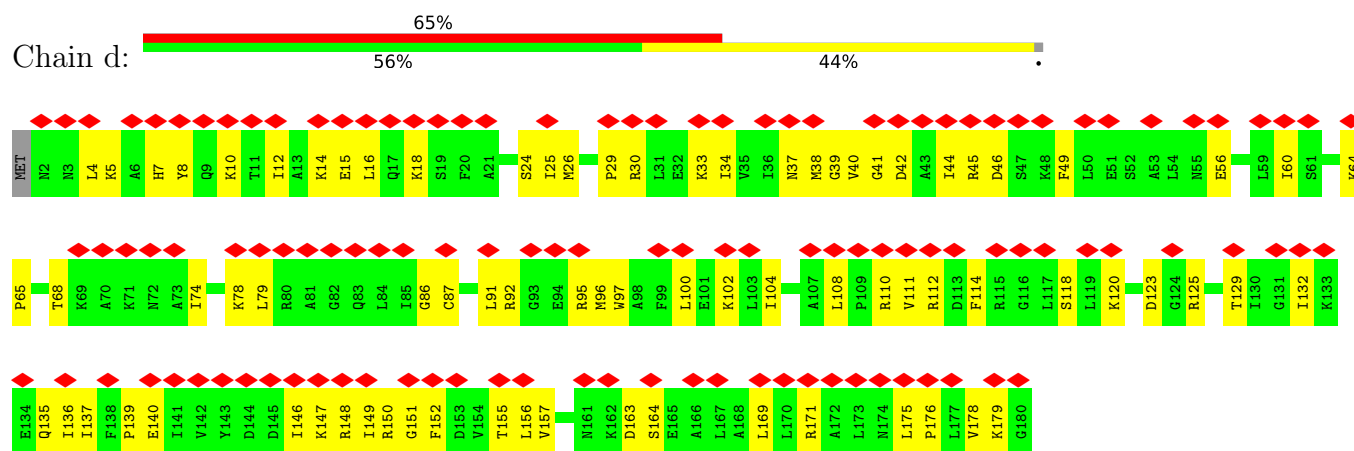
- Molecule 34: 50S ribosomal protein L3



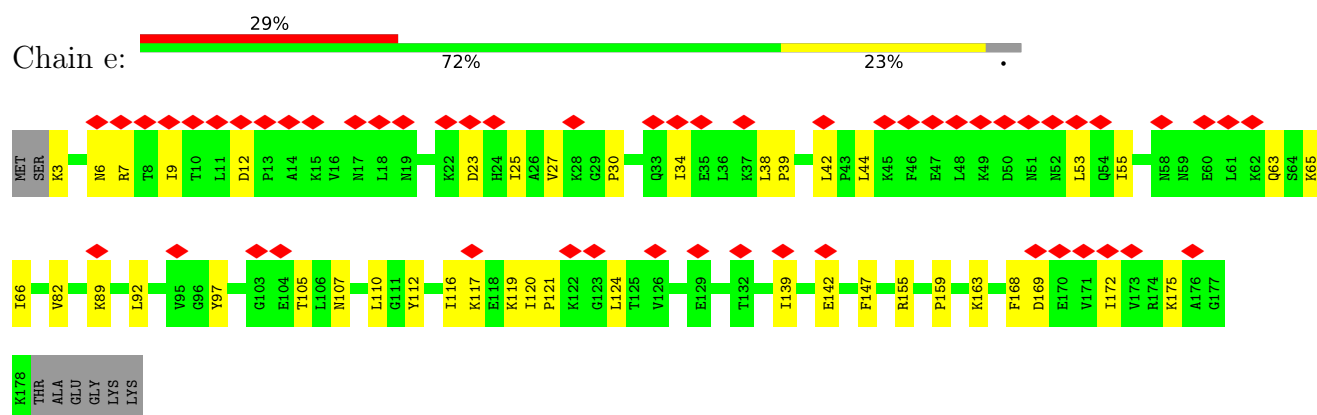
- Molecule 35: 50S ribosomal protein L4



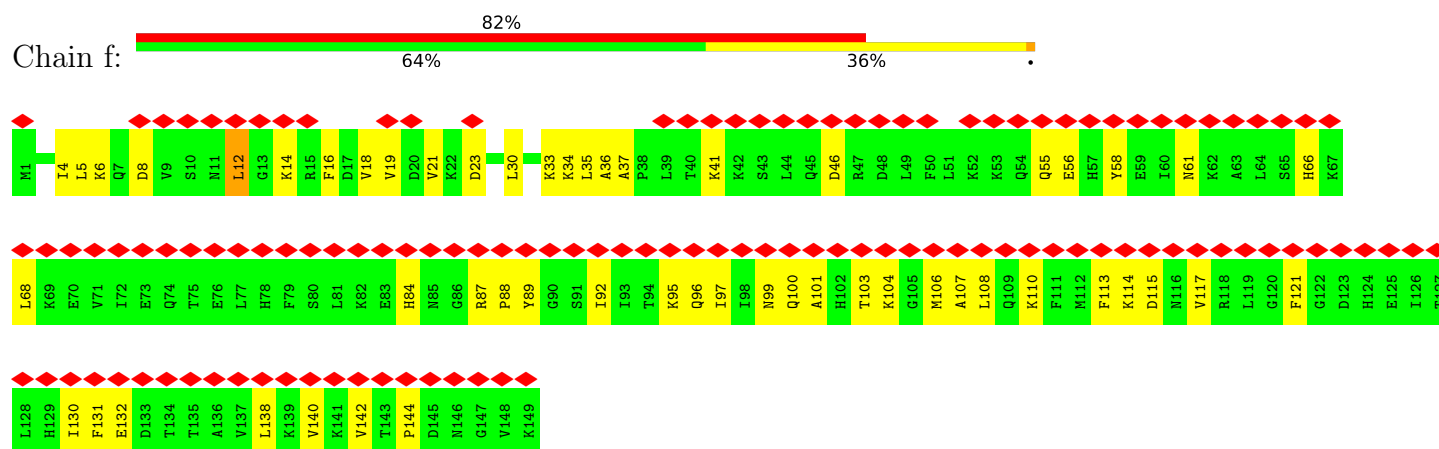
- Molecule 36: 50S ribosomal protein L5



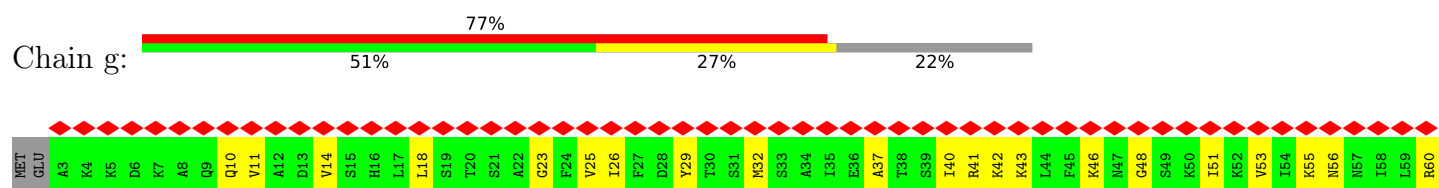
- Molecule 37: 50S ribosomal protein L6

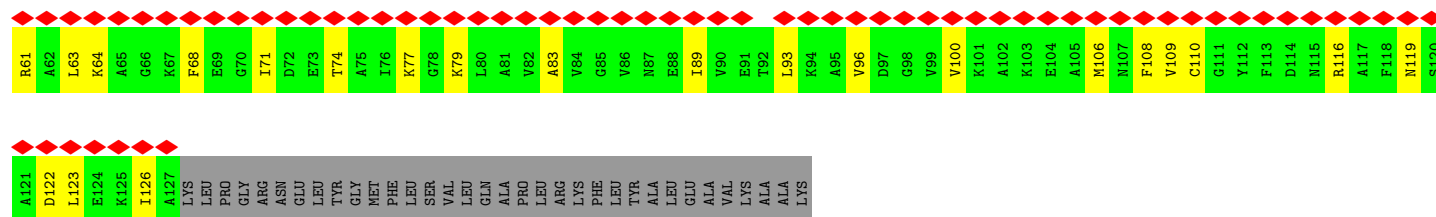


- Molecule 38: 50S ribosomal protein L9

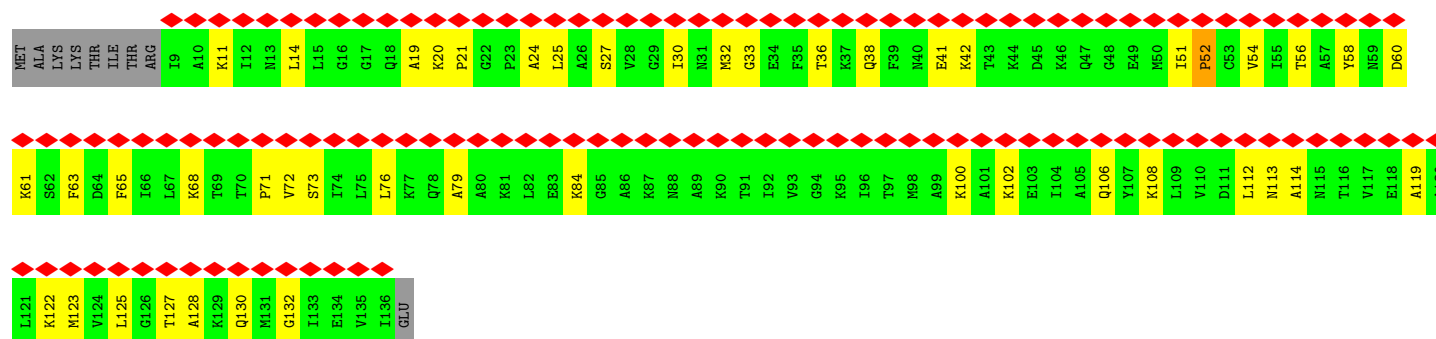


- Molecule 39: 50S ribosomal protein L10

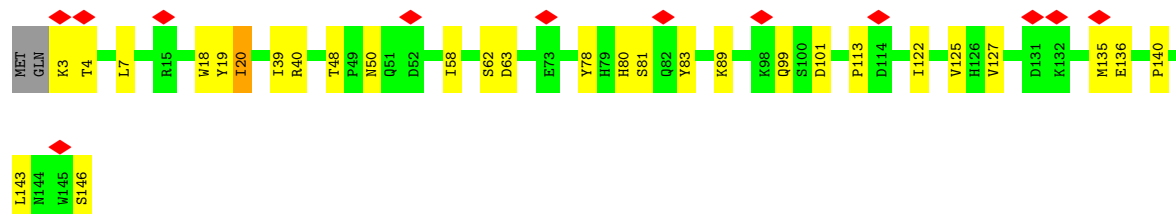
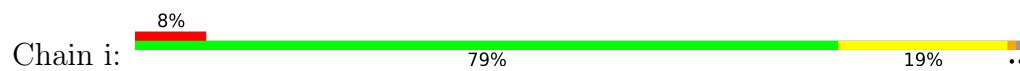




• Molecule 40: 50S ribosomal protein L11



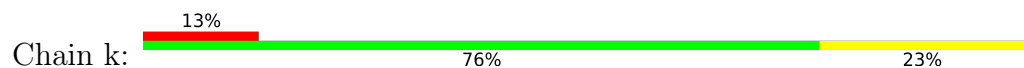
• Molecule 41: 50S ribosomal protein L13

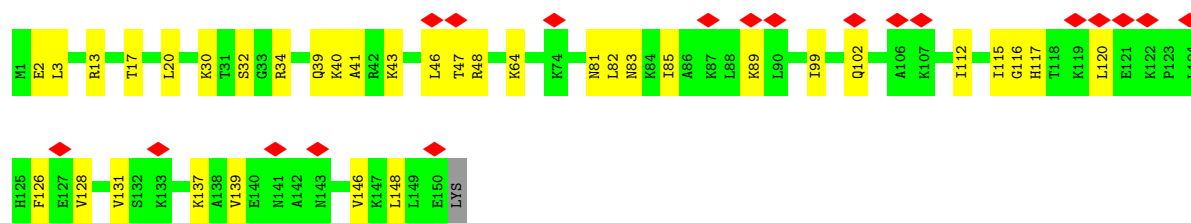


• Molecule 42: 50S ribosomal protein L14

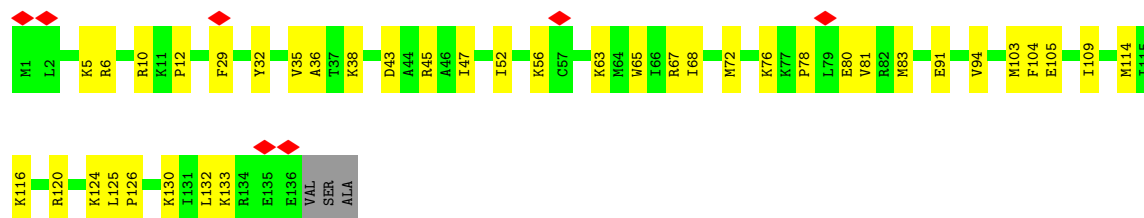


• Molecule 43: 50S ribosomal protein L15

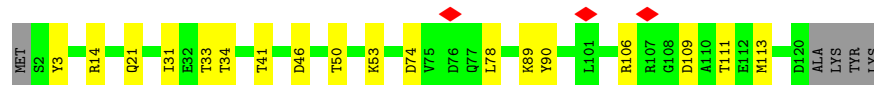
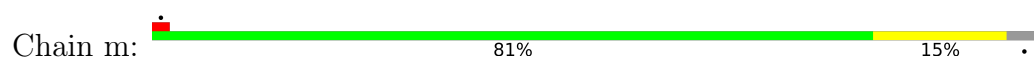




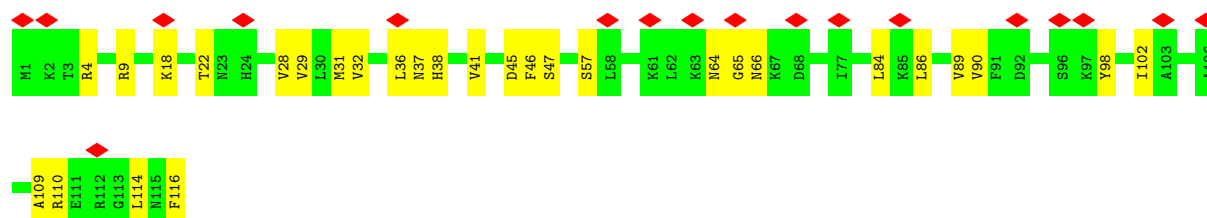
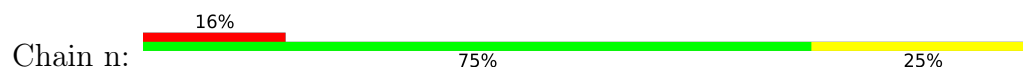
- Molecule 44: 50S ribosomal protein L16



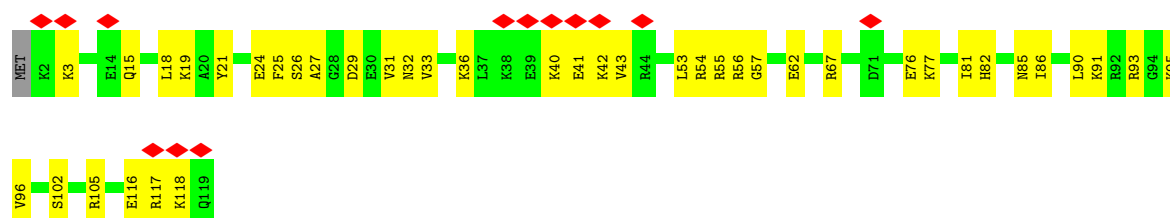
- Molecule 45: 50S ribosomal protein L17



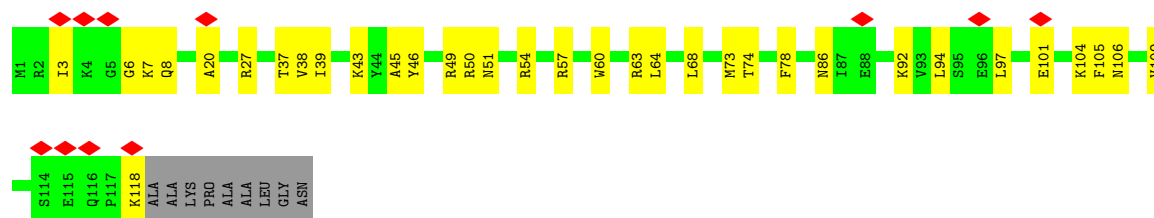
- Molecule 46: 50S ribosomal protein L18



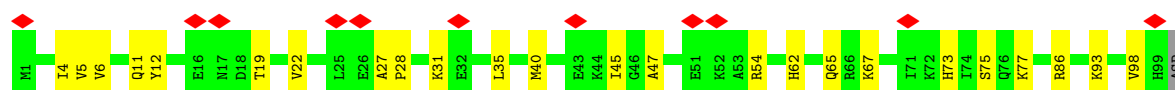
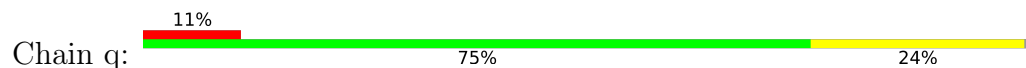
- Molecule 47: 50S ribosomal protein L19



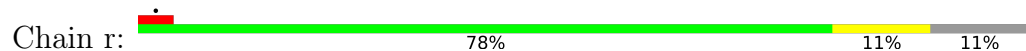
- Molecule 48: 50S ribosomal protein L20



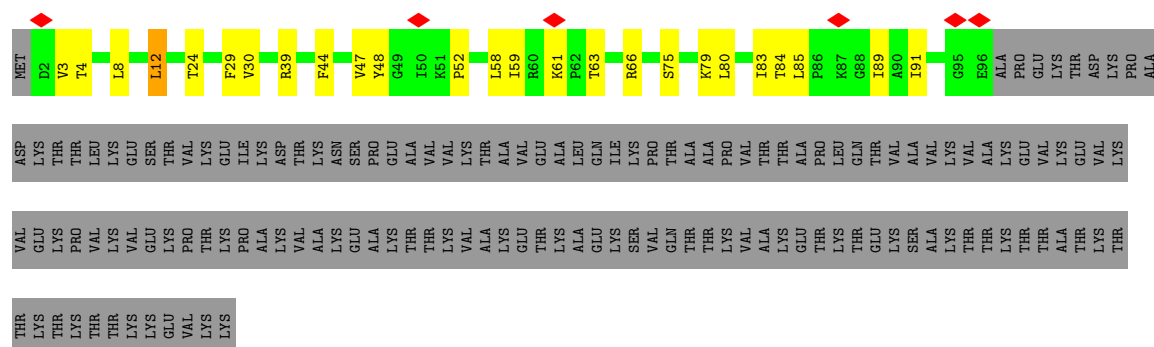
• Molecule 49: 50S ribosomal protein L21



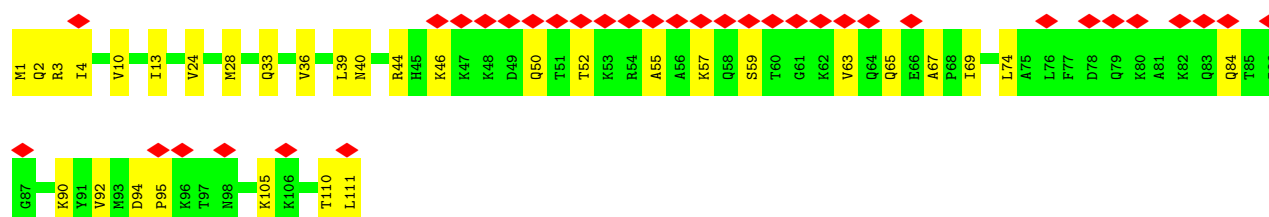
• Molecule 50: 50S ribosomal protein L22



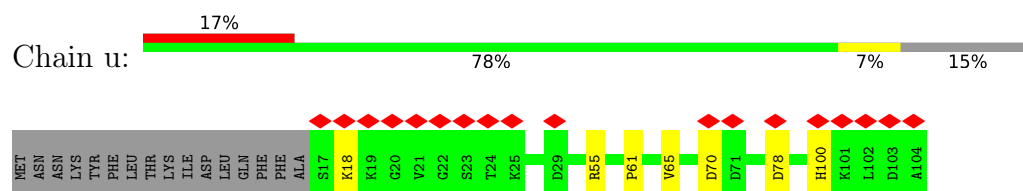
• Molecule 51: 50S ribosomal protein L23



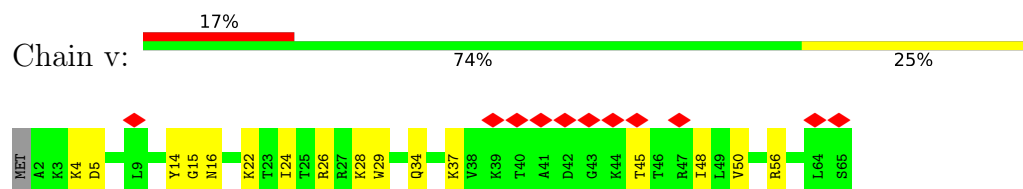
• Molecule 52: 50S ribosomal protein L24



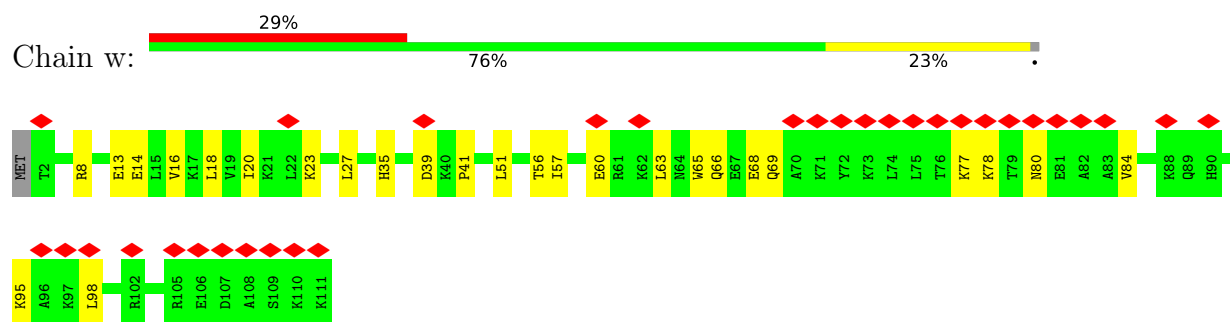
- Molecule 53: 50S ribosomal protein L27



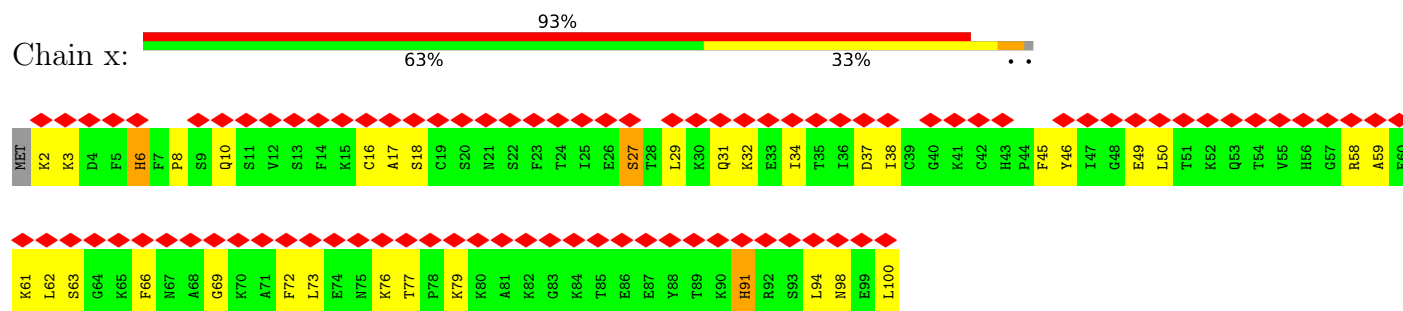
- Molecule 54: 50S ribosomal protein L28



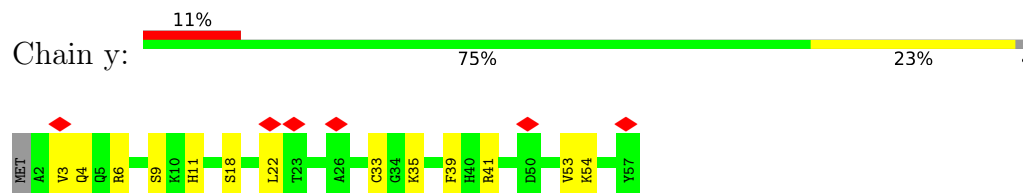
- Molecule 55: 50S ribosomal protein L29



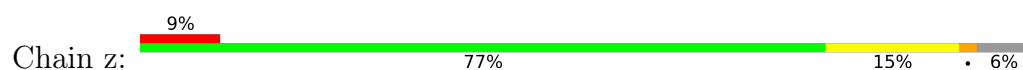
- Molecule 56: 50S ribosomal protein L31

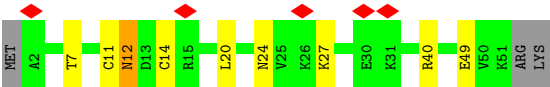


- Molecule 57: 50S ribosomal protein L32



- Molecule 58: 50S ribosomal protein L33 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	30774	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0022	Depositor
Map size (Å)	560.838, 560.838, 560.838	wwPDB
Map dimensions	422, 422, 422	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.329, 1.329, 1.329	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8T, 5MC, ZN, N2P, K, 1MG, MG, 7MG, OMG, SPM, CLM, PUT, SPD, 2MA, MA6

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	0	0.08	0/395	0.24	0/518
2	1	0.09	0/484	0.25	0/637
3	2	0.39	0/306	0.58	0/401
4	3	0.10	0/69363	0.24	8/108161 (0.0%)
5	4	0.08	0/2578	0.19	0/4016
6	5	0.08	0/35992	0.20	0/56111
7	6	0.31	0/1810	0.55	2/2817 (0.1%)
8	7	0.20	0/1785	0.38	1/2779 (0.0%)
9	8	0.22	1/1804 (0.1%)	0.31	0/2807
10	A	0.13	0/2172	0.39	0/2934
11	B	0.20	0/1863	0.57	1/2516 (0.0%)
12	C	0.29	1/1700 (0.1%)	0.63	3/2278 (0.1%)
13	D	0.14	0/1206	0.42	0/1616
14	E	0.20	0/1536	0.56	1/2072 (0.0%)
15	F	0.22	0/1274	0.60	0/1710
16	G	0.49	1/1126 (0.1%)	0.91	3/1517 (0.2%)
17	H	0.24	0/1056	0.69	1/1409 (0.1%)
18	I	0.15	0/843	0.46	1/1132 (0.1%)
19	J	0.17	0/844	0.49	0/1136
20	K	0.18	0/1089	0.51	0/1461
21	L	0.29	1/1002 (0.1%)	0.70	3/1340 (0.2%)
22	M	0.19	0/483	0.46	0/643
23	N	0.19	0/695	0.55	0/926
24	O	0.22	0/718	0.60	1/962 (0.1%)
25	P	0.19	0/702	0.54	1/934 (0.1%)
26	Q	0.45	0/601	0.70	1/801 (0.1%)
27	R	0.18	0/716	0.62	1/958 (0.1%)
28	S	0.18	0/645	0.54	0/857
29	T	0.18	0/524	0.56	0/685
30	X	0.14	0/245	0.44	0/325
31	Y	0.18	0/498	0.39	0/773
32	Z	0.89	0/26	1.70	0/33

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.12	0/2267	0.34	0/3044
34	b	0.17	0/1812	0.39	0/2436
35	c	0.13	0/1681	0.38	0/2257
36	d	0.17	0/1437	0.48	0/1931
37	e	0.14	0/1420	0.42	1/1912 (0.1%)
38	f	0.15	0/1231	0.48	0/1650
39	g	0.15	0/960	0.46	0/1284
40	h	0.35	1/968 (0.1%)	0.88	5/1298 (0.4%)
41	i	0.12	0/1186	0.31	0/1592
42	j	0.12	0/953	0.34	0/1275
43	k	0.14	0/1187	0.43	0/1581
44	l	0.14	0/1104	0.39	0/1481
45	m	0.10	0/973	0.26	0/1309
46	n	0.13	0/927	0.35	0/1239
47	o	0.13	0/976	0.37	0/1296
48	p	0.11	0/996	0.30	0/1325
49	q	0.12	0/828	0.37	0/1111
50	r	0.10	0/1100	0.27	0/1471
51	s	0.11	0/752	0.34	0/1015
52	t	0.14	0/878	0.53	4/1165 (0.3%)
53	u	0.10	0/678	0.30	0/902
54	v	0.09	0/526	0.28	0/703
55	w	0.11	0/916	0.34	0/1222
56	x	0.17	0/776	0.52	0/1033
57	y	0.10	0/457	0.35	0/601
58	z	0.09	0/412	0.29	0/547
All	All	0.14	5/163482 (0.0%)	0.33	38/243945 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	N	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	14	PRO	CG-CD	-14.04	1.03	1.50
12	C	188	PRO	CG-CD	-7.56	1.25	1.50
9	8	76	A	C6-N6	6.06	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	96	PRO	CG-CD	-5.92	1.30	1.50
40	h	52	PRO	N-CD	-5.30	1.40	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	14	PRO	N-CD-CG	-21.16	71.46	103.20
40	h	52	PRO	CA-N-CD	-20.31	83.57	112.00
16	G	14	PRO	CA-CB-CG	-17.18	71.86	104.50
40	h	71	PRO	N-CD-CG	-10.54	87.39	103.20
4	3	2184	A	C4'-C3'-O3'	10.18	128.27	113.00
12	C	188	PRO	N-CD-CG	-10.17	87.95	103.20
21	L	96	PRO	CA-N-CD	-9.98	98.03	112.00
4	3	2184	A	C5'-C4'-C3'	9.85	130.77	116.00
12	C	188	PRO	CA-CB-CG	-9.34	86.75	104.50
4	3	2184	A	P-O5'-C5'	8.81	134.12	120.90
16	G	14	PRO	N-CA-CB	-8.45	95.60	103.46
40	h	71	PRO	CA-N-CD	-8.38	100.26	112.00
12	C	188	PRO	N-CA-CB	-8.31	94.53	103.25
52	t	95	PRO	CA-N-CD	-8.27	100.42	112.00
7	6	32	U	P-O3'-C3'	-7.88	108.38	120.20
11	B	230	PRO	CA-N-CD	-7.80	101.08	112.00
40	h	71	PRO	CA-CB-CG	-7.78	89.72	104.50
37	e	30	PRO	CA-N-CD	-7.71	101.20	112.00
21	L	96	PRO	N-CD-CG	-7.44	92.03	103.20
24	O	41	PRO	CA-N-CD	-7.31	101.76	112.00
8	7	73	C	P-O3'-C3'	-6.69	110.17	120.20
25	P	33	PRO	CA-N-CD	-6.68	102.65	112.00
4	3	2183	U	O3'-P-O5'	6.55	113.82	104.00
7	6	54	U	P-O3'-C3'	-6.42	110.57	120.20
4	3	2183	U	O5'-C5'-C4'	-6.25	102.33	111.70
4	3	2183	U	C4'-C3'-C2'	-6.15	96.45	102.60
26	Q	72	PRO	N-CD-CG	-6.14	93.99	103.20
4	3	2184	A	P-O3'-C3'	-6.05	111.13	120.20
17	H	12	ARG	CA-CB-CG	6.01	126.12	114.10
27	R	76	PRO	CA-N-CD	-5.94	103.69	112.00
52	t	95	PRO	CB-CG-CD	-5.92	87.16	106.10
40	h	52	PRO	CB-CG-CD	-5.90	87.23	106.10
52	t	95	PRO	CA-CB-CG	-5.86	93.36	104.50
52	t	95	PRO	N-CD-CG	-5.86	94.41	103.20
14	E	128	PRO	CA-N-CD	-5.65	104.09	112.00
21	L	75	LEU	CA-CB-CG	5.31	134.88	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	2183	U	C2'-C3'-O3'	5.15	117.22	109.50
18	I	46	LEU	C-N-CD	-5.02	104.42	125.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	N	51	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	392	0	442	7	0
2	1	477	0	530	8	0
3	2	304	0	347	1	0
4	3	61995	0	31115	457	0
5	4	2305	0	1164	15	0
6	5	32258	0	16206	376	0
7	6	1620	0	818	25	0
8	7	1599	0	805	22	0
9	8	1615	0	816	21	0
10	A	2138	0	2204	80	0
11	B	1835	0	1909	79	0
12	C	1669	0	1729	87	0
13	D	1191	0	1284	52	0
14	E	1509	0	1520	72	0
15	F	1254	0	1320	58	0
16	G	1110	0	1226	50	0
17	H	1040	0	1107	56	0
18	I	832	0	918	30	0
19	J	829	0	855	40	0
20	K	1071	0	1165	45	0
21	L	991	0	1061	61	0
22	M	474	0	505	25	0
23	N	689	0	746	25	0
24	O	705	0	755	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	P	693	0	753	33	0
26	Q	590	0	625	28	0
27	R	700	0	709	34	0
28	S	643	0	694	29	0
29	T	519	0	578	31	0
30	X	242	0	263	6	0
31	Y	446	0	227	13	0
32	Z	187	0	68	6	0
33	a	2225	0	2301	46	0
34	b	1778	0	1821	42	0
35	c	1654	0	1744	51	0
36	d	1416	0	1500	67	0
37	e	1396	0	1481	28	0
38	f	1208	0	1254	39	0
39	g	951	0	1001	32	0
40	h	959	0	1039	40	0
41	i	1164	0	1192	27	0
42	j	944	0	1019	27	0
43	k	1170	0	1274	30	0
44	l	1079	0	1134	28	0
45	m	958	0	1011	11	0
46	n	918	0	979	24	0
47	o	966	0	1042	28	0
48	p	981	0	1062	32	0
49	q	811	0	858	16	0
50	r	1091	0	1178	15	0
51	s	740	0	819	16	0
52	t	871	0	972	22	0
53	u	670	0	704	6	0
54	v	520	0	565	11	0
55	w	906	0	981	17	0
56	x	761	0	766	25	0
57	y	452	0	471	13	0
58	z	408	0	436	8	0
59	2	1	0	0	0	0
59	M	1	0	0	0	0
59	Q	1	0	0	0	0
59	x	1	0	0	0	0
59	y	1	0	0	0	0
59	z	1	0	0	0	0
60	3	20	0	11	4	0
61	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	3	218	0	0	0	0
62	4	1	0	0	0	0
62	5	89	0	0	0	0
62	6	1	0	0	0	0
62	7	2	0	0	0	0
62	8	2	0	0	0	0
62	K	1	0	0	0	0
62	P	1	0	0	0	0
62	S	1	0	0	0	0
62	Y	2	0	0	0	0
62	a	1	0	0	0	0
62	b	2	0	0	0	0
62	i	1	0	0	0	0
62	y	2	0	0	0	0
63	3	42	0	84	2	0
63	5	6	0	12	0	0
64	3	42	0	78	6	0
64	b	14	0	26	0	0
65	3	160	0	304	4	0
65	5	20	0	38	1	0
66	3	21	0	42	0	0
66	5	7	0	14	0	0
67	8	9	0	12	0	0
All	All	151591	0	103689	2240	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2240) 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)
11:B:105:THR:HG21	11:B:232:ARG:HD2	1.25	1.12
11:B:105:THR:CG2	11:B:232:ARG:HD2	1.82	1.09
11:B:105:THR:OG1	11:B:232:ARG:HG2	1.61	1.00
21:L:6:GLY:HA3	36:d:112:ARG:HH22	1.24	0.99
10:A:214:ILE:HG22	10:A:216:PRO:HD3	1.47	0.95
8:7:34:G:H1	31:Y:42:U:H3	1.15	0.94
11:B:224:HIS:HB3	11:B:225:PRO:HD3	1.55	0.89
4:3:2165:A:H1'	4:3:2166:U:OP1	1.74	0.88
18:I:15:LYS:HB3	18:I:105:ARG:HB2	1.56	0.87
28:S:35:PHE:HZ	28:S:76:LEU:HD11	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:715:A:N7	26:Q:69:LYS:NZ	2.21	0.87
6:5:372:G:H5''	24:O:5:ARG:HD2	1.58	0.86
9:8:50:G:H1	9:8:64:U:H3	1.22	0.86
10:A:199:VAL:HG12	10:A:213:PHE:HB2	1.57	0.86
39:g:110:CYS:HA	39:g:123:LEU:HD11	1.59	0.85
18:I:48:LEU:HD21	18:I:79:LEU:HD23	1.59	0.85
56:x:10:GLN:HE22	56:x:31:GLN:HG2	1.41	0.85
45:m:109:ASP:HB3	45:m:111:THR:HG23	1.59	0.84
6:5:1269:U:O2'	21:L:14:ARG:NH2	2.11	0.84
38:f:41:LYS:HB3	38:f:46:ASP:HB3	1.58	0.83
20:K:79:TYR:HD2	20:K:100:VAL:HG21	1.42	0.83
38:f:96:GLN:HE22	38:f:121:PHE:HB3	1.41	0.83
47:o:62:GLU:HB3	47:o:81:ILE:HD12	1.57	0.83
10:A:293:ARG:HE	29:T:50:GLN:HG2	1.42	0.82
4:3:2111:U:H3	4:3:2194:G:H1'	1.45	0.82
11:B:167:ARG:HD3	31:Y:49:U:H3	1.44	0.82
11:B:37:ASP:HB2	11:B:58:ILE:HD13	1.60	0.81
40:h:122:LYS:HA	40:h:125:LEU:HD13	1.62	0.81
19:J:119:ARG:HG2	29:T:34:TYR:HB2	1.60	0.81
46:n:64:ASN:OD1	46:n:65:GLY:N	2.13	0.81
6:5:335:C:OP2	42:j:97:ARG:NH1	2.14	0.81
11:B:6:ASN:HD22	22:M:49:TYR:HB3	1.44	0.80
36:d:146:ILE:HG22	36:d:148:ARG:H	1.46	0.80
11:B:105:THR:OG1	11:B:232:ARG:CG	2.29	0.80
4:3:2312:G:H22	4:3:2320:U:H3	1.25	0.80
11:B:105:THR:CG2	11:B:232:ARG:CD	2.59	0.80
6:5:669:U:O2'	14:E:84:ARG:NH1	2.15	0.79
15:F:25:ILE:HB	15:F:100:LEU:HD22	1.65	0.79
28:S:17:ARG:O	28:S:21:ASN:ND2	2.15	0.79
14:E:6:ILE:HD13	26:Q:96:LEU:HD13	1.63	0.79
4:3:2111:U:H5'	4:3:2112:A:H5''	1.63	0.79
6:5:946:G:OP2	21:L:101:ARG:NH1	2.11	0.79
39:g:25:VAL:HG11	39:g:93:LEU:HD21	1.64	0.79
4:3:47:G:H5''	4:3:48:G:H5'	1.64	0.78
6:5:233:C:OP1	25:P:41:ARG:NH1	2.16	0.78
6:5:1049:G:OP1	11:B:202:LYS:NZ	2.17	0.78
11:B:119:ILE:HD12	11:B:205:ILE:HD11	1.65	0.77
15:F:92:GLN:HA	15:F:95:LYS:HD3	1.67	0.77
11:B:34:LEU:HD11	22:M:47:LEU:HD21	1.66	0.77
20:K:57:LYS:HB3	20:K:58:PRO:HD3	1.67	0.77
21:L:14:ARG:HD3	21:L:42:ASP:HA	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:35:PHE:CZ	28:S:76:LEU:HD11	2.20	0.76
15:F:19:ASN:HD22	15:F:58:LEU:HD11	1.50	0.76
36:d:104:ILE:HA	36:d:108:LEU:HD12	1.66	0.76
8:7:10:G:H1	8:7:25:U:H3	1.33	0.76
24:O:9:MET:HE1	24:O:18:ARG:HH21	1.50	0.76
11:B:105:THR:HG23	11:B:232:ARG:HG3	1.67	0.76
10:A:208:PRO:HB2	14:E:174:TYR:CD2	2.21	0.75
41:i:3:LYS:HG3	41:i:4:THR:H	1.52	0.75
36:d:44:ILE:HD12	36:d:78:LYS:HB2	1.67	0.75
42:j:13:ASN:ND2	42:j:96:THR:OG1	2.19	0.75
26:Q:53:LEU:HD11	26:Q:96:LEU:HD12	1.69	0.75
30:X:29:LYS:HE3	30:X:30:GLN:HG2	1.67	0.74
14:E:161:GLN:HB3	16:G:59:VAL:HG12	1.69	0.74
37:e:107:ASN:HB3	37:e:117:LYS:HG2	1.69	0.74
4:3:2137:A:O2'	4:3:2165:A:N6	2.20	0.74
4:3:2144:C:H2'	4:3:2145:A:H8	1.51	0.74
23:N:9:ILE:HD11	23:N:19:VAL:HG12	1.70	0.74
25:P:43:LYS:NZ	25:P:45:TYR:OH	2.17	0.73
52:t:1:MET:HG2	52:t:2:GLN:H	1.54	0.73
6:5:681:U:H1'	19:J:33:ASN:HA	1.69	0.73
6:5:206:G:N2	6:5:209:A:OP2	2.21	0.73
10:A:293:ARG:HH21	29:T:50:GLN:HG2	1.52	0.73
17:H:20:TYR:HB2	17:H:66:ASN:HB3	1.70	0.73
11:B:82:ASN:O	11:B:82:ASN:ND2	2.20	0.73
10:A:49:ARG:HG3	10:A:50:LYS:H	1.54	0.73
37:e:112:TYR:HB2	37:e:116:ILE:HD11	1.70	0.73
38:f:5:LEU:HA	38:f:36:ALA:HA	1.70	0.73
44:l:35:VAL:HG21	44:l:132:LEU:HD22	1.71	0.73
39:g:100:VAL:HG12	39:g:106:MET:HG3	1.71	0.73
33:a:179:TYR:HB3	33:a:191:LYS:HB3	1.69	0.72
10:A:32:MET:SD	10:A:281:ARG:NH1	2.63	0.72
1:0:9:LYS:NZ	4:3:1338:G:OP2	2.23	0.72
17:H:86:VAL:HG22	17:H:100:LEU:HD21	1.71	0.72
6:5:196:G:O2'	6:5:197:A:OP1	2.08	0.72
15:F:115:MET:HA	15:F:118:LYS:HB2	1.70	0.72
10:A:82:ILE:HG22	10:A:175:LEU:HB3	1.72	0.72
27:R:11:VAL:HG12	27:R:13:ALA:H	1.53	0.72
4:3:2688:C:H5'	34:b:198:ALA:HA	1.72	0.71
6:5:181:G:O2'	25:P:3:ARG:NH1	2.23	0.71
15:F:74:LEU:HD22	15:F:85:GLN:HB3	1.71	0.71
7:6:49:G:H1	7:6:65:U:H3	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:61:THR:HG22	11:B:62:GLN:H	1.53	0.71
10:A:286:ARG:O	10:A:287:ASN:ND2	2.22	0.71
27:R:11:VAL:HG22	27:R:38:SER:HB3	1.72	0.71
28:S:68:LEU:O	28:S:72:ASN:ND2	2.23	0.71
35:c:30:LYS:H	35:c:114:THR:HG21	1.54	0.71
6:5:1270:C:H5'	21:L:14:ARG:NH2	2.05	0.71
6:5:399:C:H5''	12:C:132:PRO:HD2	1.73	0.71
48:p:6:GLY:O	48:p:8:GLN:NE2	2.24	0.71
6:5:933:A:O3'	15:F:94:ARG:NH2	2.24	0.71
6:5:1012:A:OP1	22:M:15:LYS:NZ	2.18	0.71
47:o:15:GLN:HA	47:o:18:LEU:HD12	1.71	0.71
4:3:1031:U:O2'	48:p:92:LYS:NZ	2.23	0.71
4:3:2140:G:N3	4:3:2165:A:N6	2.38	0.71
15:F:14:ASP:HB3	15:F:19:ASN:H	1.55	0.71
4:3:2756:A:H2	37:e:66:ILE:HD11	1.56	0.70
10:A:46:GLU:N	10:A:46:GLU:OE2	2.24	0.70
4:3:1446:G:O2'	4:3:1613:A:N6	2.24	0.70
4:3:2111:U:H5''	4:3:2112:A:H8	1.55	0.70
4:3:2060:G:O2'	34:b:157:GLN:NE2	2.25	0.70
11:B:140:SER:HA	11:B:143:LYS:HE3	1.72	0.70
22:M:45:ARG:HE	22:M:49:TYR:HE2	1.39	0.70
16:G:26:ARG:HG3	16:G:82:PRO:HG3	1.73	0.70
52:t:90:LYS:HG3	52:t:105:LYS:HG2	1.72	0.70
12:C:10:ARG:HH21	12:C:14:LEU:HD21	1.55	0.70
10:A:182:VAL:HG23	10:A:206:THR:HG22	1.71	0.70
39:g:25:VAL:HG23	39:g:83:ALA:HB3	1.72	0.70
21:L:15:ILE:O	21:L:19:LEU:HD22	1.92	0.69
10:A:93:LYS:HG3	10:A:109:THR:HB	1.74	0.69
47:o:116:GLU:OE2	47:o:117:ARG:N	2.25	0.69
50:r:12:ILE:HG12	50:r:43:ALA:HB2	1.74	0.69
33:a:125:GLU:N	33:a:125:GLU:OE1	2.23	0.69
6:5:369:A:O2'	6:5:448:A:N7	2.25	0.69
20:K:84:GLY:O	20:K:112:ARG:NH2	2.25	0.69
4:3:619:A:H62	4:3:1281:A:H2	1.39	0.69
6:5:136:U:H3	6:5:157:A:H62	1.39	0.69
6:5:452:A:N6	6:5:476:U:O2	2.25	0.69
19:J:77:LEU:HD13	19:J:100:ILE:HG23	1.74	0.69
30:X:31:THR:O	30:X:35:THR:OG1	2.11	0.69
4:3:530:G:N3	50:r:61:ASN:ND2	2.41	0.69
39:g:29:TYR:HA	39:g:32:MET:HE1	1.75	0.69
43:k:126:PHE:HB2	43:k:146:VAL:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:93:A:H5'	6:5:94:A:H5''	1.75	0.69
10:A:65:LEU:HD21	10:A:231:LEU:HD13	1.73	0.69
55:w:23:LYS:HD2	55:w:51:LEU:HD21	1.75	0.69
8:7:48:G:H1	8:7:64:U:H3	1.40	0.68
4:3:1029:A:OP1	48:p:49:ARG:NH1	2.26	0.68
27:R:9:ALA:HB1	27:R:39:THR:HG21	1.74	0.68
6:5:543:C:OP1	12:C:57:LYS:NZ	2.27	0.68
39:g:23:GLY:HA3	39:g:89:ILE:HD12	1.76	0.68
4:3:1344:U:O2'	30:X:44:ARG:NH2	2.25	0.68
43:k:89:LYS:HA	43:k:89:LYS:HE3	1.75	0.68
14:E:157:TRP:HB3	16:G:60:LEU:HD21	1.74	0.68
25:P:32:HIS:CD2	25:P:33:PRO:HD3	2.28	0.68
10:A:181:PRO:HD3	10:A:200:ALA:HB1	1.75	0.68
24:O:18:ARG:HA	24:O:38:HIS:HA	1.76	0.68
35:c:205:LYS:HA	35:c:208:GLU:OE2	1.94	0.68
40:h:58:TYR:CE1	40:h:60:ASP:HB3	2.28	0.67
49:q:6:VAL:HG22	49:q:11:GLN:HG2	1.75	0.67
57:y:53:VAL:HG12	57:y:54:LYS:HG2	1.74	0.67
6:5:416:U:O2'	6:5:421:G:N2	2.27	0.67
44:l:72:MET:HA	44:l:72:MET:HE3	1.75	0.67
6:5:1354:G:O6	15:F:2:ARG:NH2	2.27	0.67
6:5:1000:A:HO2'	6:5:1029:C:HO2'	1.41	0.67
5:4:83:U:H5'	5:4:84:C:H5'	1.77	0.67
10:A:28:THR:O	10:A:61:GLN:NE2	2.27	0.67
52:t:28:MET:HE2	52:t:33:GLN:HB2	1.76	0.67
4:3:656:G:H4'	4:3:657:A:H5'	1.77	0.67
6:5:169:G:N2	6:5:219:A:O2'	2.28	0.67
47:o:36:LYS:HB3	47:o:85:ASN:HB2	1.76	0.67
34:b:227:GLU:HG3	47:o:19:LYS:HD2	1.77	0.67
6:5:1009:G:N2	6:5:1012:A:OP2	2.25	0.67
52:t:57:LYS:HE3	52:t:59:SER:HB3	1.76	0.67
4:3:788:G:N2	45:m:3:TYR:OH	2.28	0.66
4:3:2122:G:H3'	4:3:2123:A:H5''	1.78	0.66
4:3:2502:G:H4'	44:l:80:GLU:HG2	1.77	0.66
4:3:2026:A:OP2	57:y:6:ARG:NH2	2.28	0.66
14:E:99:SER:O	14:E:105:GLN:NE2	2.27	0.66
16:G:44:ILE:HG22	16:G:122:VAL:HG11	1.77	0.66
18:I:13:LYS:HG3	18:I:81:ILE:HG22	1.75	0.66
25:P:61:VAL:HG12	25:P:80:ILE:HG12	1.77	0.66
20:K:29:ASN:ND2	20:K:32:ASN:OD1	2.28	0.66
4:3:925:C:H4'	4:3:926:U:O4'	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:2799:U:OP1	4:3:2896:G:N1	2.23	0.66
7:6:9:A:H5'	7:6:46:G:H1'	1.76	0.66
10:A:95:LEU:HD11	10:A:226:CYS:HA	1.77	0.66
6:5:521:A:N6	20:K:102:ASP:OD2	2.26	0.66
11:B:46:VAL:HG23	11:B:47:ASN:H	1.59	0.66
12:C:34:ILE:HG13	12:C:39:GLY:HA2	1.76	0.66
20:K:79:TYR:CD2	20:K:100:VAL:HG21	2.28	0.66
21:L:98:ARG:HB2	21:L:100:GLN:NE2	2.10	0.66
25:P:30:PHE:HD2	25:P:41:ARG:HE	1.44	0.66
48:p:68:LEU:HD12	48:p:73:MET:HG2	1.76	0.66
27:R:36:ARG:HB3	27:R:72:GLY:HA3	1.77	0.66
27:R:50:ALA:HB1	27:R:57:PHE:HB3	1.78	0.66
4:3:2135:C:H2'	4:3:2136:A:H8	1.61	0.66
6:5:1068:G:N2	6:5:1071:A:OP2	2.22	0.66
17:H:6:TYR:HB2	17:H:21:LEU:HB2	1.78	0.66
7:6:3:G:H1	7:6:70:U:H3	1.44	0.66
10:A:30:VAL:O	10:A:218:ASN:ND2	2.26	0.66
6:5:1321:G:C8	17:H:111:ARG:HG2	2.31	0.65
16:G:14:PRO:HB2	16:G:40:LEU:HD21	1.77	0.65
21:L:98:ARG:HB2	21:L:100:GLN:HE22	1.60	0.65
17:H:19:VAL:HG11	17:H:85:ILE:HD12	1.79	0.65
29:T:6:VAL:HG12	29:T:8:ASN:H	1.61	0.65
1:0:24:THR:HG23	1:0:27:GLY:H	1.61	0.65
38:f:12:LEU:HD12	38:f:19:VAL:HB	1.77	0.65
39:g:41:ARG:NH1	39:g:51:ILE:O	2.30	0.65
42:j:7:ARG:HE	42:j:18:GLN:HG2	1.61	0.65
6:5:735:C:OP2	14:E:92:ARG:NH2	2.30	0.65
35:c:132:LEU:HA	35:c:135:LYS:HB2	1.79	0.65
21:L:52:GLU:OE1	21:L:52:GLU:N	2.26	0.65
4:3:1096:U:H1'	4:3:1105:A:H1'	1.79	0.65
4:3:2141:A:H8	4:3:2164:G:H21	1.44	0.65
12:C:78:VAL:HG21	12:C:89:LEU:HB3	1.77	0.65
13:D:138:HIS:HA	16:G:109:ASN:HD21	1.62	0.65
49:q:28:PRO:HD2	49:q:31:LYS:HE3	1.79	0.65
4:3:1806:G:OP1	33:a:268:ARG:NH1	2.30	0.64
6:5:424:U:OP1	12:C:12:ARG:NH2	2.16	0.64
10:A:249:LYS:HG3	10:A:250:PRO:HD2	1.79	0.64
4:3:1029:A:OP2	48:p:50:ARG:NH2	2.30	0.64
28:S:24:GLN:NE2	28:S:50:GLN:OE1	2.30	0.64
48:p:86:ASN:OD1	48:p:118:LYS:NZ	2.31	0.64
6:5:1425:A:H2'	6:5:1427:U:H3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1600:A:N3	33:a:62:ASN:ND2	2.44	0.64
4:3:1115:G:H21	40:h:123:MET:HE1	1.62	0.64
4:3:2688:C:OP2	34:b:117:ARG:NH2	2.31	0.64
6:5:662:G:H1'	6:5:730:G:H5'	1.80	0.64
14:E:16:GLU:OE1	14:E:16:GLU:N	2.28	0.64
21:L:19:LEU:HB2	21:L:30:SER:HB2	1.80	0.64
39:g:29:TYR:HB2	39:g:79:LYS:HD3	1.80	0.64
6:5:195:U:H2'	6:5:196:G:H8	1.62	0.64
15:F:17:PHE:HB3	15:F:58:LEU:HD22	1.80	0.64
17:H:103:LYS:HG3	17:H:105:LEU:HD23	1.80	0.64
33:a:41:LEU:HG	33:a:66:TYR:HB2	1.79	0.64
38:f:96:GLN:NE2	38:f:121:PHE:HB3	2.11	0.64
52:t:63:VAL:O	52:t:65:GLN:NE2	2.31	0.64
14:E:165:ASN:OD1	16:G:58:GLN:NE2	2.27	0.63
18:I:98:ILE:HD12	18:I:102:VAL:HG23	1.79	0.63
11:B:105:THR:HG23	11:B:232:ARG:CG	2.28	0.63
16:G:17:ASP:OD2	16:G:41:LYS:NZ	2.30	0.63
6:5:623:G:H4'	24:O:16:THR:HG21	1.80	0.63
20:K:14:LYS:NZ	20:K:15:LYS:O	2.30	0.63
23:N:22:ILE:O	23:N:26:VAL:HG23	1.98	0.63
47:o:93:ARG:HE	47:o:118:LYS:HE2	1.61	0.63
6:5:1051:U:OP1	22:M:45:ARG:NH2	2.31	0.63
14:E:4:ASN:HB2	14:E:90:LEU:HD11	1.80	0.63
20:K:83:GLU:N	20:K:83:GLU:OE1	2.31	0.63
21:L:34:LEU:HD12	21:L:39:ILE:HG23	1.80	0.63
6:5:469:C:O2'	24:O:80:LYS:NZ	2.32	0.63
10:A:293:ARG:NE	29:T:50:GLN:HG2	2.12	0.63
33:a:137:PRO:HA	33:a:197:ARG:HA	1.79	0.63
35:c:64:LYS:NZ	35:c:68:GLN:OE1	2.31	0.63
38:f:96:GLN:HB3	38:f:100:GLN:HE22	1.64	0.63
56:x:94:LEU:O	56:x:98:ASN:ND2	2.32	0.63
4:3:2589:G:N2	4:3:2589:G:OP2	2.30	0.63
6:5:509:C:OP1	12:C:41:ARG:NH1	2.31	0.63
10:A:45:ILE:HD11	10:A:204:THR:HG23	1.81	0.63
11:B:36:GLU:OE1	11:B:96:ILE:HA	1.99	0.63
51:s:59:ILE:HD11	51:s:79:LYS:HE2	1.80	0.63
6:5:983:G:H21	6:5:1012:A:H8	1.47	0.63
6:5:1290:G:N1	6:5:1293:A:OP2	2.31	0.63
4:3:1518:C:N4	4:3:2220:A:OP1	2.32	0.62
4:3:1619:A:H2'	4:3:1620:A:C8	2.34	0.62
42:j:93:PRO:HG3	42:j:114:ILE:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:104:ARG:HH12	42:j:121:VAL:HG13	1.64	0.62
15:F:92:GLN:OE1	15:F:92:GLN:N	2.32	0.62
4:3:2823:A:O2'	4:3:2825:A:N7	2.31	0.62
6:5:1264:G:OP1	15:F:34:LYS:NZ	2.32	0.62
14:E:10:ASP:O	14:E:17:GLN:NE2	2.31	0.62
4:3:2667:G:N2	4:3:2670:A:OP2	2.29	0.62
4:3:2805:A:H4'	4:3:2807:G:H5''	1.82	0.62
6:5:1009:G:H21	6:5:1012:A:H2	1.45	0.62
44:l:47:ILE:HD11	44:l:68:ILE:HD11	1.82	0.62
4:3:487:C:N4	4:3:490:A:OP2	2.27	0.62
6:5:545:A:OP1	12:C:69:LYS:NZ	2.32	0.62
17:H:125:ARG:NH1	17:H:126:ALA:O	2.33	0.62
5:4:6:U:OP2	46:n:9:ARG:NH1	2.33	0.62
6:5:408:U:H1'	12:C:28:GLY:HA2	1.81	0.62
21:L:48:LEU:HB3	21:L:53:PHE:CE1	2.35	0.62
24:O:7:MET:SD	24:O:20:VAL:HG11	2.40	0.62
36:d:5:LYS:HD3	36:d:97:TRP:CG	2.34	0.62
39:g:63:LEU:HD21	39:g:71:ILE:HB	1.82	0.62
4:3:619:A:N1	4:3:844:G:O2'	2.32	0.62
51:s:52:PRO:HB3	51:s:83:ILE:HG23	1.81	0.62
6:5:1153:G:N2	6:5:1156:G:OP2	2.32	0.62
6:5:1241:G:N2	6:5:1244:A:OP2	2.24	0.62
14:E:24:LYS:HE2	14:E:75:THR:HG22	1.81	0.62
16:G:36:ILE:HA	16:G:69:ILE:HG22	1.81	0.62
19:J:22:ASN:OD1	19:J:23:THR:N	2.32	0.62
4:3:499:G:N2	4:3:502:A:OP2	2.30	0.61
6:5:164:C:H2'	6:5:165:A:H8	1.65	0.61
22:M:47:LEU:HG	22:M:52:ALA:HB3	1.81	0.61
6:5:1508:C:H42	10:A:294:GLU:HA	1.65	0.61
40:h:41:GLU:HG3	40:h:42:LYS:HG3	1.82	0.61
44:l:32:TYR:HD2	44:l:114:MET:HE3	1.64	0.61
45:m:50:THR:HA	45:m:53:LYS:HE3	1.82	0.61
6:5:257:U:OP1	28:S:64:ARG:NH1	2.33	0.61
21:L:3:ARG:HD3	21:L:53:PHE:HB3	1.83	0.61
47:o:27:ALA:HB3	47:o:96:VAL:HG21	1.81	0.61
56:x:73:LEU:O	56:x:76:LYS:HG2	2.00	0.61
6:5:953:A:N6	27:R:77:THR:O	2.33	0.61
15:F:108:ARG:HB2	15:F:115:MET:HE1	1.82	0.61
49:q:40:MET:HG3	49:q:45:ILE:HB	1.82	0.61
29:T:54:ARG:HD3	29:T:57:ARG:HH12	1.65	0.61
33:a:128:ILE:HG22	33:a:129:ASP:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:h:24:ALA:O	40:h:27:SER:OG	2.19	0.61
12:C:97:LEU:HD12	12:C:136:LEU:HD21	1.82	0.61
31:Y:49:U:H4'	31:Y:50:U:O5'	2.01	0.61
33:a:33:PRO:HB2	33:a:38:LEU:HD11	1.82	0.61
4:3:881:A:H1'	4:3:882:C:H5''	1.83	0.61
4:3:2308:U:H2'	4:3:2309:A:H8	1.65	0.61
5:4:49:G:OP2	46:n:66:ASN:ND2	2.33	0.61
44:l:78:PRO:HG2	44:l:81:VAL:HG21	1.81	0.61
4:3:1557:G:O6	4:3:1571:G:O2'	2.18	0.61
19:J:16:VAL:HG23	19:J:79:VAL:HA	1.81	0.61
35:c:115:VAL:HG21	35:c:188:VAL:HG13	1.83	0.61
35:c:183:LEU:HD12	35:c:203:VAL:HG13	1.82	0.61
44:l:104:PHE:HE2	44:l:125:LEU:HD11	1.65	0.61
12:C:100:ILE:HG22	12:C:104:MET:HE3	1.83	0.60
13:D:152:LYS:HB3	13:D:179:TYR:HB2	1.81	0.60
4:3:2098:U:O2	54:v:34:GLN:NE2	2.34	0.60
6:5:358:G:OP1	20:K:71:THR:OG1	2.19	0.60
13:D:212:ARG:NH1	16:G:111:LEU:O	2.34	0.60
4:3:2481:U:OP1	4:3:2483:C:N4	2.34	0.60
6:5:1432:A:H5''	28:S:26:THR:HG22	1.84	0.60
11:B:216:ASN:C	11:B:218:THR:H	2.08	0.60
17:H:12:ARG:HD2	17:H:13:LYS:HG3	1.83	0.60
40:h:52:PRO:HD2	40:h:52:PRO:O	1.86	0.60
4:3:9:G:H5'	41:i:135:MET:HE1	1.82	0.60
4:3:196:G:N2	4:3:196:G:OP2	2.33	0.60
4:3:1786:U:OP2	4:3:1791:A:N6	2.26	0.60
9:8:40:C:O3'	21:L:119:LYS:NZ	2.34	0.60
21:L:6:GLY:HA3	36:d:112:ARG:NH2	2.07	0.60
27:R:69:HIS:HB2	27:R:74:PHE:CZ	2.36	0.60
4:3:354:C:O2	35:c:174:ASN:ND2	2.34	0.60
18:I:47:PRO:HA	18:I:78:ARG:HD2	1.83	0.60
4:3:600:U:OP2	43:k:30:LYS:NZ	2.35	0.60
41:i:136:GLU:OE1	41:i:136:GLU:N	2.27	0.60
4:3:341:G:N1	4:3:344:A:OP2	2.33	0.60
4:3:2465:U:H3	4:3:2502:G:H1	1.50	0.60
15:F:70:PRO:HG3	15:F:98:LEU:HD22	1.84	0.60
28:S:72:ASN:O	28:S:75:VAL:HG22	2.02	0.60
38:f:130:ILE:HD11	38:f:144:PRO:HG3	1.84	0.60
4:3:1906:G:H21	4:3:1909:C:H41	1.48	0.60
13:D:160:ILE:HG12	13:D:176:SER:O	2.02	0.60
18:I:63:VAL:HG23	18:I:64:ASP:CG	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:110:VAL:HG11	34:b:197:ILE:HD12	1.84	0.60
4:3:477:U:O2	35:c:47:GLN:NE2	2.34	0.59
11:B:229:GLN:HB3	11:B:230:PRO:HD3	1.83	0.59
16:G:115:ILE:HG22	16:G:138:LEU:HD13	1.84	0.59
41:i:80:HIS:ND1	41:i:81:SER:O	2.35	0.59
58:z:14:CYS:HB2	58:z:40:ARG:HH11	1.67	0.59
13:D:143:ARG:NH2	13:D:145:GLY:O	2.35	0.59
15:F:21:LEU:HD11	15:F:100:LEU:HD21	1.82	0.59
21:L:120:LYS:HG2	27:R:87:ARG:NE	2.17	0.59
50:r:7:GLN:HB2	50:r:50:LEU:HD11	1.84	0.59
4:3:2009:U:OP1	45:m:14:ARG:NH1	2.32	0.59
35:c:24:LEU:HD11	35:c:208:GLU:OE1	2.02	0.59
46:n:45:ASP:OD1	46:n:47:SER:OG	2.16	0.59
4:3:13:C:H3'	4:3:14:U:H5'	1.85	0.59
6:5:837:G:OP1	14:E:148:LYS:NZ	2.35	0.59
12:C:68:ASP:OD1	12:C:69:LYS:N	2.34	0.59
13:D:154:ALA:HB3	13:D:177:ASP:HB2	1.84	0.59
18:I:99:PRO:O	18:I:102:VAL:HG22	2.02	0.59
21:L:7:ILE:HG12	21:L:22:ILE:HG23	1.83	0.59
51:s:39:ARG:HG2	51:s:39:ARG:HH11	1.66	0.59
4:3:2098:U:H3'	4:3:2099:U:H5''	1.83	0.59
35:c:150:ALA:O	35:c:151:LYS:HG2	2.03	0.59
37:e:27:VAL:HG12	37:e:82:VAL:HG21	1.84	0.59
40:h:14:LEU:HD13	40:h:19:ALA:HB1	1.84	0.59
41:i:4:THR:HA	49:q:12:TYR:HE2	1.67	0.59
4:3:2475:C:O2	44:l:124:LYS:NZ	2.32	0.59
16:G:38:SER:OG	16:G:40:LEU:HD23	2.03	0.59
23:N:5:LYS:O	23:N:9:ILE:HG22	2.02	0.59
34:b:56:THR:HA	34:b:78:THR:HG22	1.84	0.59
37:e:25:ILE:HG13	37:e:38:LEU:HD21	1.82	0.59
19:J:43:MET:SD	19:J:58:ILE:HG22	2.42	0.59
4:3:512:G:N1	4:3:515:A:OP2	2.33	0.59
7:6:54:U:H2'	7:6:55:U:C6	2.36	0.59
16:G:52:GLY:O	16:G:75:LYS:NZ	2.35	0.59
36:d:26:MET:HA	36:d:30:ARG:HH21	1.67	0.59
4:3:2060:G:H4'	34:b:157:GLN:HG2	1.85	0.59
6:5:1213:A:H5'	6:5:1310:C:H41	1.67	0.59
13:D:212:ARG:NH2	16:G:51:GLU:OE1	2.36	0.59
18:I:49:PRO:O	18:I:77:LYS:NZ	2.35	0.59
27:R:13:ALA:HB2	56:x:73:LEU:HD21	1.85	0.59
6:5:1448:A:H2'	6:5:1449:G:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:f:33:LYS:HD3	38:f:113:PHE:HB2	1.85	0.59
46:n:32:VAL:HG12	46:n:41:VAL:HG13	1.84	0.59
6:5:212:G:O2'	6:5:464:A:N6	2.26	0.58
6:5:1215:U:H5	15:F:115:MET:HE3	1.68	0.58
28:S:13:GLN:O	28:S:17:ARG:HD2	2.03	0.58
33:a:143:GLU:CD	33:a:143:GLU:H	2.11	0.58
38:f:88:PRO:HG2	38:f:89:TYR:HD1	1.68	0.58
4:3:1137:C:H2'	4:3:1138:A:H8	1.66	0.58
4:3:2538:A:N7	37:e:175:LYS:NZ	2.51	0.58
60:3:3001:CLM:CL2	32:Z:33:LYS:HG2	2.39	0.58
6:5:373:A:H2'	6:5:374:G:H8	1.67	0.58
25:P:79:LYS:HZ3	25:P:81:ILE:HG23	1.68	0.58
36:d:25:ILE:H	36:d:25:ILE:HD12	1.68	0.58
36:d:148:ARG:HE	36:d:149:ILE:H	1.51	0.58
4:3:1095:U:H1'	4:3:1096:U:H3'	1.84	0.58
29:T:54:ARG:HD3	29:T:57:ARG:NH1	2.18	0.58
36:d:45:ARG:HG3	36:d:46:ASP:H	1.68	0.58
11:B:56:VAL:HG22	11:B:69:VAL:HG22	1.85	0.58
16:G:90:ILE:HG22	16:G:97:ILE:HG13	1.85	0.58
36:d:74:ILE:HD12	36:d:79:LEU:HD23	1.86	0.58
38:f:97:ILE:HA	38:f:100:GLN:HB2	1.85	0.58
41:i:7:LEU:HD23	41:i:7:LEU:H	1.69	0.58
4:3:1129:U:N3	4:3:1132:C:OP2	2.27	0.58
6:5:672:A:H1'	19:J:111:HIS:ND1	2.18	0.58
26:Q:53:LEU:HG	26:Q:54:ILE:HG13	1.86	0.58
4:3:620:G:H1	43:k:34:ARG:HH11	1.50	0.58
6:5:116:A:H5'	25:P:67:ARG:NH1	2.18	0.58
6:5:145:G:N2	6:5:148:A:OP2	2.32	0.58
13:D:69:ARG:HD3	13:D:172:LEU:HD21	1.84	0.58
15:F:46:PHE:HD2	15:F:57:PRO:HB2	1.68	0.58
20:K:47:CYS:HA	20:K:68:VAL:HA	1.86	0.58
46:n:57:SER:OG	46:n:64:ASN:ND2	2.20	0.58
6:5:1320:A:H62	6:5:1349:A:H5''	1.69	0.58
10:A:293:ARG:NH2	29:T:50:GLN:HG2	2.17	0.58
17:H:106:THR:O	17:H:106:THR:HG22	2.04	0.58
6:5:293:G:N2	6:5:296:A:OP2	2.35	0.57
6:5:350:G:O2'	6:5:385:A:OP1	2.21	0.57
6:5:1142:G:O2'	6:5:1144:A:N6	2.34	0.57
35:c:194:ALA:C	35:c:196:ALA:H	2.12	0.57
58:z:24:ASN:HD22	58:z:27:LYS:HB2	1.69	0.57
6:5:1078:G:H5'	6:5:1078:G:H8	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:70:LYS:HB3	14:E:74:ARG:HH21	1.68	0.57
36:d:56:GLU:O	36:d:60:ILE:HG13	2.04	0.57
17:H:89:LEU:HD13	17:H:96:LEU:HD21	1.86	0.57
4:3:648:G:O6	35:c:181:LYS:NZ	2.29	0.57
4:3:1093:U:H3	4:3:1115:G:H22	1.53	0.57
6:5:354:U:H2'	6:5:355:A:H8	1.69	0.57
6:5:1330:A:H2'	6:5:1331:A:C8	2.39	0.57
9:8:29:U:H3	9:8:41:A:H61	1.50	0.57
14:E:5:ILE:HD11	14:E:62:PHE:HE2	1.69	0.57
30:X:53:ALA:HB3	30:X:54:LYS:HE2	1.85	0.57
38:f:115:ASP:HA	38:f:132:GLU:HA	1.86	0.57
47:o:31:VAL:HG12	47:o:90:LEU:HA	1.87	0.57
4:3:1830:G:H21	33:a:262:HIS:HE1	1.52	0.57
6:5:55:C:H2'	6:5:348:C:H41	1.70	0.57
15:F:42:LEU:HG	15:F:46:PHE:HE1	1.69	0.57
42:j:27:SER:OG	42:j:28:THR:N	2.38	0.57
4:3:1092:A:N6	4:3:1122:G:OP1	2.37	0.57
33:a:2:PRO:HB2	33:a:24:LYS:HZ1	1.69	0.57
6:5:1497:U:H2'	6:5:1498:G:H8	1.68	0.57
27:R:9:ALA:H	56:x:69:GLY:HA3	1.69	0.57
8:7:19:A:H61	8:7:55:C:H42	1.51	0.57
12:C:101:VAL:HG23	12:C:113:ALA:HB1	1.87	0.57
14:E:43:LYS:HE3	14:E:57:TYR:CD2	2.40	0.57
36:d:40:VAL:HG22	36:d:42:ASP:H	1.70	0.57
65:3:3249:SPD:H31	34:b:133:LEU:HD13	1.86	0.57
6:5:1123:G:O2'	6:5:1124:U:O5'	2.23	0.57
13:D:132:HIS:HE1	13:D:205:PRO:HD3	1.70	0.57
13:D:177:ASP:N	13:D:177:ASP:OD1	2.36	0.57
24:O:9:MET:HE1	24:O:18:ARG:NH2	2.19	0.57
38:f:100:GLN:OE1	38:f:110:LYS:NZ	2.38	0.57
4:3:334:A:OP2	52:t:105:LYS:NZ	2.38	0.56
4:3:2068:G:OP1	35:c:69:LYS:NZ	2.29	0.56
6:5:874:C:OP1	20:K:9:ARG:NH2	2.38	0.56
12:C:38:HIS:HB3	12:C:41:ARG:HD2	1.85	0.56
14:E:93:GLU:N	14:E:93:GLU:OE1	2.38	0.56
24:O:11:ARG:HH11	24:O:11:ARG:HG3	1.69	0.56
27:R:41:PHE:CE1	56:x:66:PHE:HB3	2.40	0.56
30:X:38:MET:HG2	30:X:38:MET:O	2.05	0.56
38:f:87:ARG:HB2	38:f:88:PRO:HD3	1.87	0.56
46:n:84:LEU:HB3	46:n:86:LEU:HD12	1.87	0.56
4:3:1833:G:O2'	4:3:1978:U:OP2	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:232:G:H5''	25:P:45:TYR:OH	2.05	0.56
14:E:98:ALA:HB3	26:Q:49:LEU:HD21	1.86	0.56
20:K:115:LEU:HG	20:K:116:ASP:H	1.70	0.56
36:d:136:ILE:HD11	36:d:149:ILE:HG12	1.87	0.56
51:s:3:VAL:HG23	55:w:65:TRP:HZ2	1.70	0.56
1:0:1:MET:HE3	4:3:788:G:H5'	1.87	0.56
4:3:1055:A:N1	4:3:1176:U:O2'	2.35	0.56
4:3:2005:G:OP2	34:b:142:ARG:NH2	2.38	0.56
6:5:145:G:O2'	6:5:147:A:N6	2.36	0.56
6:5:224:A:O4'	24:O:61:LYS:HE3	2.06	0.56
6:5:1438:U:H2'	6:5:1439:G:H8	1.70	0.56
11:B:114:LEU:O	11:B:207:ARG:NH2	2.38	0.56
12:C:179:VAL:HG12	12:C:180:ARG:H	1.69	0.56
23:N:76:ARG:HG3	23:N:80:LYS:NZ	2.19	0.56
35:c:8:LYS:NZ	35:c:14:GLU:OE1	2.39	0.56
42:j:89:GLU:CD	42:j:89:GLU:H	2.12	0.56
4:3:2228:U:H5'	38:f:95:LYS:HG2	1.88	0.56
6:5:838:A:OP2	14:E:110:GLN:NE2	2.37	0.56
13:D:166:ILE:H	13:D:166:ILE:HD12	1.69	0.56
4:3:2189:U:H2'	4:3:2190:G:C8	2.40	0.56
6:5:435:U:O2'	6:5:437:U:O4	2.22	0.56
34:b:180:ARG:NH2	34:b:220:ILE:HD13	2.19	0.56
40:h:119:ALA:O	40:h:123:MET:HG2	2.05	0.56
43:k:117:HIS:ND1	43:k:117:HIS:O	2.38	0.56
4:3:720:A:OP1	4:3:721:G:N2	2.39	0.56
4:3:2131:G:H8	4:3:2131:G:O5'	1.89	0.56
4:3:2756:A:C2	37:e:66:ILE:HD11	2.40	0.56
6:5:704:U:OP1	19:J:80:LYS:NZ	2.30	0.56
6:5:1321:G:O5'	17:H:111:ARG:HG3	2.06	0.56
10:A:99:ILE:HD13	10:A:233:ALA:HB2	1.88	0.56
11:B:134:ARG:HH11	11:B:134:ARG:HG3	1.71	0.56
21:L:48:LEU:HB3	21:L:53:PHE:HE1	1.69	0.56
4:3:140:G:N2	4:3:143:A:OP2	2.30	0.56
4:3:196:G:O2'	4:3:712:A:N1	2.38	0.56
4:3:1909:C:O2'	33:a:251:ARG:O	2.21	0.56
4:3:2427:U:H5''	58:z:20:LEU:HD22	1.87	0.56
6:5:1192:C:OP1	22:M:9:LYS:NZ	2.38	0.56
18:I:98:ILE:HG13	18:I:98:ILE:O	2.06	0.56
26:Q:65:SER:N	26:Q:69:LYS:O	2.39	0.56
46:n:64:ASN:CG	46:n:65:GLY:H	2.11	0.56
4:3:343:A:N3	4:3:363:G:O2'	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:304:U:H2'	6:5:305:A:H8	1.71	0.56
24:O:39:LEU:HD12	24:O:40:ASN:H	1.70	0.56
35:c:116:TRP:CE2	35:c:191:LEU:HD11	2.40	0.56
41:i:63:ASP:OD1	41:i:63:ASP:N	2.35	0.56
11:B:110:GLY:HA3	11:B:225:PRO:HD2	1.87	0.56
11:B:158:GLY:HA3	11:B:199:ILE:HD13	1.88	0.56
20:K:7:LEU:HB3	25:P:35:TYR:CZ	2.40	0.56
39:g:119:ASN:H	39:g:122:ASP:HB2	1.69	0.56
6:5:373:A:H2'	6:5:374:G:C8	2.41	0.56
6:5:1113:U:O4	6:5:1114:A:N6	2.39	0.56
10:A:127:ILE:HG21	10:A:166:VAL:HG12	1.87	0.56
4:3:695:G:H5''	35:c:101:LEU:HD22	1.88	0.55
4:3:1000:U:O2'	4:3:2281:A:N3	2.36	0.55
4:3:1123:A:N7	40:h:130:GLN:NE2	2.49	0.55
4:3:2296:A:H1'	65:3:3247:SPD:H91	1.87	0.55
14:E:52:GLN:OE1	14:E:53:LEU:N	2.38	0.55
23:N:63:LEU:HD12	23:N:64:LEU:N	2.21	0.55
34:b:230:PRO:HG3	47:o:21:TYR:CD1	2.41	0.55
4:3:193:G:OP2	54:v:26:ARG:NH1	2.39	0.55
6:5:1321:G:O6	17:H:12:ARG:NH2	2.39	0.55
17:H:53:PRO:HG3	17:H:105:LEU:HD12	1.89	0.55
35:c:120:LEU:HA	35:c:125:THR:HG21	1.87	0.55
38:f:66:HIS:ND1	38:f:138:LEU:HD11	2.20	0.55
39:g:55:LYS:H	39:g:55:LYS:HE2	1.71	0.55
4:3:517:G:O5'	52:t:44:ARG:NH1	2.39	0.55
18:I:54:VAL:HG11	22:M:61:TRP:CZ3	2.40	0.55
23:N:36:LEU:HB3	23:N:53:LEU:HD13	1.86	0.55
36:d:175:LEU:HD12	36:d:176:PRO:HD2	1.89	0.55
4:3:1386:G:O2'	4:3:1401:A:N6	2.39	0.55
33:a:39:VAL:O	33:a:66:TYR:N	2.39	0.55
40:h:25:LEU:HB3	40:h:30:ILE:HD12	1.88	0.55
6:5:426:U:H5'	12:C:8:PHE:CG	2.42	0.55
33:a:128:ILE:HG22	33:a:129:ASP:N	2.21	0.55
6:5:681:U:O2'	19:J:34:VAL:O	2.21	0.55
12:C:85:LEU:HD22	12:C:88:ASN:ND2	2.21	0.55
13:D:171:GLU:OE1	13:D:172:LEU:HD22	2.07	0.55
15:F:25:ILE:O	15:F:29:ILE:HG12	2.06	0.55
19:J:115:LYS:HD2	29:T:35:HIS:CE1	2.41	0.55
20:K:46:VAL:HG22	20:K:92:VAL:HG22	1.89	0.55
42:j:104:ARG:HH11	42:j:104:ARG:HG3	1.72	0.55
47:o:76:GLU:OE1	47:o:105:ARG:NH1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:201:A:N6	4:3:2438:A:O2'	2.39	0.55
4:3:1583:G:O2'	4:3:1584:U:OP1	2.25	0.55
4:3:2630:U:O2'	4:3:2829:G:N7	2.39	0.55
6:5:1022:G:O2'	6:5:1023:G:O4'	2.25	0.55
36:d:135:GLN:OE1	36:d:149:ILE:HG23	2.05	0.55
6:5:223:G:N2	24:O:61:LYS:HZ1	2.05	0.55
6:5:1330:A:H2'	6:5:1331:A:H8	1.72	0.55
11:B:46:VAL:O	11:B:49:ARG:HG3	2.07	0.55
29:T:36:LEU:HD13	29:T:40:MET:HE3	1.89	0.55
29:T:57:ARG:NH1	29:T:57:ARG:HB3	2.22	0.55
39:g:37:ALA:O	39:g:40:ILE:HG22	2.06	0.55
49:q:5:VAL:HG11	49:q:35:LEU:HD23	1.87	0.55
57:y:39:PHE:O	57:y:41:ARG:NH1	2.40	0.55
6:5:1110:C:H2'	6:5:1111:G:H8	1.72	0.55
6:5:1269:U:HO2'	21:L:14:ARG:NH2	2.04	0.55
10:A:244:THR:OG1	10:A:249:LYS:NZ	2.32	0.55
17:H:47:ILE:HA	17:H:50:MET:HE3	1.89	0.55
24:O:5:ARG:HG2	24:O:6:LEU:H	1.72	0.55
24:O:23:ASP:HB3	24:O:26:VAL:HG23	1.89	0.55
36:d:110:ARG:HD3	36:d:137:ILE:O	2.06	0.55
6:5:1144:A:H2'	6:5:1145:A:C8	2.42	0.55
6:5:1332:U:H3	6:5:1338:A:N6	2.03	0.55
11:B:37:ASP:OD2	11:B:41:ARG:NH2	2.40	0.55
13:D:137:TYR:O	16:G:109:ASN:ND2	2.40	0.55
36:d:132:ILE:HB	36:d:152:PHE:HB2	1.88	0.55
4:3:2140:G:H2'	4:3:2164:G:H22	1.71	0.54
4:3:2185:C:H2'	4:3:2186:C:O4'	2.06	0.54
4:3:2641:A:O2'	34:b:66:GLN:NE2	2.41	0.54
6:5:710:G:H2'	6:5:711:G:C8	2.42	0.54
6:5:1224:C:O2'	17:H:73:GLY:O	2.25	0.54
11:B:130:ARG:HH12	11:B:195:THR:HG22	1.72	0.54
4:3:195:A:H3'	4:3:196:G:H21	1.72	0.54
6:5:87:G:H2'	6:5:88:A:H8	1.73	0.54
6:5:1019:G:O2'	6:5:1020:G:OP2	2.21	0.54
11:B:105:THR:CG2	11:B:232:ARG:CG	2.85	0.54
35:c:5:LYS:HE2	35:c:13:PHE:CE2	2.42	0.54
54:v:48:ILE:HG23	54:v:50:VAL:HG13	1.88	0.54
4:3:733:C:O2'	4:3:769:A:N6	2.40	0.54
13:D:206:ARG:NH1	13:D:210:ILE:HD11	2.21	0.54
14:E:59:ARG:HH22	14:E:88:ILE:HD11	1.72	0.54
25:P:62:GLN:NE2	25:P:79:LYS:HB3	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:55:ASP:OD2	34:b:79:LYS:NZ	2.40	0.54
37:e:44:LEU:HD12	37:e:55:ILE:HG21	1.89	0.54
52:t:3:ARG:NH2	52:t:74:LEU:O	2.40	0.54
4:3:933:A:O2'	9:8:56:C:N3	2.41	0.54
4:3:1094:G:H5''	40:h:68:LYS:HZ1	1.72	0.54
4:3:2513:G:C4	32:Z:33:LYS:HD2	2.43	0.54
6:5:399:C:H5'	12:C:131:THR:HG23	1.89	0.54
15:F:19:ASN:O	15:F:22:VAL:HG23	2.07	0.54
21:L:17:ILE:O	21:L:20:THR:OG1	2.23	0.54
25:P:8:VAL:HG12	25:P:64:VAL:HG22	1.88	0.54
27:R:69:HIS:HB2	27:R:74:PHE:HZ	1.72	0.54
4:3:996:A:H61	44:l:83:MET:HE2	1.73	0.54
11:B:223:LEU:HD12	11:B:224:HIS:N	2.22	0.54
14:E:86:LEU:HB2	26:Q:96:LEU:HD21	1.88	0.54
19:J:67:VAL:HA	19:J:70:MET:SD	2.48	0.54
4:3:1716:A:H61	4:3:1740:U:H3	1.55	0.54
6:5:223:G:H21	24:O:61:LYS:HZ1	1.55	0.54
11:B:52:GLN:HB2	11:B:72:ALA:HB3	1.90	0.54
11:B:220:ALA:O	11:B:221:HIS:ND1	2.41	0.54
4:3:184:A:O2'	4:3:186:A:N7	2.35	0.54
4:3:1103:G:N2	4:3:1130:A:O2'	2.40	0.54
4:3:1292:A:H61	4:3:2024:C:H42	1.55	0.54
6:5:684:A:H4'	19:J:42:THR:HG22	1.88	0.54
8:7:27:U:H3	8:7:43:G:H1	1.56	0.54
8:7:50:G:H1	8:7:62:C:H42	1.55	0.54
12:C:82:ARG:HD3	12:C:83:GLY:N	2.23	0.54
12:C:123:LEU:HD21	12:C:145:LYS:HE2	1.90	0.54
14:E:157:TRP:CB	16:G:60:LEU:HD21	2.37	0.54
21:L:72:GLU:O	21:L:75:LEU:HD12	2.08	0.54
21:L:95:LEU:HB3	21:L:96:PRO:HD3	1.88	0.54
56:x:32:LYS:HE3	56:x:34:ILE:HG12	1.89	0.54
4:3:1166:G:N2	4:3:1167:U:O4	2.38	0.54
4:3:2266:C:O2'	4:3:2435:C:OP2	2.25	0.54
6:5:409:G:H22	6:5:425:G:H1'	1.72	0.54
6:5:923:G:O2'	6:5:1508:C:OP1	2.26	0.54
12:C:81:GLN:HB2	12:C:85:LEU:HD11	1.90	0.54
18:I:103:THR:HG21	56:x:91:HIS:CE1	2.43	0.54
52:t:46:LYS:HE3	52:t:63:VAL:HB	1.90	0.54
2:1:15:LYS:HD3	4:3:664:G:H5''	1.89	0.54
4:3:9:G:H2'	4:3:10:U:C6	2.43	0.54
4:3:2181:A:H3'	4:3:2182:C:C5	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:76:G:N2	6:5:79:A:OP2	2.40	0.54
6:5:250:G:H2'	6:5:251:G:H8	1.73	0.54
6:5:1215:U:C5	15:F:115:MET:HE3	2.42	0.54
25:P:53:VAL:O	25:P:55:ALA:N	2.41	0.54
36:d:65:PRO:HB2	36:d:87:CYS:HB2	1.88	0.54
48:p:64:LEU:HD11	48:p:94:LEU:HB3	1.90	0.54
4:3:1076:U:H3	4:3:1149:G:H1	1.56	0.54
4:3:1569:A:H2'	4:3:1570:A:C2	2.43	0.54
4:3:1798:A:O2'	33:a:213:ILE:O	2.20	0.54
6:5:22:G:H2'	6:5:23:G:C8	2.43	0.54
24:O:8:ARG:HB2	24:O:28:ARG:NH1	2.21	0.54
31:Y:53:A:H2'	31:Y:54:A:C8	2.43	0.54
34:b:37:ALA:HB3	34:b:51:LEU:HD23	1.90	0.54
4:3:585:U:H2'	4:3:586:G:H8	1.73	0.53
6:5:1347:U:OP1	17:H:75:THR:OG1	2.17	0.53
13:D:86:MET:HE1	31:Y:49:U:C6	2.43	0.53
14:E:17:GLN:HG3	14:E:56:HIS:CD2	2.42	0.53
38:f:23:ASP:N	38:f:23:ASP:OD1	2.40	0.53
38:f:41:LYS:HE2	38:f:46:ASP:HB3	1.89	0.53
4:3:924:C:H5''	21:L:92:ARG:NH2	2.23	0.53
24:O:66:THR:H	24:O:69:VAL:HB	1.73	0.53
26:Q:42:ARG:O	26:Q:46:ILE:HD12	2.08	0.53
36:d:49:PHE:HZ	36:d:147:LYS:HB2	1.73	0.53
37:e:23:ASP:OD1	37:e:23:ASP:N	2.41	0.53
47:o:25:PHE:HB3	47:o:90:LEU:HD13	1.91	0.53
4:3:897:A:N3	5:4:77:G:O2'	2.42	0.53
6:5:1351:U:H2'	6:5:1352:A:C8	2.43	0.53
47:o:41:GLU:OE1	47:o:42:LYS:HB2	2.09	0.53
49:q:27:ALA:O	49:q:62:HIS:NE2	2.41	0.53
2:1:5:SER:HA	2:1:8:LYS:HE2	1.89	0.53
4:3:410:G:H4'	4:3:411:U:O5'	2.08	0.53
4:3:879:U:O4	4:3:968:U:O2'	2.24	0.53
4:3:1125:U:H2'	4:3:1126:G:C8	2.44	0.53
4:3:2299:U:H2'	4:3:2300:A:C8	2.44	0.53
4:3:2477:A:H2'	4:3:2478:G:O4'	2.08	0.53
6:5:510:U:H2'	6:5:511:A:H8	1.74	0.53
11:B:105:THR:HG23	11:B:232:ARG:CD	2.35	0.53
27:R:21:ASP:O	27:R:24:LYS:HG2	2.07	0.53
34:b:150:GLY:HA3	34:b:155:SER:HB3	1.89	0.53
35:c:97:ARG:HD2	35:c:99:TYR:CZ	2.43	0.53
44:l:5:LYS:HD2	44:l:6:ARG:HH22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:s:48:TYR:HD1	51:s:91:ILE:HD13	1.73	0.53
55:w:56:THR:O	55:w:60:GLU:HG2	2.09	0.53
4:3:2195:U:H2'	4:3:2196:G:C8	2.43	0.53
4:3:2321:C:O4'	36:d:37:ASN:ND2	2.41	0.53
6:5:1261:A:H2'	6:5:1262:A:C8	2.44	0.53
36:d:42:ASP:O	36:d:46:ASP:N	2.42	0.53
39:g:56:ASN:CG	39:g:60:ARG:HH21	2.16	0.53
40:h:58:TYR:HD1	40:h:60:ASP:H	1.57	0.53
6:5:197:A:H2'	6:5:198:A:C8	2.43	0.53
6:5:394:U:H2'	6:5:395:G:H8	1.74	0.53
14:E:86:LEU:HD13	26:Q:95:TYR:CE1	2.44	0.53
40:h:72:VAL:HG11	40:h:108:LYS:HD2	1.90	0.53
41:i:101:ASP:HB2	41:i:127:VAL:HG13	1.91	0.53
6:5:670:G:H2'	6:5:671:G:C8	2.43	0.53
6:5:1197:G:OP2	6:5:1296:C:N4	2.40	0.53
19:J:27:ALA:O	19:J:35:LEU:HD23	2.08	0.53
4:3:666:G:N2	4:3:669:A:OP2	2.34	0.53
4:3:2028:G:OP1	57:y:9:SER:OG	2.27	0.53
6:5:195:U:H2'	6:5:196:G:C8	2.41	0.53
14:E:170:GLN:O	16:G:80:ARG:NH2	2.41	0.53
27:R:35:SER:OG	27:R:38:SER:OG	2.17	0.53
28:S:54:LEU:HB3	28:S:60:ILE:HG13	1.91	0.53
35:c:5:LYS:HE2	35:c:13:PHE:HE2	1.74	0.53
4:3:2032:G:OP1	34:b:158:ARG:NH1	2.42	0.53
16:G:19:LEU:HD22	16:G:87:VAL:HG11	1.89	0.53
40:h:38:GLN:HB3	40:h:65:PHE:CZ	2.43	0.53
52:t:52:THR:H	52:t:55:ALA:HB3	1.73	0.53
6:5:1062:C:H2'	6:5:1063:G:H8	1.74	0.53
12:C:84:ASN:HB3	13:D:156:GLN:O	2.09	0.53
13:D:67:GLU:OE2	13:D:68:GLU:N	2.37	0.53
15:F:119:ILE:O	15:F:123:ILE:HG12	2.08	0.53
21:L:10:PRO:HB2	21:L:13:LYS:HB2	1.90	0.53
21:L:73:ILE:O	21:L:77:ILE:HG12	2.08	0.53
27:R:30:PRO:HA	27:R:48:THR:HG23	1.90	0.53
33:a:129:ASP:O	33:a:136:MET:HE1	2.08	0.53
35:c:97:ARG:NH1	35:c:99:TYR:OH	2.42	0.53
36:d:92:ARG:O	36:d:95:ARG:HG2	2.09	0.53
4:3:823:A:OP1	4:3:826:C:N4	2.38	0.52
4:3:1111:C:H2'	4:3:1112:A:O4'	2.08	0.52
6:5:36:G:H21	20:K:128:SER:HG	1.56	0.52
6:5:190:A:H2'	6:5:191:A:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:1115:G:H1'	6:5:1116:U:H5	1.74	0.52
6:5:1193:U:H2'	6:5:1194:A:C8	2.44	0.52
12:C:68:ASP:O	12:C:72:ARG:HG3	2.08	0.52
50:r:51:LEU:O	50:r:55:ILE:HG13	2.09	0.52
10:A:181:PRO:HG2	10:A:206:THR:HG21	1.91	0.52
18:I:30:LYS:O	18:I:34:VAL:HG23	2.10	0.52
39:g:46:LYS:HG2	39:g:48:GLY:H	1.75	0.52
39:g:108:PHE:CE1	39:g:123:LEU:HD13	2.43	0.52
55:w:80:ASN:O	55:w:84:VAL:HG13	2.09	0.52
4:3:892:G:H2'	4:3:893:A:C8	2.44	0.52
4:3:1391:U:O2'	4:3:1816:A:N3	2.35	0.52
4:3:2490:A:HO2'	9:8:63:C:HO2'	1.55	0.52
6:5:1138:U:H3	6:5:1149:G:H1	1.56	0.52
23:N:29:LEU:O	23:N:33:ILE:HG12	2.09	0.52
51:s:4:THR:O	51:s:4:THR:HG22	2.09	0.52
52:t:94:ASP:OD1	52:t:94:ASP:N	2.42	0.52
4:3:2173:G:H2'	4:3:2174:G:C8	2.44	0.52
6:5:1051:U:H5'	22:M:45:ARG:HH12	1.74	0.52
11:B:42:ASN:O	11:B:46:VAL:HG22	2.09	0.52
11:B:115:SER:HB2	11:B:221:HIS:NE2	2.23	0.52
37:e:142:GLU:OE1	37:e:142:GLU:N	2.40	0.52
38:f:4:ILE:HG22	38:f:18:VAL:HG22	1.90	0.52
40:h:76:LEU:HD11	40:h:127:THR:HG23	1.91	0.52
6:5:80:U:H2'	6:5:81:A:H8	1.74	0.52
6:5:577:G:H5'	6:5:725:A:H1'	1.92	0.52
10:A:20:LEU:HG	10:A:62:ARG:HH21	1.73	0.52
41:i:3:LYS:HG3	41:i:4:THR:N	2.23	0.52
4:3:620:G:H5'	64:3:3226:SPM:H82	1.91	0.52
4:3:697:U:H5''	43:k:17:THR:HG22	1.90	0.52
4:3:728:A:O2'	4:3:1381:A:N3	2.42	0.52
4:3:1648:A:N1	50:r:93:SER:OG	2.43	0.52
6:5:550:U:H2'	6:5:551:A:H8	1.75	0.52
6:5:892:G:N2	6:5:895:A:OP2	2.42	0.52
14:E:118:ILE:O	14:E:121:ARG:HG2	2.09	0.52
21:L:14:ARG:HD2	21:L:16:GLU:OE2	2.10	0.52
28:S:35:PHE:HD2	28:S:47:VAL:HG21	1.74	0.52
47:o:26:SER:N	47:o:29:ASP:OD2	2.35	0.52
4:3:2383:G:N2	4:3:2386:A:OP2	2.39	0.52
15:F:118:LYS:O	15:F:122:GLU:HG2	2.09	0.52
30:X:35:THR:HG23	30:X:48:VAL:HB	1.92	0.52
35:c:40:VAL:HG22	35:c:101:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:5:LYS:HD3	36:d:97:TRP:CD1	2.43	0.52
36:d:41:GLY:O	36:d:44:ILE:HG12	2.10	0.52
37:e:121:PRO:HG2	37:e:124:LEU:HD22	1.91	0.52
27:R:31:ILE:HB	27:R:49:PHE:HD1	1.74	0.52
28:S:35:PHE:C	28:S:35:PHE:CD1	2.87	0.52
37:e:159:PRO:HA	37:e:172:ILE:HD13	1.90	0.52
41:i:7:LEU:HD13	48:p:60:TRP:HE1	1.74	0.52
51:s:8:LEU:HB2	51:s:30:VAL:HG23	1.91	0.52
4:3:2004:G:OP2	65:3:3249:SPD:H41	2.10	0.52
4:3:2196:G:H2'	4:3:2197:U:C6	2.45	0.52
6:5:68:C:H2'	6:5:69:G:C8	2.45	0.52
6:5:941:A:H2'	6:5:942:G:C8	2.45	0.52
6:5:1283:G:O3'	21:L:76:ASN:ND2	2.43	0.52
10:A:46:GLU:HB3	10:A:57:VAL:HG22	1.91	0.52
11:B:11:ARG:NH1	11:B:180:THR:O	2.42	0.52
17:H:10:GLY:O	17:H:11:ARG:HD3	2.10	0.52
18:I:83:VAL:HG23	18:I:84:ASP:H	1.75	0.52
33:a:65:LYS:O	33:a:67:ARG:NH1	2.42	0.52
4:3:86:A:N6	4:3:101:C:O4'	2.43	0.52
4:3:2118:U:O4	4:3:2155:G:N2	2.43	0.52
6:5:192:A:H2'	6:5:193:G:H8	1.75	0.52
6:5:671:G:H2'	6:5:672:A:H8	1.75	0.52
7:6:36:C:H2'	7:6:37:A:O4'	2.10	0.52
18:I:54:VAL:HG11	22:M:61:TRP:HZ3	1.75	0.52
19:J:17:SER:HA	19:J:80:LYS:HB3	1.92	0.52
8:7:36:C:H2'	8:7:37:A:C8	2.44	0.51
50:r:41:LYS:HE3	57:y:22:LEU:HD11	1.92	0.51
6:5:1406:U:O4	6:5:1407:A:N6	2.42	0.51
40:h:11:LYS:HD3	40:h:54:VAL:HG22	1.92	0.51
6:5:808:C:O2'	6:5:895:A:N1	2.43	0.51
13:D:215:ASN:HB2	13:D:218:GLU:HB3	1.91	0.51
17:H:41:PHE:C	17:H:43:ASN:H	2.16	0.51
21:L:34:LEU:HD21	21:L:41:PRO:HB3	1.92	0.51
28:S:36:HIS:ND1	28:S:36:HIS:O	2.43	0.51
38:f:97:ILE:O	38:f:101:ALA:N	2.42	0.51
55:w:77:LYS:HG2	55:w:78:LYS:H	1.75	0.51
6:5:715:A:C4	19:J:111:HIS:CD2	2.98	0.51
11:B:105:THR:HG21	11:B:232:ARG:CD	2.17	0.51
19:J:10:SER:O	19:J:72:MET:HG3	2.10	0.51
24:O:19:ILE:N	24:O:37:GLY:O	2.43	0.51
25:P:12:ILE:HG12	25:P:60:LYS:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:590:G:H1	6:5:644:U:H3	1.58	0.51
13:D:186:ASN:OD1	13:D:186:ASN:N	2.43	0.51
15:F:14:ASP:OD1	15:F:15:PRO:HD2	2.11	0.51
15:F:98:LEU:HD21	15:F:102:TRP:CH2	2.46	0.51
43:k:20:LEU:O	43:k:32:SER:OG	2.17	0.51
48:p:6:GLY:H	48:p:8:GLN:NE2	2.08	0.51
4:3:916:U:H3	4:3:935:U:H3	1.59	0.51
4:3:1521:A:N3	4:3:1611:C:O2'	2.41	0.51
4:3:2135:C:H2'	4:3:2136:A:C8	2.42	0.51
12:C:104:MET:HA	12:C:167:VAL:HG11	1.91	0.51
15:F:110:ARG:HG2	15:F:112:GLU:HG3	1.91	0.51
18:I:93:LEU:HD12	18:I:96:ILE:HD12	1.91	0.51
23:N:33:ILE:O	23:N:37:THR:HG23	2.11	0.51
24:O:43:LEU:HD23	24:O:47:LYS:HA	1.92	0.51
37:e:12:ASP:OD1	37:e:12:ASP:N	2.44	0.51
42:j:86:LEU:HB3	42:j:94:ARG:HD2	1.93	0.51
4:3:1588:A:H2'	4:3:1589:A:C8	2.46	0.51
4:3:1807:C:OP2	33:a:190:ARG:NH2	2.43	0.51
6:5:223:G:H21	24:O:61:LYS:NZ	2.08	0.51
6:5:823:C:H1'	16:G:24:ASN:HD22	1.76	0.51
14:E:6:ILE:HG21	26:Q:96:LEU:HD11	1.93	0.51
22:M:7:LYS:HG2	22:M:23:ARG:HD3	1.93	0.51
50:r:129:VAL:O	50:r:133:GLN:HG3	2.11	0.51
4:3:408:G:OP2	4:3:459:A:N6	2.44	0.51
4:3:1805:U:O2'	4:3:1809:A:N3	2.42	0.51
4:3:2665:A:O2'	37:e:163:LYS:NZ	2.43	0.51
8:7:36:C:H2'	8:7:37:A:H8	1.75	0.51
15:F:130:THR:O	15:F:130:THR:OG1	2.27	0.51
34:b:45:ASP:O	34:b:46:LYS:HB2	2.11	0.51
40:h:14:LEU:HD22	40:h:19:ALA:HA	1.93	0.51
4:3:622:U:H2'	4:3:623:A:C8	2.46	0.51
4:3:901:C:H4'	4:3:902:U:C5'	2.41	0.51
4:3:933:A:H3'	4:3:934:C:O4'	2.11	0.51
4:3:947:A:H62	44:l:12:PRO:HA	1.75	0.51
6:5:664:A:H2'	6:5:665:G:C8	2.46	0.51
10:A:22:LYS:HZ2	10:A:251:ASP:HA	1.75	0.51
11:B:61:THR:HB	11:B:64:THR:HG22	1.92	0.51
35:c:153:LEU:HD12	35:c:153:LEU:H	1.76	0.51
12:C:124:LEU:HD22	12:C:127:ARG:HG2	1.93	0.51
17:H:51:GLU:HG3	17:H:51:GLU:O	2.10	0.51
22:M:39:VAL:HG13	22:M:44:PHE:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:252:ASP:OD2	33:a:261:ARG:NH1	2.44	0.51
47:o:102:SER:O	47:o:105:ARG:HG2	2.11	0.51
4:3:1033:A:OP2	48:p:57:ARG:NH1	2.44	0.50
4:3:1617:U:H5''	4:3:1619:A:C4	2.46	0.50
13:D:219:LEU:H	13:D:219:LEU:HD12	1.76	0.50
27:R:3:ARG:NH2	27:R:10:PHE:HB2	2.25	0.50
28:S:21:ASN:OD1	28:S:59:ILE:HG12	2.10	0.50
35:c:7:ILE:HG22	35:c:127:LEU:O	2.11	0.50
37:e:3:LYS:HG2	37:e:6:ASN:H	1.75	0.50
42:j:90:ASP:O	42:j:91:LYS:HB2	2.10	0.50
4:3:2150:C:H2'	4:3:2151:G:C8	2.46	0.50
6:5:111:A:OP1	6:5:603:U:O2'	2.29	0.50
6:5:821:U:O2	16:G:11:HIS:NE2	2.44	0.50
6:5:1214:A:H62	6:5:1273:A:H62	1.57	0.50
10:A:293:ARG:HH21	29:T:50:GLN:CG	2.24	0.50
11:B:46:VAL:HG23	11:B:47:ASN:N	2.25	0.50
16:G:125:ASP:OD1	16:G:126:LYS:N	2.44	0.50
19:J:109:ILE:HD11	29:T:28:LEU:HD22	1.93	0.50
4:3:1106:G:N2	4:3:1124:G:O2'	2.44	0.50
6:5:433:C:H2'	6:5:434:U:C6	2.47	0.50
6:5:825:A:N3	10:A:39:PRO:HG2	2.26	0.50
7:6:73:A:H2'	7:6:74:C:O4'	2.11	0.50
10:A:107:PHE:HD2	10:A:109:THR:HG23	1.77	0.50
10:A:208:PRO:CG	14:E:174:TYR:CE2	2.94	0.50
11:B:41:ARG:HH22	22:M:52:ALA:HB1	1.76	0.50
11:B:105:THR:OG1	11:B:232:ARG:CD	2.59	0.50
14:E:85:GLU:OE1	14:E:87:ILE:HG13	2.12	0.50
19:J:29:ASP:OD1	19:J:30:PRO:HD2	2.12	0.50
20:K:94:LEU:HD22	20:K:114:THR:HG21	1.92	0.50
33:a:112:PRO:HG2	33:a:115:ILE:HG12	1.93	0.50
34:b:74:ASN:HD22	34:b:74:ASN:C	2.19	0.50
36:d:108:LEU:HB3	36:d:114:PHE:CE2	2.46	0.50
39:g:26:ILE:HG22	39:g:109:VAL:HB	1.93	0.50
6:5:57:U:H2'	6:5:58:G:H8	1.77	0.50
22:M:29:ARG:NH1	22:M:31:ARG:HG3	2.26	0.50
33:a:84:LYS:HE2	33:a:100:THR:HG21	1.93	0.50
43:k:112:ILE:HG22	43:k:128:VAL:HG12	1.94	0.50
4:3:2813:A:H2'	4:3:2814:A:C8	2.46	0.50
6:5:1049:G:H5''	11:B:189:LEU:HD11	1.94	0.50
6:5:1292:A:H1'	27:R:37:ARG:HH22	1.77	0.50
12:C:94:GLU:OE1	12:C:99:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:180:ARG:HG3	12:C:180:ARG:O	2.12	0.50
13:D:181:LYS:HG2	13:D:183:LEU:HD22	1.93	0.50
28:S:54:LEU:HD22	28:S:59:ILE:HD12	1.94	0.50
37:e:23:ASP:HA	37:e:38:LEU:HB2	1.92	0.50
55:w:16:VAL:O	55:w:20:ILE:HD12	2.11	0.50
4:3:620:G:H5'	64:3:3226:SPM:H61	1.93	0.50
4:3:917:G:H2'	4:3:918:G:C8	2.47	0.50
4:3:2111:U:N3	4:3:2194:G:H1'	2.19	0.50
6:5:813:A:OP1	6:5:1501:G:O2'	2.24	0.50
14:E:25:GLN:O	14:E:25:GLN:NE2	2.41	0.50
14:E:165:ASN:HD21	16:G:58:GLN:HG3	1.75	0.50
15:F:15:PRO:HG3	17:H:45:LEU:HD21	1.93	0.50
17:H:32:VAL:HA	17:H:67:VAL:HB	1.92	0.50
24:O:56:LEU:HD21	24:O:78:LEU:HD11	1.92	0.50
56:x:10:GLN:NE2	56:x:29:LEU:O	2.45	0.50
4:3:663:A:N7	43:k:81:ASN:ND2	2.56	0.50
4:3:2308:U:H2'	4:3:2309:A:C8	2.46	0.50
10:A:223:GLN:HE22	10:A:277:ILE:HD13	1.77	0.50
12:C:148:THR:O	12:C:151:ILE:HG22	2.11	0.50
15:F:15:PRO:HG2	17:H:45:LEU:HD11	1.94	0.50
17:H:21:LEU:HD22	17:H:63:PHE:HB3	1.92	0.50
35:c:128:VAL:HG23	35:c:132:LEU:HD21	1.92	0.50
4:3:853:G:N1	4:3:1219:U:OP2	2.38	0.50
7:6:8:U:O2'	7:6:21:A:N1	2.41	0.50
7:6:76:A:C8	7:6:76:A:H5'	2.46	0.50
11:B:86:GLN:O	11:B:89:THR:OG1	2.27	0.50
13:D:212:ARG:HA	16:G:75:LYS:HZ1	1.77	0.50
19:J:16:VAL:HG12	19:J:25:VAL:HG13	1.94	0.50
43:k:82:LEU:HB2	43:k:116:GLY:HA3	1.94	0.50
43:k:102:GLN:OE1	43:k:102:GLN:HA	2.11	0.50
5:4:2:U:O2	5:4:107:G:N2	2.45	0.50
6:5:250:G:H2'	6:5:251:G:C8	2.47	0.50
6:5:423:U:OP1	12:C:31:ARG:HD3	2.12	0.50
10:A:37:TRP:HB2	10:A:204:THR:HG22	1.93	0.50
12:C:172:LYS:O	12:C:172:LYS:HG2	2.11	0.50
13:D:87:ARG:HG2	13:D:109:LEU:HD22	1.94	0.50
13:D:219:LEU:C	16:G:126:LYS:HZ3	2.20	0.50
4:3:436:G:O6	54:v:56:ARG:NH2	2.44	0.49
4:3:1166:G:O4'	41:i:80:HIS:HD2	1.95	0.49
5:4:40:U:H5''	36:d:64:LYS:HD2	1.93	0.49
13:D:80:THR:OG1	13:D:81:LYS:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:129:ASP:O	14:E:132:VAL:HG23	2.11	0.49
36:d:49:PHE:CZ	36:d:147:LYS:HB2	2.47	0.49
4:3:2736:U:O2'	4:3:2737:G:H8	1.95	0.49
11:B:152:ILE:HG23	11:B:205:ILE:HG12	1.93	0.49
15:F:128:ASN:O	15:F:130:THR:HG23	2.13	0.49
17:H:12:ARG:CD	17:H:13:LYS:HG3	2.42	0.49
17:H:14:SER:O	17:H:14:SER:OG	2.27	0.49
21:L:96:PRO:HG2	21:L:102:THR:HG22	1.92	0.49
35:c:110:ALA:O	35:c:114:THR:HG23	2.12	0.49
36:d:148:ARG:NE	36:d:149:ILE:H	2.10	0.49
38:f:6:LYS:HE3	38:f:37:ALA:HB2	1.92	0.49
38:f:88:PRO:HG2	38:f:89:TYR:CD1	2.47	0.49
4:3:2107:A:H3'	4:3:2108:C:C6	2.48	0.49
6:5:386:U:H4'	24:O:28:ARG:HH21	1.76	0.49
6:5:460:A:H2'	6:5:461:G:C8	2.47	0.49
9:8:28:A:H2'	9:8:29:U:C6	2.46	0.49
36:d:15:GLU:HG3	36:d:16:LEU:N	2.27	0.49
47:o:36:LYS:HE3	47:o:85:ASN:HA	1.94	0.49
4:3:818:A:H2'	4:3:819:U:H4'	1.95	0.49
6:5:1279:G:H21	6:5:1306:A:H2	1.58	0.49
10:A:147:LYS:O	10:A:151:MET:HG3	2.12	0.49
12:C:17:SER:O	12:C:63:MET:HE1	2.13	0.49
14:E:103:LYS:O	14:E:107:LEU:HG	2.12	0.49
25:P:21:THR:HG22	25:P:73:LYS:NZ	2.28	0.49
29:T:34:TYR:O	29:T:41:ARG:NH2	2.44	0.49
38:f:106:MET:SD	38:f:107:ALA:HB2	2.51	0.49
51:s:59:ILE:O	51:s:61:LYS:NZ	2.44	0.49
4:3:549:A:N3	4:3:614:C:O2'	2.45	0.49
4:3:1031:U:O2'	41:i:4:THR:HG21	2.12	0.49
6:5:424:U:OP2	12:C:31:ARG:NH1	2.44	0.49
6:5:577:G:O2'	23:N:51:ARG:NH1	2.45	0.49
6:5:1022:G:O2'	6:5:1023:G:O5'	2.30	0.49
6:5:1121:U:C4	17:H:34:ARG:HD3	2.47	0.49
14:E:59:ARG:HH12	14:E:88:ILE:HD11	1.77	0.49
16:G:97:ILE:HG23	16:G:99:ARG:HD3	1.95	0.49
24:O:86:LYS:C	24:O:86:LYS:HD3	2.37	0.49
46:n:28:VAL:HG12	46:n:89:VAL:HG12	1.95	0.49
46:n:98:TYR:HA	46:n:102:ILE:HG21	1.94	0.49
4:3:604:A:O2'	4:3:606:G:OP2	2.29	0.49
4:3:788:G:H2'	4:3:789:A:H8	1.77	0.49
4:3:2493:G:O3'	44:l:126:PRO:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:133:G:H2'	6:5:134:G:C8	2.47	0.49
6:5:275:A:H5''	6:5:276:U:H3'	1.95	0.49
11:B:47:ASN:OD1	11:B:48:TYR:HD2	1.96	0.49
11:B:192:ALA:HB3	11:B:199:ILE:HB	1.94	0.49
21:L:39:ILE:HD11	21:L:48:LEU:HD21	1.94	0.49
36:d:135:GLN:HE22	36:d:149:ILE:HG12	1.76	0.49
38:f:33:LYS:HB3	38:f:35:LEU:HG	1.92	0.49
43:k:20:LEU:HB3	43:k:32:SER:HB3	1.94	0.49
48:p:39:ILE:HG22	48:p:43:LYS:HE3	1.95	0.49
4:3:180:A:H5'	4:3:181:G:C8	2.47	0.49
6:5:672:A:H1'	19:J:111:HIS:CE1	2.47	0.49
6:5:1096:A:H2'	6:5:1097:G:H8	1.78	0.49
6:5:1350:A:P	15:F:27:ASN:HD22	2.35	0.49
9:8:40:C:H2'	9:8:41:A:C8	2.48	0.49
12:C:179:VAL:HG12	12:C:180:ARG:N	2.27	0.49
37:e:89:LYS:HB3	37:e:168:PHE:HB2	1.94	0.49
44:l:130:LYS:HE2	44:l:132:LEU:HD11	1.94	0.49
56:x:6:HIS:ND1	56:x:6:HIS:O	2.46	0.49
4:3:1665:G:N1	4:3:1668:G:OP2	2.36	0.49
6:5:855:G:HO2'	6:5:868:G:HO2'	1.61	0.49
6:5:929:C:O2'	6:5:1318:C:OP2	2.19	0.49
20:K:78:THR:HG21	20:K:95:LEU:HD22	1.95	0.49
35:c:82:PRO:HB3	35:c:90:VAL:HG23	1.93	0.49
36:d:29:PRO:HG2	36:d:169:LEU:HB2	1.94	0.49
36:d:39:GLY:HA2	36:d:86:GLY:HA2	1.93	0.49
4:3:1566:A:H2'	4:3:1567:U:O4'	2.13	0.49
4:3:2142:U:H2'	4:3:2143:G:C8	2.48	0.49
6:5:507:A:H1'	12:C:54:LEU:HD22	1.95	0.49
15:F:66:GLY:HA2	15:F:69:MET:HG3	1.95	0.49
26:Q:36:ARG:HB2	26:Q:38:LYS:HG2	1.95	0.49
36:d:8:TYR:O	36:d:12:ILE:HB	2.13	0.49
4:3:619:A:OP1	64:3:3226:SPM:N14	2.46	0.49
4:3:2111:U:H5''	4:3:2112:A:C8	2.43	0.49
6:5:840:C:H4'	26:Q:40:TYR:CZ	2.47	0.49
13:D:103:TYR:HE2	13:D:193:HIS:HE1	1.60	0.49
14:E:94:TYR:HB3	26:Q:85:HIS:CD2	2.48	0.49
37:e:39:PRO:HG2	37:e:42:LEU:HD13	1.93	0.49
38:f:56:GLU:OE1	38:f:56:GLU:N	2.38	0.49
43:k:81:ASN:OD1	43:k:83:ASN:ND2	2.46	0.49
4:3:1920:A:C8	6:5:1469:G:H4'	2.48	0.48
4:3:2820:G:N3	4:3:2887:A:O2'	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:2854:A:N7	4:3:2872:A:O2'	2.34	0.48
6:5:1241:G:H21	6:5:1243:A:H8	1.61	0.48
6:5:1332:U:OP1	22:M:35:SER:OG	2.31	0.48
7:6:59:G:H2'	7:6:60:A:C8	2.47	0.48
24:O:40:ASN:HB3	24:O:43:LEU:HB2	1.94	0.48
25:P:18:ASN:HB2	25:P:21:THR:OG1	2.12	0.48
33:a:137:PRO:HG2	33:a:140:PHE:CE2	2.47	0.48
46:n:110:ARG:HG3	46:n:116:PHE:CZ	2.48	0.48
4:3:204:U:H4'	54:v:22:LYS:HB2	1.95	0.48
4:3:995:A:N6	44:l:83:MET:HE1	2.27	0.48
4:3:1104:A:H5''	4:3:1105:A:C5	2.48	0.48
4:3:2169:G:O3'	4:3:2173:G:N2	2.46	0.48
6:5:680:G:H21	19:J:33:ASN:H	1.61	0.48
10:A:84:PHE:CE1	10:A:177:ILE:HD12	2.47	0.48
10:A:208:PRO:HG2	14:E:174:TYR:CE2	2.48	0.48
14:E:114:LYS:O	14:E:118:ILE:HD12	2.13	0.48
35:c:52:ILE:HG21	35:c:92:GLY:HA3	1.94	0.48
4:3:87:G:O2'	4:3:104:A:N1	2.38	0.48
4:3:1445:U:H2'	4:3:1446:G:O4'	2.12	0.48
4:3:2847:C:H2'	4:3:2848:A:H8	1.79	0.48
6:5:192:A:H2'	6:5:193:G:C8	2.49	0.48
6:5:259:A:H2'	6:5:260:C:C6	2.48	0.48
6:5:394:U:H2'	6:5:395:G:C8	2.48	0.48
6:5:447:G:H5''	6:5:448:A:H3'	1.95	0.48
6:5:1215:U:O4'	15:F:41:ILE:HD11	2.13	0.48
8:7:10:G:O2'	8:7:11:U:OP1	2.25	0.48
28:S:67:ARG:NH1	28:S:67:ARG:HB3	2.28	0.48
41:i:78:TYR:CE1	41:i:89:LYS:HB3	2.48	0.48
47:o:19:LYS:HE2	47:o:82:HIS:HA	1.96	0.48
4:3:638:A:H62	4:3:660:U:H3	1.61	0.48
4:3:1392:G:N2	4:3:1395:A:OP2	2.40	0.48
6:5:775:G:O2'	19:J:114:CYS:SG	2.70	0.48
6:5:998:G:O2'	6:5:1000:A:OP1	2.31	0.48
11:B:183:ALA:HB3	11:B:185:ILE:HD11	1.96	0.48
13:D:187:THR:O	13:D:191:MET:HG3	2.13	0.48
14:E:133:THR:HG22	14:E:136:LEU:HD12	1.95	0.48
14:E:139:THR:OG1	14:E:140:GLN:N	2.45	0.48
19:J:21:ASN:O	19:J:21:ASN:ND2	2.31	0.48
40:h:112:LEU:HG	40:h:114:ALA:H	1.78	0.48
4:3:316:C:H2'	4:3:392:A:H61	1.78	0.48
6:5:196:G:HO2'	6:5:197:A:P	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:256:G:OP2	28:S:71:ARG:NH2	2.43	0.48
11:B:221:HIS:CG	11:B:221:HIS:O	2.67	0.48
12:C:85:LEU:HD22	12:C:88:ASN:HD22	1.78	0.48
12:C:104:MET:HE2	12:C:176:GLY:O	2.13	0.48
21:L:39:ILE:HD12	21:L:52:GLU:HB3	1.94	0.48
24:O:66:THR:HG22	24:O:67:ASP:H	1.78	0.48
43:k:131:VAL:HG12	43:k:148:LEU:HD21	1.96	0.48
2:1:42:ARG:NH1	4:3:2358:U:OP2	2.46	0.48
4:3:518:A:O2'	4:3:532:A:N1	2.44	0.48
4:3:1115:G:N2	40:h:123:MET:HE1	2.28	0.48
4:3:1465:U:HO2'	4:3:1542:G:HO2'	1.57	0.48
5:4:55:A:C4	36:d:26:MET:HE1	2.48	0.48
6:5:369:A:H4'	6:5:448:A:H62	1.79	0.48
6:5:1348:G:P	17:H:75:THR:HG21	2.54	0.48
10:A:202:CYS:SG	10:A:214:ILE:HG23	2.54	0.48
4:3:1239:G:O2'	4:3:1267:A:N1	2.40	0.48
4:3:2165:A:H1'	4:3:2166:U:P	2.54	0.48
6:5:510:U:H2'	6:5:511:A:C8	2.48	0.48
9:8:38:A:C2	21:L:124:LYS:HA	2.49	0.48
17:H:65:ILE:HG22	17:H:67:VAL:HG23	1.96	0.48
34:b:21:ASN:OD1	42:j:73:ASP:HB3	2.14	0.48
34:b:47:TYR:HB2	34:b:85:ARG:HH21	1.78	0.48
35:c:157:VAL:HA	35:c:196:ALA:O	2.14	0.48
41:i:4:THR:HA	49:q:12:TYR:CE2	2.46	0.48
42:j:15:GLY:HA3	42:j:47:ILE:HG12	1.95	0.48
42:j:51:MET:HG3	42:j:52:VAL:HG13	1.96	0.48
4:3:799:A:H5''	33:a:217:GLY:HA3	1.95	0.48
4:3:1023:C:O2'	4:3:1036:A:N3	2.43	0.48
4:3:1618:U:H4'	4:3:1619:A:OP2	2.13	0.48
6:5:1361:G:H2'	6:5:1362:G:H8	1.78	0.48
6:5:1387:U:H2'	6:5:1388:A:C8	2.49	0.48
7:6:76:A:H5'	7:6:76:A:H8	1.77	0.48
10:A:53:ASN:ND2	10:A:279:SER:O	2.47	0.48
10:A:115:GLY:HA2	10:A:118:THR:HG22	1.95	0.48
12:C:26:SER:OG	12:C:27:LYS:N	2.45	0.48
20:K:20:LYS:HB2	20:K:20:LYS:NZ	2.29	0.48
21:L:16:GLU:OE1	21:L:16:GLU:N	2.34	0.48
23:N:6:ASN:O	23:N:10:LYS:HG2	2.14	0.48
33:a:72:LYS:HB3	33:a:74:THR:HG22	1.95	0.48
44:l:43:ASP:HA	44:l:94:VAL:HA	1.95	0.48
4:3:274:A:OP2	4:3:294:G:N1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:427:A:H1'	4:3:447:G:O4'	2.14	0.48
4:3:2299:U:H2'	4:3:2300:A:H8	1.79	0.48
4:3:2623:U:H1'	57:y:4:GLN:HB3	1.95	0.48
6:5:821:U:H2'	6:5:822:A:C8	2.49	0.48
6:5:1045:C:H42	31:Y:46:G:H22	1.61	0.48
6:5:1158:A:O2'	6:5:1159:A:OP1	2.29	0.48
9:8:38:A:H2	21:L:124:LYS:HA	1.78	0.48
11:B:153:LYS:HB3	11:B:204:TRP:HB2	1.96	0.48
12:C:194:SER:O	12:C:197:VAL:HG12	2.14	0.48
40:h:79:ALA:O	40:h:100:LYS:NZ	2.46	0.48
46:n:109:ALA:HB1	46:n:114:LEU:HD12	1.96	0.48
4:3:527:A:N1	50:r:7:GLN:NE2	2.61	0.48
4:3:1230:U:H1'	48:p:3:ILE:HG13	1.96	0.48
4:3:2299:U:OP1	4:3:2388:C:O2'	2.31	0.48
6:5:111:A:H2'	6:5:112:U:O4'	2.13	0.48
7:6:71:C:H3'	7:6:72:C:H6	1.79	0.48
11:B:9:GLY:HA3	22:M:49:TYR:CD1	2.49	0.48
12:C:9:LYS:HE2	12:C:9:LYS:HB3	1.59	0.48
21:L:55:ALA:O	21:L:59:VAL:HG23	2.14	0.48
25:P:21:THR:HG22	25:P:73:LYS:HZ1	1.79	0.48
36:d:171:ARG:HA	36:d:171:ARG:CZ	2.43	0.48
38:f:96:GLN:HE21	38:f:117:VAL:HG21	1.79	0.48
39:g:42:LYS:HZ1	40:h:113:ASN:C	2.19	0.48
41:i:40:ARG:HG2	41:i:40:ARG:HH11	1.79	0.48
50:r:134:LYS:NZ	50:r:134:LYS:HB3	2.29	0.48
4:3:118:G:OP2	4:3:120:A:O2'	2.30	0.47
4:3:230:G:O2'	4:3:232:A:N6	2.46	0.47
60:3:3001:CLM:CL1	32:Z:35:ALA:HB2	2.50	0.47
6:5:516:C:H4'	6:5:517:C:H5''	1.95	0.47
6:5:711:G:H2'	6:5:712:A:C8	2.48	0.47
6:5:1289:U:O2'	6:5:1334:A:N3	2.46	0.47
6:5:1400:A:H2'	6:5:1401:A:C8	2.49	0.47
21:L:95:LEU:HB3	21:L:96:PRO:CD	2.43	0.47
23:N:76:ARG:HG3	23:N:80:LYS:HZ2	1.79	0.47
36:d:68:THR:N	36:d:86:GLY:O	2.28	0.47
36:d:118:SER:C	36:d:120:LYS:H	2.22	0.47
52:t:40:ASN:HB2	52:t:69:ILE:HD11	1.96	0.47
4:3:615:G:H2'	4:3:616:G:H8	1.79	0.47
4:3:1132:C:H3'	4:3:1133:A:H8	1.79	0.47
4:3:1919:A:HO2'	6:5:1469:G:HO2'	1.57	0.47
4:3:2017:G:H5''	50:r:42:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:118:THR:HA	10:A:194:LEU:HD11	1.96	0.47
10:A:178:VAL:HG13	10:A:184:GLU:HG3	1.95	0.47
11:B:134:ARG:HG3	11:B:134:ARG:NH1	2.29	0.47
11:B:136:ALA:O	11:B:139:GLN:HG2	2.14	0.47
14:E:172:ASN:HB3	14:E:175:ARG:HE	1.80	0.47
20:K:22:PRO:HD2	20:K:107:ARG:HH21	1.79	0.47
20:K:52:THR:HG22	20:K:64:LYS:HD3	1.96	0.47
20:K:94:LEU:HD23	20:K:111:VAL:HB	1.95	0.47
24:O:48:CYS:SG	24:O:72:LEU:HD22	2.54	0.47
26:Q:53:LEU:O	26:Q:57:LEU:HD13	2.14	0.47
29:T:35:HIS:C	29:T:35:HIS:CD2	2.91	0.47
34:b:50:THR:HB	34:b:87:MET:HB3	1.96	0.47
34:b:97:THR:HG23	34:b:99:GLN:H	1.78	0.47
35:c:197:LEU:HD13	35:c:199:VAL:HG23	1.96	0.47
44:l:116:LYS:O	44:l:120:ARG:HG2	2.13	0.47
4:3:1603:A:O5'	33:a:63:LYS:NZ	2.47	0.47
4:3:2155:G:H2'	4:3:2156:G:C8	2.50	0.47
5:4:11:A:H2'	5:4:12:U:H5''	1.96	0.47
6:5:998:G:H5'	6:5:999:C:C4	2.49	0.47
6:5:1116:U:C4	18:I:46:LEU:HD21	2.50	0.47
12:C:124:LEU:HD23	12:C:125:ASN:N	2.29	0.47
19:J:115:LYS:HD2	29:T:35:HIS:ND1	2.29	0.47
20:K:78:THR:HG23	20:K:108:TYR:C	2.39	0.47
27:R:12:ASP:OD2	27:R:37:ARG:HD3	2.14	0.47
34:b:50:THR:OG1	34:b:87:MET:O	2.23	0.47
58:z:7:THR:OG1	58:z:49:GLU:OE2	2.19	0.47
4:3:1568:C:H3'	4:3:1569:A:C8	2.49	0.47
4:3:2114:C:H42	4:3:2191:G:H1	1.62	0.47
6:5:196:G:H5'	28:S:49:SER:HA	1.95	0.47
6:5:576:A:O2'	6:5:725:A:N3	2.41	0.47
6:5:787:A:OP1	8:7:38:C:O2'	2.33	0.47
6:5:1205:C:N4	21:L:104:THR:OG1	2.47	0.47
19:J:65:LYS:HA	19:J:68:LYS:HD3	1.95	0.47
5:4:2:U:H2'	5:4:3:U:C6	2.50	0.47
6:5:1269:U:H2'	6:5:1270:C:C6	2.49	0.47
10:A:221:GLN:NE2	10:A:279:SER:HB2	2.30	0.47
11:B:230:PRO:HB2	11:B:231:ASN:H	1.41	0.47
19:J:14:ILE:HD12	19:J:27:ALA:HB2	1.94	0.47
22:M:7:LYS:O	22:M:11:THR:HG23	2.14	0.47
56:x:72:PHE:CD1	56:x:72:PHE:C	2.93	0.47
4:3:12:A:H2'	4:3:13:C:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1415:A:H5'	4:3:1495:A:H1'	1.96	0.47
6:5:433:C:O2'	12:C:151:ILE:HD11	2.15	0.47
6:5:473:A:H2'	6:5:474:G:C8	2.49	0.47
6:5:1138:U:H2'	6:5:1139:A:H8	1.80	0.47
10:A:171:ARG:HG2	10:A:172:LEU:H	1.79	0.47
16:G:15:VAL:O	16:G:19:LEU:HG	2.14	0.47
54:v:37:LYS:HB3	54:v:45:THR:HG22	1.97	0.47
56:x:37:ASP:OD1	56:x:38:ILE:HG13	2.13	0.47
4:3:253:C:O2'	43:k:64:LYS:NZ	2.34	0.47
4:3:700:U:H2'	4:3:701:A:H8	1.80	0.47
4:3:1031:U:HO2'	48:p:92:LYS:NZ	2.12	0.47
4:3:2181:A:H3'	4:3:2182:C:C6	2.49	0.47
4:3:2376:C:H2'	4:3:2377:A:H8	1.80	0.47
4:3:2490:A:O2'	9:8:63:C:O2'	2.24	0.47
6:5:625:U:H2'	6:5:626:G:H8	1.80	0.47
6:5:1343:G:H5''	17:H:116:LYS:HB3	1.95	0.47
6:5:1490:G:H2'	6:5:1491:A:C8	2.50	0.47
9:8:5:C:H2'	9:8:6:U:H6	1.80	0.47
10:A:93:LYS:HE3	10:A:93:LYS:HB2	1.80	0.47
12:C:74:LEU:O	12:C:78:VAL:HG12	2.14	0.47
16:G:19:LEU:HD13	16:G:87:VAL:HG12	1.95	0.47
16:G:38:SER:HG	16:G:40:LEU:HD23	1.80	0.47
17:H:61:LYS:HG2	17:H:63:PHE:CZ	2.50	0.47
21:L:25:ILE:HD13	21:L:29:ARG:HH12	1.79	0.47
24:O:23:ASP:OD1	24:O:24:SER:N	2.46	0.47
27:R:7:LYS:HE2	56:x:72:PHE:CE1	2.50	0.47
29:T:45:LYS:O	29:T:48:ILE:HG12	2.15	0.47
35:c:20:LEU:HD21	35:c:204:LEU:HD11	1.97	0.47
36:d:7:HIS:HA	36:d:10:LYS:HD2	1.96	0.47
36:d:24:SER:OG	36:d:26:MET:SD	2.62	0.47
40:h:128:ALA:O	40:h:132:GLY:N	2.47	0.47
56:x:63:SER:HA	56:x:66:PHE:HD1	1.80	0.47
4:3:125:G:OP1	4:3:1404:C:O2'	2.28	0.47
4:3:1544:G:H2'	4:3:1545:A:H8	1.80	0.47
6:5:927:C:N4	15:F:1:MET:HE3	2.28	0.47
17:H:15:SER:OG	17:H:72:GLY:HA3	2.15	0.47
17:H:86:VAL:O	17:H:90:LEU:HD23	2.15	0.47
20:K:7:LEU:HD12	20:K:12:ARG:HG2	1.97	0.47
34:b:26:ILE:HD12	34:b:192:LEU:HG	1.96	0.47
36:d:96:MET:HG3	36:d:97:TRP:N	2.29	0.47
4:3:1485:A:H4'	4:3:1486:U:C4	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1696:C:O2'	4:3:2695:U:OP1	2.32	0.47
4:3:2452:G:OP2	35:c:69:LYS:HD2	2.15	0.47
4:3:2813:A:H61	4:3:2894:G:H2'	1.79	0.47
6:5:527:G:O6	20:K:59:ASN:HA	2.14	0.47
6:5:1097:G:O3'	11:B:175:ASN:HA	2.15	0.47
7:6:33:U:H4'	15:F:82:SER:HA	1.96	0.47
15:F:45:ALA:O	15:F:49:ILE:HG13	2.15	0.47
28:S:12:ARG:O	28:S:15:ILE:HG22	2.15	0.47
39:g:96:VAL:O	39:g:100:VAL:HG22	2.15	0.47
41:i:80:HIS:HE1	41:i:83:TYR:O	1.98	0.47
4:3:1436:C:H2'	4:3:1437:A:C8	2.50	0.47
6:5:520:C:H41	20:K:63:ARG:NH2	2.13	0.47
6:5:941:A:H2'	6:5:942:G:H8	1.78	0.47
7:6:28:C:H2'	7:6:29:U:C6	2.50	0.47
8:7:46:U:O2'	8:7:47:U:OP1	2.24	0.47
11:B:170:MET:HG3	11:B:171:TYR:N	2.29	0.47
14:E:147:GLU:C	14:E:149:ALA:H	2.22	0.47
17:H:26:ASP:O	17:H:27:LYS:HB2	2.14	0.47
23:N:26:VAL:HG22	23:N:63:LEU:HD11	1.96	0.47
52:t:84:GLN:H	52:t:84:GLN:HG3	1.56	0.47
4:3:615:G:H2'	4:3:616:G:C8	2.50	0.46
4:3:2838:G:H2'	4:3:2883:A:H61	1.80	0.46
6:5:1463:A:H2'	6:5:1464:G:C8	2.50	0.46
11:B:9:GLY:HA3	22:M:49:TYR:HD1	1.80	0.46
12:C:166:PHE:CD1	12:C:182:PRO:HG3	2.50	0.46
14:E:49:ILE:HG23	14:E:83:LEU:HD23	1.97	0.46
14:E:132:VAL:HG12	14:E:132:VAL:O	2.15	0.46
24:O:61:LYS:HA	24:O:61:LYS:HD2	1.60	0.46
43:k:40:LYS:HD2	43:k:46:LEU:HD22	1.97	0.46
48:p:46:TYR:HA	48:p:49:ARG:NH1	2.30	0.46
4:3:1270:C:H2'	4:3:1271:A:H8	1.79	0.46
6:5:354:U:H2'	6:5:355:A:C8	2.50	0.46
6:5:458:G:H2'	6:5:459:C:C6	2.50	0.46
13:D:68:GLU:HB3	13:D:94:VAL:HG12	1.96	0.46
21:L:120:LYS:HG2	27:R:87:ARG:HE	1.80	0.46
32:Z:2:UNK:HA	52:t:50:GLN:HB2	1.97	0.46
33:a:3:ILE:HD13	33:a:210:LEU:HB2	1.98	0.46
36:d:102:LYS:NZ	36:d:139:PRO:HG2	2.30	0.46
38:f:30:LEU:HB3	38:f:36:ALA:HB3	1.97	0.46
4:3:1081:A:H2	39:g:11:VAL:HG11	1.80	0.46
6:5:452:A:OP1	24:O:70:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:63:ARG:NE	15:F:127:SER:OG	2.48	0.46
16:G:14:PRO:O	16:G:41:LYS:HE2	2.15	0.46
34:b:63:ASN:OD1	34:b:64:LYS:N	2.47	0.46
41:i:19:TYR:HD2	41:i:143:LEU:HD22	1.81	0.46
42:j:77:LEU:HD13	47:o:77:LYS:HE2	1.97	0.46
4:3:1117:U:H2'	4:3:1118:U:O4'	2.16	0.46
4:3:1137:C:H2'	4:3:1138:A:C8	2.48	0.46
4:3:1246:U:OP2	48:p:7:LYS:NZ	2.49	0.46
4:3:1306:G:H2'	4:3:1307:G:H8	1.81	0.46
4:3:2254:G:H2'	4:3:2255:A:H8	1.81	0.46
6:5:9:A:O2'	12:C:202:ARG:NH2	2.49	0.46
6:5:677:C:H2'	6:5:678:A:H8	1.80	0.46
10:A:158:ARG:O	10:A:161:LYS:HG2	2.15	0.46
12:C:124:LEU:HD22	12:C:127:ARG:CG	2.45	0.46
13:D:135:SER:HB3	13:D:177:ASP:OD1	2.16	0.46
15:F:112:GLU:HB2	15:F:118:LYS:HG2	1.97	0.46
17:H:45:LEU:O	17:H:48:GLN:HG2	2.15	0.46
21:L:100:GLN:H	21:L:100:GLN:CD	2.23	0.46
27:R:16:LEU:O	27:R:20:ILE:HG13	2.15	0.46
28:S:32:VAL:HG12	28:S:47:VAL:HG13	1.98	0.46
29:T:44:GLU:O	29:T:48:ILE:HG23	2.16	0.46
42:j:17:LYS:N	42:j:45:ASP:O	2.44	0.46
47:o:95:LYS:HA	47:o:95:LYS:HD2	1.72	0.46
54:v:14:TYR:CZ	54:v:28:LYS:HD3	2.50	0.46
4:3:892:G:H2'	4:3:893:A:H8	1.81	0.46
4:3:1413:A:O2'	4:3:1424:U:O2	2.34	0.46
4:3:1812:C:O2	4:3:1819:G:N2	2.32	0.46
4:3:1830:G:OP1	33:a:58:GLN:NE2	2.48	0.46
4:3:2580:A:OP2	34:b:151:ARG:N	2.49	0.46
8:7:74:C:H5''	8:7:75:A:OP2	2.16	0.46
11:B:35:ILE:HG12	22:M:25:GLN:HB2	1.97	0.46
20:K:18:LYS:HB2	20:K:18:LYS:HE2	1.69	0.46
27:R:19:VAL:HG11	27:R:44:PHE:HD1	1.81	0.46
58:z:11:CYS:SG	58:z:12:ASN:N	2.88	0.46
4:3:1440:U:H2'	4:3:1441:A:C8	2.51	0.46
4:3:1529:U:H2'	4:3:1530:G:H8	1.81	0.46
6:5:403:A:H2'	6:5:404:A:C8	2.50	0.46
6:5:515:G:N2	6:5:528:G:OP1	2.47	0.46
6:5:945:U:H3'	21:L:101:ARG:HH22	1.80	0.46
10:A:192:ASN:HD21	10:A:210:LEU:HA	1.81	0.46
15:F:78:ARG:HB3	15:F:83:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:151:GLU:OE2	33:a:154:PRO:HA	2.15	0.46
43:k:47:THR:OG1	43:k:48:ARG:N	2.49	0.46
56:x:62:LEU:O	56:x:66:PHE:CD1	2.69	0.46
4:3:652:U:H2'	4:3:653:G:H8	1.81	0.46
6:5:61:A:N1	6:5:92:G:O2'	2.47	0.46
6:5:943:C:H2'	6:5:944:A:H8	1.81	0.46
10:A:18:VAL:HG11	10:A:231:LEU:HD11	1.98	0.46
16:G:63:LYS:HG3	16:G:63:LYS:O	2.15	0.46
35:c:112:LEU:HD23	35:c:211:PHE:HE1	1.80	0.46
42:j:104:ARG:HH12	42:j:121:VAL:CG1	2.29	0.46
51:s:58:LEU:HB2	51:s:80:LEU:HB2	1.97	0.46
51:s:66:ARG:HA	51:s:66:ARG:HD2	1.59	0.46
56:x:2:LYS:HG3	56:x:3:LYS:H	1.81	0.46
4:3:50:G:H22	4:3:180:A:H5''	1.81	0.46
4:3:524:G:N2	4:3:527:A:OP2	2.32	0.46
4:3:1096:U:C5	40:h:11:LYS:HG3	2.50	0.46
4:3:1124:G:N2	4:3:1125:U:O4	2.48	0.46
4:3:2299:U:O2'	4:3:2382:A:N3	2.47	0.46
4:3:2797:C:H5'	4:3:2798:A:O5'	2.16	0.46
6:5:96:G:H1	6:5:326:C:H41	1.63	0.46
6:5:378:A:H2'	6:5:379:A:C8	2.50	0.46
6:5:399:C:OP1	12:C:133:SER:HB3	2.16	0.46
6:5:1166:A:H5''	11:B:4:LYS:HE3	1.98	0.46
12:C:102:TYR:CD2	12:C:110:ARG:HB2	2.50	0.46
14:E:71:ASP:N	14:E:71:ASP:OD1	2.47	0.46
19:J:106:LYS:HB3	19:J:106:LYS:HE3	1.55	0.46
20:K:62:LEU:O	20:K:64:LYS:NZ	2.45	0.46
21:L:20:THR:HG22	21:L:27:LEU:HA	1.98	0.46
22:M:19:ARG:HH11	22:M:19:ARG:HG3	1.81	0.46
40:h:123:MET:O	40:h:127:THR:HG22	2.16	0.46
45:m:33:THR:OG1	45:m:34:THR:N	2.49	0.46
46:n:4:ARG:HH12	46:n:36:LEU:HD11	1.80	0.46
51:s:85:LEU:HB3	51:s:89:ILE:HG23	1.96	0.46
4:3:333:A:N3	4:3:353:G:O2'	2.43	0.46
4:3:917:G:H2'	4:3:918:G:H8	1.81	0.46
4:3:1093:U:H3	4:3:1115:G:H1	1.62	0.46
4:3:1121:A:H5''	4:3:1122:G:H5'	1.97	0.46
4:3:1296:G:O2'	4:3:2019:G:O6	2.29	0.46
4:3:1436:C:H2'	4:3:1437:A:H8	1.80	0.46
6:5:521:A:H61	20:K:102:ASP:CG	2.20	0.46
6:5:1022:G:H21	6:5:1026:A:H62	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:1202:A:OP2	21:L:110:LYS:NZ	2.32	0.46
8:7:50:G:H2'	8:7:51:G:C8	2.51	0.46
10:A:49:ARG:CG	10:A:50:LYS:H	2.25	0.46
20:K:55:PRO:HB3	20:K:102:ASP:HB3	1.98	0.46
23:N:26:VAL:HG22	23:N:63:LEU:CD1	2.45	0.46
35:c:191:LEU:HD23	35:c:191:LEU:HA	1.81	0.46
53:u:61:PRO:HB3	53:u:65:VAL:HG12	1.98	0.46
56:x:45:PHE:CE1	56:x:50:LEU:HB2	2.51	0.46
4:3:1306:G:H4'	45:m:31:ILE:HD12	1.97	0.46
4:3:1797:C:O2'	33:a:216:ALA:HB2	2.16	0.46
6:5:265:U:H2'	6:5:266:A:C8	2.51	0.46
6:5:821:U:H2'	6:5:822:A:H8	1.80	0.46
6:5:945:U:H2'	6:5:946:G:H8	1.80	0.46
10:A:43:PHE:CE2	14:E:173:PRO:HD2	2.50	0.46
10:A:234:ASP:OD1	10:A:245:MET:N	2.30	0.46
11:B:74:PRO:HB3	11:B:106:ILE:HD11	1.97	0.46
12:C:8:PHE:CE1	12:C:23:LYS:HD2	2.51	0.46
16:G:78:GLN:OE1	16:G:78:GLN:HA	2.15	0.46
17:H:82:ARG:O	17:H:85:ILE:HG22	2.16	0.46
19:J:76:LYS:NZ	19:J:102:GLU:OE1	2.49	0.46
28:S:3:ASN:C	28:S:4:ILE:HD13	2.41	0.46
28:S:56:ARG:HH12	28:S:57:LYS:NZ	2.13	0.46
33:a:177:GLY:O	33:a:178:LYS:HG2	2.16	0.46
34:b:16:VAL:HG13	34:b:26:ILE:HD13	1.97	0.46
36:d:45:ARG:HG3	36:d:46:ASP:N	2.30	0.46
44:l:43:ASP:OD2	44:l:45:ARG:NH1	2.49	0.46
4:3:355:A:O2'	4:3:374:A:N3	2.47	0.45
4:3:700:U:H5''	43:k:46:LEU:HD12	1.97	0.45
4:3:1092:A:H2'	4:3:1093:U:C6	2.51	0.45
4:3:1103:G:O2'	4:3:1104:A:H5'	2.16	0.45
10:A:202:CYS:HB3	10:A:206:THR:OG1	2.15	0.45
11:B:136:ALA:HA	11:B:139:GLN:NE2	2.30	0.45
17:H:78:ALA:O	17:H:82:ARG:HG2	2.16	0.45
26:Q:50:ARG:HB3	26:Q:50:ARG:CZ	2.46	0.45
28:S:35:PHE:CD2	28:S:47:VAL:HG21	2.51	0.45
36:d:140:GLU:OE2	56:x:27:SER:HB2	2.17	0.45
52:t:24:VAL:HG22	52:t:36:VAL:HG12	1.98	0.45
4:3:2254:G:H2'	4:3:2255:A:C8	2.51	0.45
64:3:3226:SPM:H92	64:3:3226:SPM:H121	1.76	0.45
6:5:117:U:H2'	6:5:118:C:C6	2.51	0.45
6:5:433:C:H1'	12:C:153:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:293:ARG:HH12	29:T:54:ARG:CZ	2.30	0.45
12:C:184:ARG:HD2	12:C:192:ASN:CG	2.40	0.45
13:D:91:LEU:HD21	13:D:192:ILE:HD12	1.98	0.45
25:P:31:LYS:HE3	25:P:36:HIS:HB3	1.98	0.45
34:b:30:TYR:OH	34:b:189:MET:HE3	2.17	0.45
34:b:106:GLU:HA	34:b:217:VAL:HA	1.99	0.45
35:c:128:VAL:O	35:c:200:GLU:HA	2.17	0.45
46:n:29:VAL:HG21	46:n:46:PHE:CD2	2.52	0.45
57:y:53:VAL:HG12	57:y:54:LYS:CG	2.44	0.45
2:1:19:ILE:HD12	2:1:47:VAL:HG21	1.97	0.45
4:3:1343:C:O2'	4:3:1420:A:N3	2.41	0.45
4:3:2158:C:H2'	4:3:2159:U:C6	2.52	0.45
4:3:2477:A:H4'	44:l:56:LYS:HD2	1.98	0.45
64:3:3248:SPM:H62	64:3:3248:SPM:H92	1.78	0.45
6:5:663:G:H21	23:N:48:ILE:HD12	1.81	0.45
6:5:989:A:O2'	22:M:12:ARG:NH1	2.50	0.45
6:5:1201:C:P	21:L:90:ARG:HH12	2.39	0.45
7:6:37:A:H2'	7:6:38:C:C6	2.51	0.45
10:A:208:PRO:HG2	14:E:174:TYR:HE2	1.81	0.45
17:H:117:LYS:HB2	17:H:120:LEU:HD22	1.99	0.45
24:O:39:LEU:HD12	24:O:40:ASN:N	2.31	0.45
27:R:20:ILE:HG12	27:R:43:GLU:OE2	2.16	0.45
47:o:56:ARG:HG2	47:o:57:GLY:N	2.31	0.45
48:p:64:LEU:O	48:p:68:LEU:HD23	2.16	0.45
48:p:86:ASN:HB2	49:q:47:ALA:HB1	1.98	0.45
4:3:411:U:H2'	4:3:412:A:H8	1.82	0.45
4:3:1091:G:H4'	4:3:1121:A:H8	1.82	0.45
4:3:2181:A:H8	4:3:2181:A:OP2	1.99	0.45
6:5:836:C:H1'	14:E:145:ARG:HG2	1.98	0.45
6:5:1071:A:H5''	13:D:76:ILE:HD12	1.99	0.45
13:D:131:ILE:HG22	13:D:175:TYR:CE1	2.52	0.45
14:E:28:THR:HG21	14:E:72:PHE:HA	1.98	0.45
36:d:15:GLU:HG3	36:d:16:LEU:HD22	1.99	0.45
41:i:7:LEU:HD12	48:p:63:ARG:NH1	2.31	0.45
43:k:34:ARG:HB3	43:k:41:ALA:HA	1.98	0.45
55:w:13:GLU:HG2	55:w:14:GLU:N	2.31	0.45
1:0:48:ARG:HH12	4:3:1339:U:H2'	1.81	0.45
4:3:340:U:H2'	4:3:341:G:O4'	2.17	0.45
13:D:131:ILE:C	13:D:132:HIS:HD2	2.24	0.45
34:b:14:SER:OG	34:b:15:GLN:N	2.49	0.45
35:c:162:ASN:O	35:c:162:ASN:ND2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:108:LEU:HB3	36:d:114:PHE:HE2	1.80	0.45
39:g:18:LEU:HD13	39:g:68:PHE:HE2	1.80	0.45
39:g:116:ARG:HE	39:g:116:ARG:HB3	1.66	0.45
45:m:21:GLN:HB3	45:m:41:THR:HG21	1.98	0.45
46:n:37:ASN:C	46:n:38:HIS:HD2	2.25	0.45
51:s:44:PHE:CE2	51:s:85:LEU:HD11	2.51	0.45
4:3:583:U:O4	41:i:3:LYS:HD3	2.17	0.45
4:3:652:U:H2'	4:3:653:G:C8	2.51	0.45
4:3:668:A:H2'	4:3:669:A:C8	2.52	0.45
4:3:1045:A:N3	4:3:1188:C:O2'	2.46	0.45
4:3:1797:C:H2'	4:3:1798:A:C8	2.52	0.45
6:5:499:U:H2'	6:5:500:G:C8	2.52	0.45
6:5:704:U:H2'	6:5:705:A:H8	1.82	0.45
8:7:34:G:O6	31:Y:42:U:O4	2.35	0.45
12:C:149:ILE:HD11	12:C:174:PHE:CE2	2.51	0.45
14:E:17:GLN:OE1	14:E:17:GLN:HA	2.16	0.45
16:G:44:ILE:CG2	16:G:122:VAL:HG11	2.45	0.45
35:c:60:GLY:HA3	35:c:80:ARG:HD3	1.98	0.45
41:i:99:GLN:O	41:i:99:GLN:HG2	2.17	0.45
45:m:46:ASP:O	45:m:50:THR:HG22	2.17	0.45
4:3:54:A:OP2	4:3:118:G:N1	2.40	0.45
4:3:933:A:H2'	4:3:933:A:N3	2.32	0.45
4:3:1583:G:H2'	4:3:1584:U:C6	2.52	0.45
4:3:2409:U:OP1	58:z:40:ARG:NH2	2.48	0.45
6:5:507:A:H5''	12:C:51:ALA:HB2	1.99	0.45
6:5:1024:U:O2'	6:5:1025:U:OP1	2.33	0.45
9:8:28:A:H2'	9:8:29:U:H6	1.81	0.45
10:A:131:ASN:O	10:A:135:GLU:HG2	2.17	0.45
12:C:31:ARG:HG2	12:C:33:THR:HG22	1.99	0.45
12:C:96:ARG:HB2	12:C:99:ASN:HB3	1.99	0.45
17:H:79:GLY:O	17:H:82:ARG:HG3	2.16	0.45
26:Q:94:ARG:HB3	26:Q:101:PHE:CE1	2.51	0.45
35:c:154:ASP:OD1	35:c:154:ASP:N	2.34	0.45
42:j:73:ASP:N	42:j:73:ASP:OD1	2.50	0.45
43:k:120:LEU:HD23	43:k:120:LEU:H	1.82	0.45
47:o:24:GLU:HA	47:o:55:ARG:HH12	1.82	0.45
3:2:9:PRO:HD3	3:2:16:ILE:HD11	1.98	0.45
4:3:558:C:H1'	4:3:587:U:H1'	1.99	0.45
4:3:2797:C:O2	4:3:2895:A:O2'	2.25	0.45
6:5:233:C:H5''	25:P:41:ARG:HH12	1.82	0.45
6:5:374:G:H2'	6:5:375:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:159:ARG:NH2	11:B:163:ALA:O	2.45	0.45
13:D:71:VAL:HG11	13:D:192:ILE:HD11	1.98	0.45
15:F:55:GLU:HG2	15:F:56:LYS:H	1.81	0.45
18:I:7:VAL:HG13	18:I:8:LYS:N	2.32	0.45
18:I:55:ILE:HG21	22:M:34:LEU:HD21	1.97	0.45
21:L:65:ILE:HG22	21:L:67:GLY:H	1.82	0.45
24:O:47:LYS:HE3	24:O:47:LYS:HB2	1.83	0.45
33:a:73:ARG:HH21	33:a:123:ALA:HB2	1.80	0.45
36:d:4:LEU:O	36:d:4:LEU:HD23	2.17	0.45
36:d:12:ILE:O	36:d:16:LEU:HB2	2.17	0.45
54:v:15:GLY:HA3	54:v:29:TRP:HZ3	1.82	0.45
4:3:963:U:H2'	4:3:964:A:H8	1.82	0.45
4:3:2137:A:OP1	4:3:2139:C:O2'	2.33	0.45
6:5:57:U:H2'	6:5:58:G:C8	2.51	0.45
6:5:664:A:H2'	6:5:665:G:H8	1.82	0.45
6:5:991:A:H2'	6:5:992:U:C6	2.51	0.45
11:B:167:ARG:NH2	31:Y:50:U:O2	2.50	0.45
18:I:24:LEU:HD11	18:I:78:ARG:CG	2.47	0.45
19:J:86:LYS:NZ	29:T:26:ARG:HH21	2.14	0.45
21:L:89:LEU:O	21:L:92:ARG:HB3	2.17	0.45
38:f:130:ILE:HB	38:f:142:VAL:HB	1.98	0.45
4:3:610:G:H5''	4:3:2510:G:C2	2.52	0.45
4:3:755:C:H2'	4:3:756:A:H8	1.80	0.45
6:5:499:U:H2'	6:5:500:G:H8	1.82	0.45
6:5:1126:U:O4	6:5:1127:A:N6	2.50	0.45
6:5:1384:A:H2'	6:5:1385:A:C8	2.51	0.45
11:B:184:ASP:OD1	11:B:210:ILE:HB	2.17	0.45
13:D:78:LYS:HG2	13:D:85:ASN:HB2	1.98	0.45
13:D:212:ARG:HA	16:G:75:LYS:NZ	2.32	0.45
14:E:50:LYS:HA	14:E:50:LYS:HD2	1.69	0.45
17:H:77:GLN:O	17:H:81:ILE:HG12	2.17	0.45
34:b:22:GLU:HG2	42:j:72:LYS:HE3	1.97	0.45
39:g:42:LYS:HZ3	39:g:42:LYS:HG3	1.70	0.45
40:h:56:THR:O	40:h:58:TYR:CD2	2.70	0.45
46:n:110:ARG:HG3	46:n:116:PHE:CE1	2.52	0.45
50:r:125:VAL:O	50:r:129:VAL:HG23	2.17	0.45
4:3:223:A:N3	4:3:238:U:O2'	2.43	0.44
4:3:2027:G:H5'	57:y:9:SER:HB3	1.99	0.44
4:3:2653:G:OP2	4:3:2653:G:N2	2.29	0.44
6:5:1316:C:H2'	6:5:1317:A:C8	2.51	0.44
13:D:165:ALA:HB3	13:D:191:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:93:GLU:OE2	14:E:96:TYR:HB2	2.18	0.44
16:G:98:TYR:C	16:G:99:ARG:HD2	2.42	0.44
16:G:118:THR:OG1	16:G:119:SER:N	2.50	0.44
26:Q:67:TYR:CE1	29:T:2:PRO:HA	2.53	0.44
48:p:97:LEU:HD11	49:q:4:ILE:HD11	1.98	0.44
48:p:101:GLU:OE1	48:p:104:LYS:HE3	2.18	0.44
4:3:1437:A:H2'	4:3:1438:G:C8	2.52	0.44
4:3:2036:G:N1	4:3:2040:A:OP2	2.34	0.44
4:3:2177:G:H1'	7:6:56:U:OP1	2.17	0.44
6:5:649:U:H4'	16:G:67:LYS:HE2	2.00	0.44
6:5:737:U:OP2	23:N:2:GLN:NE2	2.50	0.44
6:5:1505:G:H2'	6:5:1506:A:C8	2.52	0.44
10:A:84:PHE:N	10:A:84:PHE:CD1	2.85	0.44
12:C:13:ARG:HE	12:C:35:PRO:HD2	1.81	0.44
13:D:95:GLY:N	13:D:172:LEU:HD12	2.32	0.44
14:E:140:GLN:HB2	14:E:141:PRO:HD2	1.99	0.44
15:F:49:ILE:HD11	15:F:123:ILE:HD12	1.99	0.44
20:K:37:ASN:O	20:K:37:ASN:OD1	2.35	0.44
35:c:125:THR:HG22	35:c:125:THR:O	2.17	0.44
37:e:120:ILE:HA	37:e:147:PHE:HE2	1.83	0.44
45:m:106:ARG:HG3	45:m:113:MET:SD	2.57	0.44
47:o:42:LYS:HG2	47:o:43:VAL:H	1.82	0.44
49:q:12:TYR:CZ	49:q:22:VAL:HG12	2.53	0.44
49:q:19:THR:HG22	49:q:93:LYS:HB2	1.99	0.44
55:w:20:ILE:HD11	55:w:69:GLN:HG3	1.99	0.44
1:0:6:GLN:O	4:3:721:G:H8	2.00	0.44
4:3:569:U:H2'	4:3:570:C:C6	2.51	0.44
4:3:2179:A:H1'	4:3:2180:U:C6	2.53	0.44
4:3:2372:C:H2'	4:3:2373:G:O4'	2.17	0.44
6:5:712:A:H2'	6:5:713:A:C8	2.52	0.44
17:H:12:ARG:NE	17:H:13:LYS:HG3	2.32	0.44
19:J:86:LYS:HB2	19:J:86:LYS:HE3	1.78	0.44
36:d:163:ASP:OD1	36:d:164:SER:N	2.49	0.44
36:d:178:VAL:C	36:d:179:LYS:HG2	2.42	0.44
39:g:60:ARG:O	39:g:64:LYS:HG2	2.17	0.44
41:i:78:TYR:HE1	41:i:89:LYS:HB3	1.81	0.44
49:q:67:LYS:HD2	49:q:86:ARG:HD2	1.98	0.44
4:3:2190:G:H2'	4:3:2191:G:C8	2.53	0.44
4:3:2459:A:C2	60:3:3001:CLM:H8	2.52	0.44
6:5:369:A:H2'	6:5:370:A:H8	1.83	0.44
6:5:1088:C:H5''	10:A:154:ARG:HH22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:1225:A:H4'	17:H:72:GLY:N	2.32	0.44
10:A:171:ARG:HG2	10:A:172:LEU:N	2.32	0.44
12:C:49:GLY:O	12:C:53:GLN:HB2	2.18	0.44
16:G:16:ALA:HA	16:G:19:LEU:HB2	2.00	0.44
16:G:104:LEU:HD23	16:G:104:LEU:HA	1.83	0.44
25:P:1:MET:HE3	25:P:3:ARG:HB2	1.99	0.44
25:P:32:HIS:CG	25:P:33:PRO:HD3	2.52	0.44
36:d:33:LYS:HG3	36:d:157:VAL:HG21	1.99	0.44
40:h:58:TYR:HE1	40:h:60:ASP:HB3	1.76	0.44
48:p:27:ARG:HD3	48:p:37:THR:HG21	1.98	0.44
53:u:55:ARG:HD3	53:u:55:ARG:HA	1.78	0.44
55:w:8:ARG:HD2	55:w:57:ILE:HG12	2.00	0.44
4:3:1135:C:H2'	4:3:1136:U:O4'	2.17	0.44
4:3:1803:U:H3	4:3:1830:G:H1	1.64	0.44
4:3:2540:G:N2	4:3:2671:G:O2'	2.51	0.44
6:5:487:A:O2'	6:5:488:U:O3'	2.36	0.44
6:5:1001:A:N7	6:5:1020:G:N2	2.65	0.44
6:5:1078:G:H5'	6:5:1078:G:C8	2.51	0.44
11:B:104:LEU:HG	11:B:231:ASN:ND2	2.32	0.44
12:C:12:ARG:HG2	12:C:33:THR:O	2.18	0.44
13:D:101:ILE:HG23	13:D:196:MET:HE1	1.99	0.44
14:E:153:LYS:HG3	14:E:153:LYS:O	2.18	0.44
21:L:7:ILE:H	21:L:7:ILE:HD12	1.83	0.44
25:P:56:LYS:H	25:P:56:LYS:HD2	1.81	0.44
35:c:4:LEU:HD12	35:c:4:LEU:HA	1.83	0.44
38:f:58:TYR:HA	38:f:61:ASN:HD21	1.83	0.44
40:h:61:LYS:HA	40:h:63:PHE:CE1	2.53	0.44
44:l:36:ALA:HB2	44:l:103:MET:HE2	2.00	0.44
52:t:1:MET:HG2	52:t:2:GLN:N	2.27	0.44
4:3:1529:U:H2'	4:3:1530:G:C8	2.52	0.44
4:3:1697:C:HO2'	4:3:1698:A:H8	1.63	0.44
4:3:1830:G:N2	33:a:262:HIS:HE1	2.15	0.44
4:3:2606:A:H5''	33:a:242:GLY:HA3	2.00	0.44
6:5:22:G:O6	13:D:185:ARG:NH2	2.48	0.44
6:5:916:U:O2	13:D:79:THR:OG1	2.31	0.44
6:5:966:A:O2'	65:5:1603:SPD:N1	2.51	0.44
8:7:73:C:H41	53:u:18:LYS:HG3	1.81	0.44
21:L:29:ARG:O	21:L:33:ILE:HG13	2.17	0.44
33:a:252:ASP:OD1	33:a:252:ASP:N	2.40	0.44
37:e:105:THR:HG22	37:e:119:LYS:HD3	1.99	0.44
38:f:5:LEU:HD23	38:f:5:LEU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:g:43:LYS:HE3	39:g:43:LYS:HB3	1.89	0.44
44:l:52:ILE:HG22	44:l:56:LYS:HE2	1.98	0.44
4:3:603:G:H2'	4:3:2037:A:N7	2.32	0.44
4:3:2863:G:H8	4:3:2863:G:OP2	2.00	0.44
64:3:3240:SPM:H121	64:3:3240:SPM:H92	1.76	0.44
6:5:476:U:H5'	6:5:477:U:OP1	2.18	0.44
6:5:1197:G:OP1	6:5:1295:U:O2'	2.33	0.44
7:6:20:U:O2'	7:6:21:A:H4'	2.18	0.44
12:C:91:ARG:HD2	12:C:181:PHE:HB2	1.99	0.44
26:Q:39:LYS:HD3	26:Q:39:LYS:HA	1.66	0.44
35:c:194:ALA:O	35:c:195:ASN:HB3	2.17	0.44
36:d:112:ARG:HE	36:d:112:ARG:HB2	1.54	0.44
43:k:39:GLN:NE2	43:k:47:THR:HG22	2.32	0.44
51:s:63:THR:H	51:s:75:SER:HB3	1.83	0.44
52:t:36:VAL:HG23	52:t:39:LEU:HB2	2.00	0.44
4:3:1091:G:H4'	4:3:1121:A:C8	2.52	0.44
4:3:1102:A:H2'	4:3:1102:A:N3	2.32	0.44
6:5:470:U:O4	6:5:471:A:N6	2.50	0.44
7:6:18:G:H1	7:6:55:U:H1'	1.83	0.44
9:8:18:G:N2	9:8:58:A:OP2	2.46	0.44
15:F:94:ARG:HH11	15:F:94:ARG:HG3	1.83	0.44
15:F:113:LYS:O	15:F:118:LYS:HE2	2.18	0.44
16:G:98:TYR:O	16:G:99:ARG:HD2	2.18	0.44
20:K:64:LYS:O	20:K:80:ILE:HD12	2.18	0.44
34:b:123:ILE:HG23	34:b:128:PHE:O	2.18	0.44
35:c:14:GLU:HG3	35:c:16:GLU:H	1.83	0.44
36:d:34:ILE:HG23	36:d:155:THR:O	2.17	0.44
43:k:13:ARG:HD2	43:k:13:ARG:HA	1.61	0.44
46:n:114:LEU:HD23	46:n:114:LEU:HA	1.86	0.44
4:3:680:A:H2'	4:3:682:A:N7	2.33	0.44
4:3:799:A:H5''	33:a:217:GLY:CA	2.48	0.44
4:3:1801:U:H2'	4:3:1802:C:C6	2.52	0.44
6:5:214:U:H2'	6:5:215:C:H6	1.83	0.44
6:5:707:G:H2'	6:5:708:A:H8	1.83	0.44
6:5:725:A:H2'	6:5:726:A:C8	2.52	0.44
6:5:1026:A:N3	6:5:1026:A:H2'	2.33	0.44
6:5:1032:G:H2'	6:5:1033:U:O4'	2.18	0.44
6:5:1332:U:H3	6:5:1338:A:H61	1.64	0.44
12:C:69:LYS:HG2	12:C:70:GLN:N	2.33	0.44
12:C:75:PHE:CD1	12:C:75:PHE:C	2.96	0.44
14:E:117:GLU:HG3	14:E:121:ARG:HH21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:66:THR:O	19:J:70:MET:HG3	2.18	0.44
27:R:19:VAL:HG21	27:R:44:PHE:CE1	2.53	0.44
36:d:100:LEU:O	36:d:104:ILE:HG22	2.18	0.44
4:3:356:A:OP2	35:c:174:ASN:HB2	2.18	0.43
4:3:894:G:N3	4:3:2276:A:H2'	2.32	0.43
6:5:311:A:O2'	6:5:326:C:O2'	2.37	0.43
6:5:331:C:H2'	6:5:332:A:C8	2.52	0.43
6:5:1472:G:H1'	6:5:1493:MA6:H2	2.00	0.43
9:8:74:C:OP1	9:8:75:C:H5'	2.18	0.43
10:A:288:PRO:HB3	29:T:57:ARG:HE	1.82	0.43
15:F:154:ARG:HG3	15:F:155:TRP:H	1.83	0.43
21:L:14:ARG:HG2	21:L:44:ARG:HD3	2.00	0.43
23:N:3:ILE:HG21	23:N:31:SER:OG	2.18	0.43
29:T:57:ARG:HB3	29:T:57:ARG:HH11	1.82	0.43
4:3:703:A:H2'	4:3:705:A:H62	1.83	0.43
4:3:1119:A:C4	39:g:53:VAL:HG21	2.52	0.43
4:3:2394:A:O2'	53:u:70:ASP:OD1	2.32	0.43
4:3:2530:U:O2'	4:3:2655:U:OP1	2.33	0.43
4:3:2548:G:O2'	4:3:2748:A:N3	2.46	0.43
4:3:2863:G:H2'	4:3:2864:A:C8	2.53	0.43
6:5:595:G:N2	16:G:98:TYR:OH	2.47	0.43
6:5:1385:A:H2'	6:5:1386:C:C6	2.53	0.43
7:6:15:A:H2'	7:6:16:C:C4	2.53	0.43
10:A:26:MET:HG2	10:A:227:LEU:HD22	1.99	0.43
10:A:68:ALA:O	10:A:72:VAL:HG12	2.18	0.43
10:A:293:ARG:HE	29:T:50:GLN:CG	2.21	0.43
25:P:52:GLU:HG2	25:P:52:GLU:O	2.16	0.43
27:R:35:SER:HG	27:R:38:SER:HG	1.52	0.43
34:b:6:ILE:HG22	34:b:207:ILE:HB	1.99	0.43
50:r:50:LEU:HD23	50:r:50:LEU:HA	1.89	0.43
56:x:61:LYS:HG3	56:x:62:LEU:HD12	2.00	0.43
4:3:1414:C:H2'	4:3:1415:A:C8	2.52	0.43
6:5:483:U:H2'	6:5:484:A:H8	1.82	0.43
8:7:35:U:H2'	8:7:36:C:C6	2.52	0.43
10:A:30:VAL:HG13	10:A:53:ASN:HB3	2.00	0.43
10:A:282:LEU:HB3	10:A:283:ASN:H	1.52	0.43
11:B:133:LEU:O	11:B:137:MET:HG3	2.18	0.43
12:C:92:VAL:O	12:C:96:ARG:NH1	2.51	0.43
17:H:41:PHE:C	17:H:43:ASN:N	2.77	0.43
20:K:86:ASN:CG	20:K:118:VAL:HG22	2.44	0.43
33:a:189:THR:HB	33:a:279:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:h:84:LYS:HA	40:h:84:LYS:HD2	1.90	0.43
43:k:115:ILE:HD13	43:k:115:ILE:HA	1.90	0.43
4:3:356:A:H5'	4:3:374:A:H1'	2.00	0.43
4:3:610:G:H2'	4:3:611:A:C8	2.54	0.43
4:3:764:G:OP1	33:a:10:SER:OG	2.36	0.43
4:3:916:U:H2'	4:3:917:G:C8	2.54	0.43
4:3:1575:C:H2'	4:3:1576:G:O4'	2.19	0.43
4:3:2438:A:H2'	4:3:2438:A:N3	2.33	0.43
6:5:36:G:N2	20:K:128:SER:OG	2.34	0.43
6:5:1019:G:OP2	6:5:1019:G:H8	2.02	0.43
9:8:37:A:H3'	9:8:38:A:H8	1.82	0.43
10:A:293:ARG:CZ	29:T:50:GLN:HG2	2.48	0.43
21:L:27:LEU:O	21:L:31:GLN:HG3	2.18	0.43
23:N:21:SER:O	23:N:25:GLN:HG3	2.17	0.43
23:N:22:ILE:H	23:N:22:ILE:HD12	1.83	0.43
24:O:77:GLY:O	24:O:81:LYS:HE3	2.18	0.43
56:x:6:HIS:O	56:x:8:PRO:HD3	2.18	0.43
4:3:756:A:H2'	4:3:757:A:C8	2.53	0.43
4:3:831:U:H2'	4:3:832:C:C6	2.52	0.43
4:3:1691:U:H2'	4:3:1692:A:C8	2.53	0.43
4:3:2358:U:H2'	4:3:2359:G:O4'	2.18	0.43
65:3:3249:SPD:C3	34:b:133:LEU:HD13	2.49	0.43
6:5:260:C:H2'	6:5:261:G:O4'	2.17	0.43
6:5:500:G:OP1	20:K:128:SER:HB3	2.18	0.43
6:5:673:A:H2'	6:5:674:U:H6	1.83	0.43
6:5:1000:A:O2'	6:5:1029:C:O2'	2.17	0.43
6:5:1214:A:H62	6:5:1273:A:N6	2.16	0.43
21:L:14:ARG:CD	21:L:42:ASP:HA	2.44	0.43
24:O:5:ARG:HA	24:O:69:VAL:HG21	2.01	0.43
24:O:69:VAL:HG12	24:O:73:PHE:CE2	2.53	0.43
24:O:73:PHE:HB3	24:O:78:LEU:HB3	2.01	0.43
25:P:60:LYS:HE2	25:P:82:GLU:HB2	2.01	0.43
26:Q:56:ASP:HB2	26:Q:59:ALA:HB3	2.01	0.43
27:R:7:LYS:HA	27:R:7:LYS:HD2	1.79	0.43
31:Y:54:A:H1'	31:Y:55:A:C8	2.53	0.43
48:p:73:MET:HE3	48:p:78:PHE:HD1	1.83	0.43
4:3:1128:G:H2'	4:3:1129:U:C6	2.54	0.43
6:5:369:A:H61	6:5:387:G:H1'	1.83	0.43
6:5:561:A:H2	20:K:12:ARG:NH1	2.17	0.43
6:5:961:G:N2	8:7:34:G:H5'	2.34	0.43
6:5:1200:G:H4'	27:R:78:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:41:A:H2'	9:8:42:U:O4'	2.18	0.43
18:I:7:VAL:HG13	18:I:8:LYS:H	1.84	0.43
18:I:50:THR:HG22	18:I:76:HIS:HA	2.00	0.43
20:K:56:LYS:HB2	20:K:56:LYS:HE2	1.90	0.43
23:N:9:ILE:O	23:N:13:GLN:HG2	2.19	0.43
28:S:44:LEU:HD22	28:S:76:LEU:HD22	1.99	0.43
42:j:22:ILE:HD11	42:j:42:SER:HB3	2.00	0.43
44:l:38:LYS:HE2	44:l:38:LYS:HB3	1.88	0.43
47:o:85:ASN:O	47:o:86:ILE:HD13	2.19	0.43
4:3:1598:U:H2'	4:3:1599:C:C6	2.54	0.43
6:5:380:G:H2'	6:5:381:C:O4'	2.19	0.43
12:C:19:LEU:HD21	12:C:188:PRO:HG3	1.99	0.43
21:L:79:HIS:CE1	21:L:83:ILE:HD11	2.54	0.43
22:M:53:ILE:O	22:M:56:VAL:HG22	2.19	0.43
26:Q:64:LEU:CD1	26:Q:99:VAL:HG11	2.48	0.43
48:p:45:ALA:O	48:p:49:ARG:HG3	2.19	0.43
55:w:65:TRP:CE2	55:w:66:GLN:HG3	2.53	0.43
4:3:299:A:H2'	4:3:300:G:C8	2.54	0.43
4:3:2081:U:O2'	4:3:2605:G:O2'	2.29	0.43
4:3:2565:G:H2'	4:3:2566:C:C6	2.54	0.43
4:3:2811:G:H2'	4:3:2812:U:C6	2.53	0.43
5:4:104:C:H2'	5:4:105:A:C8	2.54	0.43
6:5:214:U:H2'	6:5:215:C:C6	2.53	0.43
13:D:162:ALA:O	13:D:167:ARG:HD3	2.19	0.43
13:D:197:ASP:O	13:D:201:LYS:HG2	2.19	0.43
15:F:19:ASN:OD1	15:F:21:LEU:HB3	2.19	0.43
17:H:44:LYS:O	17:H:45:LEU:HB3	2.18	0.43
35:c:209:GLY:O	35:c:212:LYS:HG3	2.19	0.43
38:f:92:ILE:O	38:f:121:PHE:HE1	2.02	0.43
39:g:10:GLN:O	39:g:14:VAL:HG22	2.19	0.43
40:h:30:ILE:HG23	40:h:63:PHE:CD1	2.53	0.43
43:k:3:LEU:HD23	43:k:3:LEU:HA	1.87	0.43
48:p:43:LYS:HE2	49:q:73:HIS:HB3	2.01	0.43
4:3:749:U:H1'	4:3:752:C:H5	1.83	0.43
4:3:901:C:H4'	4:3:902:U:O5'	2.19	0.43
4:3:1096:U:H5	40:h:11:LYS:HG3	1.82	0.43
4:3:1437:A:H2'	4:3:1438:G:H8	1.84	0.43
4:3:2081:U:H2'	4:3:2082:U:C6	2.53	0.43
4:3:2132:G:H1'	4:3:2181:A:H62	1.84	0.43
4:3:2758:A:OP2	37:e:65:LYS:NZ	2.45	0.43
6:5:648:C:H2'	6:5:649:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:123:MET:HG2	16:G:127:VAL:HG13	2.01	0.43
31:Y:49:U:O2	31:Y:50:U:N3	2.52	0.43
34:b:13:MET:HB2	34:b:13:MET:HE3	1.71	0.43
34:b:19:THR:HB	34:b:221:GLU:HG2	2.01	0.43
38:f:16:PHE:HE2	38:f:55:GLN:HA	1.84	0.43
39:g:123:LEU:O	39:g:126:ILE:HG22	2.19	0.43
42:j:24:VAL:HG13	42:j:33:ALA:HB2	2.00	0.43
51:s:12:LEU:HD21	55:w:35:HIS:NE2	2.34	0.43
55:w:20:ILE:CD1	55:w:69:GLN:HG3	2.48	0.43
4:3:246:G:O2'	4:3:258:G:O6	2.29	0.43
4:3:909:U:H2'	4:3:910:G:C8	2.54	0.43
4:3:1321:C:H2'	4:3:1322:A:O4'	2.19	0.43
4:3:1585:A:N3	4:3:1585:A:H2'	2.34	0.43
4:3:1974:U:OP1	63:3:3230:PUT:N1	2.52	0.43
4:3:2814:A:H4'	34:b:64:LYS:HD2	2.00	0.43
6:5:80:U:H2'	6:5:81:A:C8	2.54	0.43
6:5:403:A:H2'	6:5:404:A:H8	1.83	0.43
6:5:518:A:N6	6:5:531:A:H61	2.17	0.43
6:5:596:U:H4'	16:G:98:TYR:CG	2.54	0.43
8:7:23:C:H2'	8:7:24:A:C8	2.54	0.43
20:K:33:LYS:HA	20:K:33:LYS:HD2	1.85	0.43
23:N:23:GLN:OE1	23:N:23:GLN:N	2.44	0.43
55:w:95:LYS:HE3	55:w:98:LEU:HD22	2.00	0.43
56:x:16:CYS:SG	56:x:17:ALA:N	2.92	0.43
1:0:32:LYS:O	1:0:36:LYS:HG3	2.19	0.42
4:3:1114:C:H3'	4:3:1115:G:H8	1.83	0.42
5:4:3:U:O2'	5:4:24:A:N1	2.48	0.42
5:4:82:U:H2'	5:4:83:U:H4'	1.99	0.42
6:5:1022:G:H2'	6:5:1023:G:C8	2.54	0.42
6:5:1204:A:OP2	21:L:113:ARG:HD3	2.19	0.42
24:O:73:PHE:CD1	24:O:78:LEU:HD23	2.54	0.42
25:P:23:THR:O	25:P:23:THR:OG1	2.35	0.42
26:Q:90:LEU:HD23	26:Q:90:LEU:HA	1.86	0.42
28:S:24:GLN:HE21	28:S:54:LEU:HD21	1.84	0.42
41:i:20:ILE:HD13	41:i:58:ILE:HB	2.00	0.42
44:l:32:TYR:CE1	44:l:133:LYS:HB3	2.54	0.42
47:o:32:ASN:HB2	47:o:91:LYS:HD2	2.01	0.42
4:3:19:G:OP1	57:y:11:HIS:ND1	2.47	0.42
4:3:174:A:H2'	4:3:175:A:H8	1.84	0.42
4:3:1081:A:C2	39:g:61:ARG:HD2	2.54	0.42
4:3:2154:A:H2'	4:3:2155:G:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:2260:G:O6	53:u:18:LYS:NZ	2.37	0.42
15:F:98:LEU:C	15:F:98:LEU:HD23	2.43	0.42
18:I:18:SER:OG	18:I:20:ASP:O	2.35	0.42
33:a:147:VAL:HA	33:a:200:VAL:HA	2.01	0.42
36:d:132:ILE:HG21	36:d:152:PHE:HD2	1.84	0.42
46:n:18:LYS:O	46:n:22:THR:HG23	2.20	0.42
46:n:38:HIS:HB3	46:n:57:SER:HB2	2.00	0.42
48:p:106:ASN:O	48:p:109:VAL:HG22	2.19	0.42
53:u:78:ASP:HB3	53:u:100:HIS:NE2	2.34	0.42
4:3:1190:A:O3'	48:p:54:ARG:NH2	2.51	0.42
4:3:1313:G:N2	4:3:1356:G:H5''	2.34	0.42
4:3:1619:A:H8	4:3:1619:A:H5''	1.82	0.42
4:3:2025:C:H2'	4:3:2026:A:H8	1.84	0.42
4:3:2386:A:H1'	46:n:90:VAL:HG23	2.02	0.42
6:5:116:A:H5'	25:P:67:ARG:CZ	2.49	0.42
6:5:259:A:H2'	6:5:260:C:H6	1.84	0.42
10:A:44:PHE:HD1	10:A:60:LEU:HD13	1.84	0.42
10:A:293:ARG:HH22	29:T:54:ARG:HB2	1.84	0.42
12:C:106:PHE:HD1	12:C:157:ALA:O	2.03	0.42
12:C:144:LEU:HG	12:C:145:LYS:H	1.84	0.42
14:E:5:ILE:CD1	14:E:62:PHE:HE2	2.31	0.42
14:E:173:PRO:HB2	14:E:174:TYR:CD1	2.55	0.42
17:H:45:LEU:HG	17:H:48:GLN:OE1	2.18	0.42
19:J:21:ASN:HD22	19:J:21:ASN:C	2.14	0.42
20:K:42:LEU:HD13	20:K:94:LEU:HG	1.99	0.42
23:N:16:ASP:O	23:N:17:LYS:HG2	2.19	0.42
24:O:6:LEU:HD22	24:O:17:TYR:CD2	2.55	0.42
25:P:24:VAL:HG21	25:P:63:ILE:HD11	2.00	0.42
35:c:162:ASN:HD22	35:c:162:ASN:C	2.20	0.42
37:e:92:LEU:HD21	37:e:97:TYR:HB3	2.00	0.42
42:j:54:LYS:HE3	42:j:54:LYS:HB3	1.82	0.42
43:k:82:LEU:HA	43:k:85:ILE:HG22	2.01	0.42
54:v:4:LYS:HG3	54:v:5:ASP:O	2.18	0.42
4:3:17:G:H4'	57:y:18:SER:HB2	2.00	0.42
4:3:449:C:H2'	4:3:450:C:C6	2.55	0.42
4:3:1112:A:H2	40:h:130:GLN:NE2	2.17	0.42
4:3:1623:U:H2'	4:3:1624:A:C8	2.54	0.42
4:3:1854:A:H1'	6:5:699:A:C4	2.54	0.42
4:3:2764:U:H1'	4:3:2765:A:H5''	2.01	0.42
6:5:147:A:H2'	6:5:148:A:C8	2.54	0.42
6:5:473:A:H2'	6:5:474:G:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:1070:G:H2'	6:5:1071:A:C8	2.55	0.42
6:5:1488:A:H2'	6:5:1489:C:C6	2.54	0.42
10:A:208:PRO:HB2	14:E:174:TYR:CE2	2.55	0.42
18:I:59:ARG:CZ	18:I:69:GLU:HB3	2.49	0.42
20:K:16:LYS:HE3	20:K:16:LYS:HB3	1.91	0.42
27:R:3:ARG:NH2	27:R:7:LYS:HG3	2.34	0.42
27:R:40:ILE:HD12	27:R:66:MET:HG2	2.01	0.42
31:Y:47:U:H3'	31:Y:48:C:H6	1.84	0.42
34:b:97:THR:HG22	34:b:100:ASN:OD1	2.20	0.42
37:e:34:ILE:HD11	37:e:139:ILE:HG13	2.01	0.42
37:e:168:PHE:C	37:e:169:ASP:OD1	2.63	0.42
40:h:51:ILE:HG23	40:h:68:LYS:O	2.19	0.42
44:l:56:LYS:HB2	44:l:56:LYS:HE3	1.82	0.42
51:s:29:PHE:CE1	51:s:83:ILE:HD12	2.54	0.42
54:v:16:ASN:HD22	54:v:24:ILE:HG23	1.84	0.42
4:3:869:U:H2'	4:3:870:A:H8	1.85	0.42
4:3:1385:U:H2'	4:3:1386:G:O4'	2.19	0.42
6:5:1329:G:H2'	6:5:1330:A:C8	2.54	0.42
6:5:1401:A:H2'	6:5:1402:U:H6	1.84	0.42
11:B:9:GLY:HA2	11:B:12:PHE:HD2	1.83	0.42
11:B:92:ILE:O	11:B:96:ILE:HG12	2.19	0.42
12:C:188:PRO:O	12:C:188:PRO:HG2	2.19	0.42
13:D:205:PRO:HA	16:G:111:LEU:HD11	2.02	0.42
18:I:14:ILE:HD12	18:I:80:MET:HG3	2.01	0.42
25:P:67:ARG:O	25:P:69:LEU:HD22	2.20	0.42
42:j:2:VAL:HG22	42:j:6:THR:HG21	2.01	0.42
42:j:104:ARG:NH2	42:j:122:VAL:OXT	2.53	0.42
48:p:6:GLY:O	48:p:7:LYS:HB3	2.19	0.42
49:q:65:GLN:O	49:q:86:ARG:NH2	2.53	0.42
1:0:44:VAL:O	1:0:47:GLU:HG3	2.19	0.42
4:3:1118:U:H5''	39:g:41:ARG:CZ	2.49	0.42
4:3:2122:G:H3'	4:3:2123:A:C5'	2.48	0.42
4:3:2655:U:H2'	4:3:2656:G:H8	1.85	0.42
4:3:2813:A:H2'	4:3:2814:A:H8	1.84	0.42
6:5:295:G:H2'	6:5:296:A:C8	2.55	0.42
6:5:425:G:H4'	6:5:426:U:O5'	2.19	0.42
6:5:537:A:H2'	6:5:538:G:C8	2.55	0.42
6:5:631:C:H2'	6:5:632:A:C8	2.54	0.42
6:5:909:A:O2'	6:5:911:G:H5''	2.18	0.42
6:5:934:G:P	15:F:94:ARG:HH22	2.42	0.42
6:5:1193:U:H2'	6:5:1194:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:98:ASP:HA	12:C:101:VAL:HG22	2.01	0.42
12:C:201:LYS:O	12:C:201:LYS:HD2	2.19	0.42
18:I:94:LYS:HG3	56:x:100:LEU:O	2.20	0.42
28:S:25:LYS:HG2	28:S:29:LYS:HE3	2.00	0.42
33:a:240:HIS:CE1	33:a:249:VAL:HG13	2.55	0.42
38:f:68:LEU:HD22	38:f:108:LEU:HD21	2.01	0.42
42:j:8:LEU:HD11	42:j:84:CYS:HB3	2.02	0.42
4:3:783:1MG:C8	50:r:89:ALA:HB1	2.55	0.42
4:3:848:U:H2'	4:3:849:C:C6	2.53	0.42
4:3:1120:A:H2'	4:3:1121:A:N9	2.34	0.42
4:3:1279:U:H5'	48:p:3:ILE:HB	2.02	0.42
4:3:1673:U:O2'	4:3:2707:A:H4'	2.20	0.42
4:3:2896:G:H3'	4:3:2897:G:H5'	2.02	0.42
60:3:3001:CLM:CL1	32:Z:35:ALA:CB	3.04	0.42
5:4:47:C:N4	5:4:48:A:H62	2.17	0.42
6:5:573:G:H4'	6:5:574:C:O5'	2.19	0.42
6:5:737:U:OP1	23:N:35:GLN:NE2	2.53	0.42
6:5:768:G:H2'	6:5:769:U:C6	2.54	0.42
7:6:58:A:H4'	7:6:59:G:OP1	2.19	0.42
12:C:64:TYR:HD1	12:C:110:ARG:NH1	2.18	0.42
12:C:131:THR:HB	12:C:134:ILE:HD11	2.01	0.42
14:E:182:ASN:OD1	14:E:182:ASN:N	2.52	0.42
16:G:131:LYS:O	16:G:133:ILE:HG23	2.19	0.42
20:K:92:VAL:HG12	20:K:115:LEU:HD11	2.00	0.42
33:a:30:LYS:HE3	33:a:30:LYS:HB3	1.93	0.42
34:b:13:MET:HE1	34:b:196:ALA:HA	2.01	0.42
38:f:131:PHE:HA	38:f:140:VAL:O	2.20	0.42
41:i:122:ILE:HD12	41:i:122:ILE:HA	1.84	0.42
48:p:105:PHE:O	48:p:109:VAL:HG13	2.19	0.42
52:t:10:VAL:HG21	52:t:74:LEU:HB3	2.01	0.42
56:x:46:TYR:CD1	56:x:46:TYR:N	2.86	0.42
4:3:1464:G:H1	4:3:1590:U:H3	1.66	0.42
4:3:1815:U:O2'	4:3:1816:A:O4'	2.38	0.42
4:3:2323:U:O2	36:d:125:ARG:NH1	2.52	0.42
6:5:733:A:H2'	6:5:734:A:C8	2.55	0.42
6:5:1103:C:O2	11:B:182:ARG:HG3	2.20	0.42
6:5:1347:U:H5''	17:H:75:THR:HG23	2.00	0.42
8:7:10:G:H2'	8:7:11:U:C6	2.54	0.42
12:C:67:THR:HG21	12:C:69:LYS:HE2	2.02	0.42
12:C:168:GLU:HG3	12:C:177:THR:HG23	2.00	0.42
14:E:40:LEU:HD12	14:E:57:TYR:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:98:ALA:CB	26:Q:49:LEU:HD21	2.49	0.42
16:G:12:PHE:HD1	16:G:13:ASP:N	2.17	0.42
17:H:98:LYS:C	17:H:98:LYS:HD3	2.44	0.42
25:P:43:LYS:HD3	25:P:45:TYR:CE1	2.54	0.42
40:h:106:GLN:OE1	40:h:106:GLN:N	2.52	0.42
47:o:54:ARG:HD3	47:o:56:ARG:HB2	2.01	0.42
56:x:58:ARG:NH2	56:x:62:LEU:HD22	2.35	0.42
4:3:622:U:H2'	4:3:623:A:H8	1.81	0.42
4:3:1093:U:H3	4:3:1115:G:N2	2.18	0.42
4:3:1143:U:H5''	39:g:77:LYS:HA	2.00	0.42
4:3:1414:C:H2'	4:3:1415:A:H8	1.85	0.42
4:3:1460:G:H2'	4:3:1461:A:C8	2.55	0.42
4:3:1705:U:H1'	34:b:135:HIS:CE1	2.55	0.42
4:3:2107:A:H3'	4:3:2108:C:H6	1.85	0.42
4:3:2853:U:O2'	4:3:2870:U:O2	2.32	0.42
63:3:3224:PUT:H21	43:k:20:LEU:HD11	2.02	0.42
6:5:747:C:O2	23:N:20:GLY:HA3	2.18	0.42
6:5:832:G:H2'	6:5:833:G:H8	1.84	0.42
6:5:968:G:OP1	18:I:65:LYS:NZ	2.53	0.42
6:5:1351:U:H2'	6:5:1352:A:H8	1.84	0.42
13:D:110:GLU:HB2	13:D:113:ASN:OD1	2.19	0.42
15:F:124:ILE:HG13	15:F:125:ASP:N	2.34	0.42
17:H:57:THR:O	17:H:58:ASP:HB3	2.20	0.42
22:M:34:LEU:O	22:M:38:GLY:N	2.52	0.42
25:P:62:GLN:HG2	25:P:79:LYS:O	2.20	0.42
25:P:66:THR:HB	25:P:76:ARG:HD3	2.02	0.42
38:f:99:ASN:O	38:f:103:THR:HG23	2.20	0.42
40:h:72:VAL:O	40:h:73:SER:OG	2.30	0.42
43:k:2:GLU:N	43:k:2:GLU:CD	2.78	0.42
48:p:20:ALA:HB2	48:p:38:VAL:HG23	2.01	0.42
49:q:54:ARG:HB2	49:q:98:VAL:HB	2.00	0.42
50:r:1:MET:HE3	50:r:62:HIS:HB3	2.00	0.42
4:3:1306:G:H2'	4:3:1307:G:C8	2.55	0.42
4:3:1803:U:H2'	4:3:1804:A:C8	2.55	0.42
4:3:1836:A:H3'	4:3:1837:C:H6	1.85	0.42
4:3:2032:G:H2'	4:3:2033:G:C8	2.55	0.42
4:3:2271:C:H4'	4:3:2337:U:H4'	2.00	0.42
4:3:2420:A:H2'	4:3:2421:U:O4'	2.19	0.42
6:5:196:G:H2'	6:5:197:A:H5''	2.02	0.42
6:5:492:G:O2'	6:5:494:A:H1'	2.19	0.42
6:5:825:A:H2'	6:5:826:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:1199:U:O2'	6:5:1296:C:OP1	2.35	0.42
10:A:223:GLN:HG2	10:A:224:SER:H	1.85	0.42
11:B:78:ILE:HA	11:B:85:ILE:HG12	2.02	0.42
17:H:45:LEU:O	17:H:45:LEU:HD23	2.19	0.42
20:K:99:ARG:CZ	20:K:101:LYS:HG2	2.49	0.42
21:L:101:ARG:HG3	21:L:102:THR:N	2.35	0.42
24:O:39:LEU:HD22	24:O:72:LEU:HD11	2.02	0.42
35:c:133:PHE:CE2	35:c:161:VAL:HG22	2.55	0.42
40:h:25:LEU:HD12	40:h:32:MET:HE2	2.02	0.42
46:n:37:ASN:C	46:n:38:HIS:CD2	2.98	0.42
47:o:40:LYS:H	47:o:40:LYS:HG3	1.61	0.42
4:3:776:U:H2'	4:3:777:C:H6	1.85	0.41
4:3:2022:A:C2	57:y:3:VAL:HB	2.55	0.41
4:3:2239:U:H5''	54:v:29:TRP:HD1	1.85	0.41
4:3:2376:C:H2'	4:3:2377:A:C8	2.55	0.41
6:5:348:C:H4'	6:5:350:G:OP1	2.20	0.41
6:5:1002:A:H2'	6:5:1003:A:O4'	2.20	0.41
12:C:102:TYR:HD2	12:C:110:ARG:HB2	1.85	0.41
14:E:62:PHE:CD1	14:E:63:SER:N	2.88	0.41
18:I:46:LEU:HB3	18:I:79:LEU:HG	2.01	0.41
24:O:50:ILE:HG13	24:O:51:ASP:N	2.34	0.41
36:d:45:ARG:HB3	36:d:78:LYS:NZ	2.36	0.41
47:o:3:LYS:HE3	47:o:3:LYS:HB2	1.79	0.41
48:p:73:MET:HG3	48:p:74:THR:N	2.35	0.41
57:y:9:SER:HB2	57:y:11:HIS:CD2	2.54	0.41
4:3:899:A:H2'	4:3:900:G:C8	2.55	0.41
6:5:896:G:H2'	6:5:897:A:H8	1.86	0.41
6:5:1045:C:H42	31:Y:46:G:N2	2.18	0.41
8:7:61:C:H2'	8:7:62:C:H6	1.85	0.41
14:E:132:VAL:O	14:E:132:VAL:CG1	2.68	0.41
28:S:9:LYS:HE3	28:S:13:GLN:HE22	1.85	0.41
29:T:3:LYS:H	29:T:3:LYS:HG3	1.73	0.41
29:T:57:ARG:O	29:T:60:VAL:HG12	2.20	0.41
33:a:12:SER:O	33:a:12:SER:OG	2.28	0.41
34:b:57:VAL:HG23	34:b:61:LYS:HE3	2.01	0.41
39:g:74:THR:HG22	39:g:110:CYS:HB2	2.01	0.41
52:t:40:ASN:HB3	52:t:67:ALA:HB3	2.02	0.41
58:z:12:ASN:HD22	58:z:12:ASN:HA	1.64	0.41
4:3:299:A:H2'	4:3:300:G:H8	1.86	0.41
4:3:1495:A:H2'	4:3:1496:A:C8	2.55	0.41
4:3:2335:A:H2'	4:3:2336:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:271:G:H4'	25:P:18:ASN:OD1	2.20	0.41
6:5:1154:A:O3'	17:H:107:THR:HG23	2.21	0.41
10:A:22:LYS:NZ	10:A:251:ASP:HA	2.36	0.41
14:E:130:VAL:N	14:E:131:PRO:HD2	2.34	0.41
15:F:110:ARG:HB2	15:F:122:GLU:OE2	2.20	0.41
17:H:89:LEU:HD23	17:H:89:LEU:HA	1.85	0.41
33:a:146:GLN:H	33:a:146:GLN:HG2	1.69	0.41
36:d:91:LEU:C	36:d:96:MET:HB3	2.45	0.41
41:i:18:TRP:HB3	41:i:140:PRO:HB3	2.01	0.41
42:j:106:LEU:HD22	42:j:106:LEU:H	1.85	0.41
44:l:67:ARG:HD3	44:l:105:GLU:OE2	2.20	0.41
52:t:3:ARG:C	52:t:4:ILE:HD13	2.45	0.41
4:3:1119:A:C8	39:g:53:VAL:HG21	2.55	0.41
6:5:224:A:H2'	6:5:225:U:C6	2.55	0.41
6:5:258:A:O2'	28:S:63:ASN:ND2	2.54	0.41
6:5:535:A:H5''	20:K:123:ARG:NH2	2.36	0.41
6:5:733:A:H2'	6:5:734:A:H8	1.86	0.41
7:6:8:U:O2'	7:6:46:G:N2	2.54	0.41
10:A:84:PHE:N	10:A:84:PHE:HD1	2.18	0.41
10:A:119:ASN:HD21	10:A:122:THR:HG23	1.85	0.41
11:B:144:VAL:HG11	11:B:152:ILE:HG12	2.02	0.41
12:C:90:PHE:HA	12:C:93:LEU:HD23	2.03	0.41
12:C:177:THR:OG1	12:C:178:TYR:N	2.54	0.41
13:D:177:ASP:C	13:D:178:ILE:HG12	2.45	0.41
14:E:40:LEU:HD12	14:E:57:TYR:HB3	2.01	0.41
15:F:108:ARG:O	15:F:108:ARG:HG2	2.20	0.41
21:L:43:LYS:HA	21:L:43:LYS:HD3	1.86	0.41
24:O:18:ARG:HD3	24:O:35:LEU:CD1	2.50	0.41
38:f:114:LYS:HB3	38:f:132:GLU:OE2	2.20	0.41
40:h:102:LYS:HB2	40:h:102:LYS:HE2	1.80	0.41
45:m:89:LYS:HD2	45:m:90:TYR:CZ	2.56	0.41
51:s:47:VAL:HG21	55:w:27:LEU:HD22	2.03	0.41
4:3:339:U:H2'	4:3:340:U:C6	2.55	0.41
4:3:756:A:H2'	4:3:757:A:H8	1.86	0.41
4:3:1871:U:OP1	4:3:2418:G:O2'	2.35	0.41
4:3:2070:C:H1'	32:Z:36:ASP:HA	2.02	0.41
4:3:2311:G:H21	36:d:129:THR:HG21	1.85	0.41
4:3:2336:A:H2'	4:3:2337:U:C6	2.55	0.41
4:3:2403:C:H2'	4:3:2404:G:C8	2.55	0.41
6:5:426:U:H3'	12:C:8:PHE:CD1	2.55	0.41
6:5:1325:U:O2'	15:F:32:ASP:OD1	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:32:U:O3'	15:F:83:ASN:ND2	2.53	0.41
12:C:8:PHE:CZ	12:C:23:LYS:HA	2.55	0.41
12:C:83:GLY:O	12:C:85:LEU:HG	2.20	0.41
12:C:98:ASP:OD1	12:C:98:ASP:N	2.50	0.41
12:C:103:ARG:NH2	12:C:164:SER:OG	2.53	0.41
17:H:132:ARG:H	17:H:132:ARG:HG2	1.71	0.41
20:K:114:THR:HG23	20:K:115:LEU:H	1.86	0.41
21:L:9:ILE:HB	21:L:18:ALA:HB1	2.03	0.41
27:R:81:LYS:HB2	27:R:81:LYS:HE3	1.81	0.41
31:Y:45:G:H2'	31:Y:46:G:O4'	2.19	0.41
37:e:9:ILE:HG21	37:e:53:LEU:HB3	2.03	0.41
37:e:63:GLN:O	37:e:66:ILE:HG22	2.21	0.41
40:h:33:GLY:O	40:h:36:THR:OG1	2.38	0.41
42:j:13:ASN:HD21	42:j:96:THR:H	1.67	0.41
44:l:29:PHE:HB3	44:l:65:TRP:CE2	2.56	0.41
4:3:45:U:H2'	4:3:46:A:O4'	2.20	0.41
4:3:1099:C:H3'	4:3:1100:U:H6	1.86	0.41
4:3:1563:G:N2	4:3:1566:A:OP2	2.32	0.41
4:3:1954:C:H2'	4:3:1955:G:H8	1.85	0.41
4:3:2537:G:H5''	4:3:2538:A:H5''	2.02	0.41
6:5:231:U:H2'	6:5:232:G:H8	1.84	0.41
6:5:409:G:N2	6:5:425:G:H1'	2.33	0.41
6:5:1368:U:O2'	6:5:1476:C:O2'	2.37	0.41
7:6:37:A:H2'	7:6:38:C:H6	1.86	0.41
10:A:40:LYS:HB3	10:A:40:LYS:HE3	1.80	0.41
10:A:119:ASN:OD1	10:A:122:THR:OG1	2.28	0.41
17:H:95:GLU:OE1	17:H:95:GLU:N	2.47	0.41
18:I:24:LEU:HD21	18:I:78:ARG:HG2	2.02	0.41
21:L:4:ILE:HD11	21:L:57:ARG:HB2	2.01	0.41
26:Q:48:GLN:HG3	26:Q:50:ARG:O	2.21	0.41
27:R:34:TRP:CD1	27:R:34:TRP:N	2.89	0.41
44:l:76:LYS:HB3	44:l:91:GLU:HG3	2.02	0.41
46:n:28:VAL:CG1	46:n:89:VAL:HG12	2.50	0.41
46:n:31:MET:HE2	46:n:31:MET:HB3	1.76	0.41
47:o:93:ARG:HH21	47:o:118:LYS:HE2	1.86	0.41
55:w:18:LEU:HA	55:w:18:LEU:HD23	1.79	0.41
57:y:33:CYS:SG	57:y:35:LYS:HG2	2.60	0.41
4:3:196:G:O6	4:3:207:C:O2'	2.25	0.41
4:3:1572:U:H2'	4:3:1573:A:H8	1.85	0.41
6:5:18:U:H2'	6:5:19:C:C6	2.54	0.41
6:5:335:C:H2'	6:5:336:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:661:G:N2	6:5:723:C:O2'	2.46	0.41
11:B:216:ASN:O	11:B:217:ARG:HG2	2.20	0.41
12:C:82:ARG:HH11	12:C:82:ARG:C	2.28	0.41
13:D:218:GLU:O	13:D:219:LEU:C	2.63	0.41
16:G:38:SER:O	16:G:42:ILE:HG12	2.20	0.41
35:c:135:LYS:HA	35:c:135:LYS:HD2	1.70	0.41
48:p:51:ASN:O	48:p:54:ARG:HG2	2.20	0.41
52:t:13:ILE:H	52:t:13:ILE:HG13	1.75	0.41
52:t:110:THR:HG22	52:t:111:LEU:HG	2.03	0.41
4:3:567:U:H4'	4:3:568:G:C8	2.55	0.41
4:3:606:G:N2	4:3:2038:A:OP1	2.51	0.41
6:5:190:A:H2'	6:5:191:A:C8	2.54	0.41
6:5:747:C:H2'	6:5:748:U:C6	2.56	0.41
11:B:113:MET:O	11:B:115:SER:N	2.46	0.41
11:B:154:VAL:O	11:B:170:MET:HA	2.21	0.41
12:C:8:PHE:HE2	12:C:26:SER:HB2	1.85	0.41
12:C:155:LYS:O	12:C:159:GLU:HG2	2.20	0.41
14:E:90:LEU:H	14:E:90:LEU:HD12	1.86	0.41
21:L:29:ARG:NH2	21:L:63:TYR:CD1	2.89	0.41
24:O:67:ASP:OD1	24:O:67:ASP:N	2.53	0.41
27:R:31:ILE:HB	27:R:49:PHE:CD1	2.56	0.41
35:c:6:LEU:HD23	35:c:127:LEU:O	2.21	0.41
38:f:34:LYS:HD2	38:f:34:LYS:N	2.36	0.41
40:h:125:LEU:H	40:h:125:LEU:HD12	1.86	0.41
47:o:53:LEU:HD11	47:o:67:ARG:HD2	2.03	0.41
49:q:77:LYS:HA	49:q:77:LYS:HD3	1.78	0.41
4:3:63:U:O2'	4:3:64:U:O2	2.38	0.41
4:3:450:C:H2'	4:3:451:A:C8	2.56	0.41
4:3:679:A:N1	4:3:2377:A:O2'	2.47	0.41
4:3:2166:U:H2'	4:3:2167:G:C8	2.56	0.41
6:5:207:C:H2'	6:5:208:A:O4'	2.21	0.41
6:5:331:C:H2'	6:5:332:A:H8	1.85	0.41
6:5:381:C:H2'	6:5:382:U:C6	2.56	0.41
6:5:685:G:O5'	19:J:42:THR:HA	2.21	0.41
6:5:990:C:O2	22:M:4:LYS:NZ	2.51	0.41
6:5:1141:U:O2'	6:5:1142:G:H8	2.03	0.41
6:5:1402:U:H2'	6:5:1403:A:H8	1.86	0.41
7:6:4:G:H2'	7:6:5:A:O4'	2.21	0.41
9:8:27:A:H61	9:8:43:U:H3	1.69	0.41
9:8:63:C:H5''	9:8:63:C:H6	1.86	0.41
11:B:61:THR:HG22	11:B:62:GLN:N	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:124:LEU:HD23	12:C:126:ASP:H	1.86	0.41
13:D:178:ILE:HG22	13:D:180:THR:HG23	2.03	0.41
14:E:45:LEU:HD12	26:Q:97:ALA:HB1	2.03	0.41
14:E:80:LYS:H	14:E:80:LYS:HG2	1.72	0.41
14:E:157:TRP:HB3	16:G:60:LEU:CD2	2.49	0.41
15:F:15:PRO:CG	17:H:45:LEU:HD21	2.51	0.41
15:F:148:LYS:HE2	15:F:148:LYS:HB2	1.84	0.41
15:F:154:ARG:HG3	15:F:155:TRP:N	2.35	0.41
16:G:51:GLU:HG3	16:G:113:ILE:HG21	2.02	0.41
17:H:54:LEU:HD12	17:H:54:LEU:HA	1.89	0.41
17:H:82:ARG:HH21	17:H:105:LEU:CD1	2.34	0.41
21:L:89:LEU:HA	21:L:92:ARG:HB3	2.03	0.41
24:O:7:MET:CG	24:O:18:ARG:HG2	2.50	0.41
26:Q:40:TYR:HD1	26:Q:40:TYR:HA	1.74	0.41
33:a:126:HIS:HB3	33:a:127:PRO:HD2	2.03	0.41
34:b:105:GLY:HA2	34:b:181:ILE:O	2.21	0.41
36:d:38:MET:HE1	36:d:150:ARG:HB2	2.02	0.41
36:d:111:VAL:HB	36:d:114:PHE:HB2	2.03	0.41
40:h:52:PRO:O	40:h:52:PRO:CD	2.61	0.41
41:i:39:ILE:HG12	41:i:125:VAL:HG22	2.02	0.41
44:l:10:ARG:HH11	44:l:10:ARG:HG2	1.86	0.41
45:m:74:ASP:O	45:m:78:LEU:HB2	2.20	0.41
50:r:29:THR:HG23	50:r:55:ILE:HD13	2.02	0.41
4:3:705:A:H5'	43:k:43:LYS:O	2.21	0.41
4:3:1043:C:O3'	41:i:113:PRO:HB3	2.20	0.41
4:3:1141:U:H2'	4:3:1142:G:C8	2.56	0.41
4:3:2322:G:N2	36:d:123:ASP:OD2	2.54	0.41
6:5:35:C:H2'	6:5:36:G:H8	1.86	0.41
6:5:483:U:H2'	6:5:484:A:C8	2.56	0.41
6:5:655:G:H2'	6:5:656:U:C6	2.55	0.41
6:5:998:G:H2'	6:5:998:G:N3	2.36	0.41
6:5:1248:U:H2'	6:5:1249:G:O4'	2.20	0.41
6:5:1273:A:H2'	6:5:1273:A:N3	2.36	0.41
9:8:48:C:OP2	9:8:48:C:H6	2.04	0.41
10:A:288:PRO:HB3	29:T:58:ASN:HD21	1.85	0.41
11:B:26:SER:OG	11:B:27:HIS:N	2.54	0.41
11:B:224:HIS:HB3	11:B:225:PRO:CD	2.36	0.41
13:D:132:HIS:CD2	13:D:132:HIS:N	2.89	0.41
14:E:9:VAL:CG1	14:E:56:HIS:HB2	2.51	0.41
17:H:44:LYS:HD2	17:H:44:LYS:HA	1.91	0.41
19:J:77:LEU:HD23	19:J:90:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:116:PRO:O	29:T:35:HIS:HB2	2.21	0.41
23:N:60:ARG:HA	23:N:63:LEU:HG	2.03	0.41
26:Q:56:ASP:OD1	26:Q:56:ASP:N	2.54	0.41
42:j:51:MET:HG3	42:j:52:VAL:N	2.35	0.41
44:l:109:ILE:HG22	44:l:114:MET:HG3	2.01	0.41
2:1:4:LYS:HG2	2:1:6:ALA:H	1.86	0.40
4:3:230:G:H2'	4:3:231:A:C8	2.57	0.40
4:3:1691:U:H2'	4:3:1692:A:H8	1.87	0.40
4:3:1915:C:O2'	8:7:12:G:H5''	2.21	0.40
6:5:421:G:H5''	6:5:422:A:OP2	2.21	0.40
6:5:870:A:H2'	6:5:871:U:H6	1.86	0.40
6:5:1164:U:OP1	18:I:59:ARG:NH2	2.54	0.40
10:A:285:THR:HG23	10:A:286:ARG:HD3	2.04	0.40
13:D:142:GLY:HA2	13:D:201:LYS:NZ	2.36	0.40
13:D:150:LEU:O	13:D:180:THR:HA	2.21	0.40
14:E:9:VAL:HG13	14:E:56:HIS:HB2	2.03	0.40
15:F:82:SER:OG	15:F:83:ASN:N	2.54	0.40
16:G:47:ILE:HG21	16:G:122:VAL:HG23	2.03	0.40
18:I:63:VAL:HG23	18:I:64:ASP:OD1	2.21	0.40
23:N:68:LYS:HE2	23:N:75:TYR:CE2	2.56	0.40
36:d:14:LYS:HG3	36:d:18:LYS:HE2	2.03	0.40
40:h:20:LYS:N	40:h:21:PRO:HD2	2.37	0.40
41:i:48:THR:HG22	41:i:50:ASN:OD1	2.21	0.40
55:w:63:LEU:HD11	55:w:68:GLU:HB2	2.03	0.40
4:3:1208:A:H2'	4:3:1209:U:H4'	2.02	0.40
4:3:1334:U:H2'	4:3:1335:A:H8	1.86	0.40
4:3:1543:U:H2'	4:3:1544:G:C8	2.57	0.40
4:3:1798:A:H8	4:3:1798:A:P	2.45	0.40
4:3:1809:A:H2'	4:3:1810:A:C8	2.56	0.40
4:3:1819:G:H21	33:a:54:THR:HG21	1.86	0.40
4:3:2204:C:H2'	4:3:2205:U:C6	2.56	0.40
5:4:26:C:OP2	46:n:37:ASN:ND2	2.36	0.40
5:4:65:G:H2'	5:4:66:A:H8	1.86	0.40
6:5:35:C:H2'	6:5:36:G:C8	2.56	0.40
6:5:1201:C:C5	21:L:103:ARG:HA	2.56	0.40
7:6:2:G:H2'	7:6:3:G:H8	1.86	0.40
8:7:61:C:H2'	8:7:62:C:C6	2.55	0.40
12:C:31:ARG:HE	12:C:31:ARG:HB2	1.62	0.40
14:E:8:LEU:HB3	14:E:83:LEU:HB2	2.02	0.40
15:F:49:ILE:HD11	15:F:123:ILE:CD1	2.51	0.40
15:F:58:LEU:HA	15:F:58:LEU:HD12	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:63:ILE:HG23	25:P:75:PHE:HB3	2.04	0.40
27:R:65:ASP:C	27:R:67:VAL:H	2.29	0.40
33:a:148:HIS:CD2	33:a:203:VAL:HG22	2.56	0.40
35:c:24:LEU:HD11	35:c:208:GLU:HB3	2.03	0.40
35:c:43:ALA:C	35:c:45:TRP:H	2.29	0.40
35:c:67:LYS:HB2	35:c:67:LYS:HE3	1.89	0.40
36:d:78:LYS:HB3	36:d:78:LYS:HE2	1.84	0.40
36:d:132:ILE:O	36:d:151:GLY:HA3	2.21	0.40
36:d:155:THR:O	36:d:156:LEU:HD13	2.20	0.40
38:f:14:LYS:C	38:f:14:LYS:HD2	2.46	0.40
38:f:19:VAL:HG23	38:f:21:VAL:HG13	2.02	0.40
43:k:137:LYS:HB3	43:k:137:LYS:HE2	1.86	0.40
55:w:39:ASP:O	55:w:41:PRO:HD3	2.22	0.40
56:x:77:THR:O	56:x:79:LYS:N	2.54	0.40
2:l:10:ARG:HG2	43:k:64:LYS:HA	2.03	0.40
4:3:1605:A:H2'	4:3:1606:A:H8	1.85	0.40
6:5:55:C:OP1	6:5:347:G:N2	2.54	0.40
6:5:212:G:H2'	6:5:213:U:C6	2.56	0.40
6:5:686:C:P	19:J:41:GLY:HA3	2.62	0.40
6:5:763:A:OP2	6:5:809:G:N2	2.54	0.40
9:8:70:U:H2'	9:8:71:G:C8	2.55	0.40
10:A:46:GLU:HB2	10:A:47:PRO:HD2	2.04	0.40
10:A:119:ASN:O	10:A:119:ASN:CG	2.63	0.40
11:B:184:ASP:O	11:B:207:ARG:HG2	2.21	0.40
20:K:123:ARG:O	20:K:127:ARG:HD3	2.22	0.40
24:O:17:TYR:O	24:O:39:LEU:N	2.50	0.40
38:f:104:LYS:HB3	38:f:104:LYS:HE3	1.83	0.40
4:3:1859:U:H5'	7:6:72:C:H5''	2.03	0.40
4:3:2334:U:H3	4:3:2397:G:H1	1.69	0.40
6:5:459:C:H2'	6:5:460:A:O4'	2.22	0.40
6:5:1485:C:H2'	6:5:1486:C:C6	2.57	0.40
11:B:109:ILE:HA	11:B:222:ILE:HG23	2.02	0.40
12:C:131:THR:HA	12:C:132:PRO:HD3	1.90	0.40
12:C:187:LEU:O	12:C:192:ASN:ND2	2.50	0.40
13:D:94:VAL:HG22	13:D:122:ALA:HB1	2.03	0.40
15:F:19:ASN:O	15:F:20:THR:C	2.64	0.40
19:J:16:VAL:CG1	19:J:25:VAL:HG13	2.52	0.40
19:J:48:SER:O	19:J:51:LYS:HG2	2.22	0.40
19:J:102:GLU:OE2	19:J:104:ASN:ND2	2.54	0.40
21:L:6:GLY:H	36:d:112:ARG:HH12	1.68	0.40
26:Q:96:LEU:HA	26:Q:96:LEU:HD23	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:11:PHE:HB3	2:1:19:ILE:HG22	2.04	0.40
2:1:31:PRO:HD3	58:z:20:LEU:HD21	2.04	0.40
4:3:1536:C:H2'	4:3:1537:A:C8	2.56	0.40
4:3:1889:U:H2'	4:3:1890:U:C6	2.57	0.40
6:5:69:G:H2'	6:5:70:A:O4'	2.21	0.40
6:5:766:G:H4'	6:5:1488:A:H4'	2.04	0.40
9:8:5:C:H2'	9:8:6:U:C6	2.56	0.40
10:A:288:PRO:CB	29:T:57:ARG:HE	2.35	0.40
12:C:149:ILE:HA	12:C:149:ILE:HD12	1.87	0.40
19:J:13:ILE:HG23	19:J:78:PHE:CD1	2.56	0.40
20:K:42:LEU:CD1	20:K:94:LEU:HG	2.51	0.40
26:Q:102:VAL:HG13	26:Q:103:LYS:HD3	2.04	0.40
28:S:10:ARG:HD3	28:S:10:ARG:HA	1.93	0.40
33:a:182:LEU:HD23	33:a:182:LEU:HA	1.83	0.40
37:e:42:LEU:HG	37:e:44:LEU:HD21	2.03	0.40
37:e:110:LEU:HG	37:e:155:ARG:HG3	2.04	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	0	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
2	1	57/59 (97%)	57 (100%)	0	0	100	100
3	2	35/37 (95%)	35 (100%)	0	0	100	100
10	A	262/294 (89%)	237 (90%)	23 (9%)	2 (1%)	16	46
11	B	230/273 (84%)	203 (88%)	22 (10%)	5 (2%)	5	23
12	C	202/205 (98%)	171 (85%)	30 (15%)	1 (0%)	24	57
13	D	153/219 (70%)	143 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	E	182/215 (85%)	153 (84%)	27 (15%)	2 (1%)	11	39
15	F	153/155 (99%)	140 (92%)	11 (7%)	2 (1%)	9	35
16	G	139/142 (98%)	131 (94%)	8 (6%)	0	100	100
17	H	127/132 (96%)	112 (88%)	15 (12%)	0	100	100
18	I	102/108 (94%)	88 (86%)	13 (13%)	1 (1%)	12	41
19	J	112/121 (93%)	106 (95%)	5 (4%)	1 (1%)	14	44
20	K	133/139 (96%)	116 (87%)	14 (10%)	3 (2%)	5	22
21	L	121/124 (98%)	109 (90%)	10 (8%)	2 (2%)	7	29
22	M	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
23	N	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
24	O	85/94 (90%)	80 (94%)	4 (5%)	1 (1%)	10	37
25	P	83/85 (98%)	73 (88%)	9 (11%)	1 (1%)	10	37
26	Q	69/104 (66%)	65 (94%)	4 (6%)	0	100	100
27	R	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
28	S	77/87 (88%)	74 (96%)	2 (3%)	1 (1%)	9	35
29	T	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	X	28/444 (6%)	24 (86%)	4 (14%)	0	100	100
32	Z	3/36 (8%)	3 (100%)	0	0	100	100
33	a	283/287 (99%)	266 (94%)	16 (6%)	1 (0%)	30	61
34	b	229/287 (80%)	221 (96%)	8 (4%)	0	100	100
35	c	209/212 (99%)	198 (95%)	11 (5%)	0	100	100
36	d	177/180 (98%)	170 (96%)	7 (4%)	0	100	100
37	e	174/184 (95%)	161 (92%)	13 (8%)	0	100	100
38	f	147/149 (99%)	134 (91%)	12 (8%)	1 (1%)	18	49
39	g	123/161 (76%)	118 (96%)	5 (4%)	0	100	100
40	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
41	i	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
42	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
43	k	148/151 (98%)	139 (94%)	9 (6%)	0	100	100
44	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
45	m	117/124 (94%)	112 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	n	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
47	o	116/119 (98%)	107 (92%)	9 (8%)	0	100	100
48	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
49	q	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
50	r	140/159 (88%)	136 (97%)	4 (3%)	0	100	100
51	s	93/237 (39%)	89 (96%)	4 (4%)	0	100	100
52	t	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
53	u	86/104 (83%)	83 (96%)	3 (4%)	0	100	100
54	v	62/65 (95%)	62 (100%)	0	0	100	100
55	w	108/111 (97%)	103 (95%)	5 (5%)	0	100	100
56	x	94/97 (97%)	67 (71%)	24 (26%)	3 (3%)	3	16
57	y	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
58	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	6047/7150 (85%)	5615 (93%)	405 (7%)	27 (0%)	31	61

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	B	229	GLN
11	B	230	PRO
20	K	56	LYS
25	P	54	LEU
11	B	217	ARG
12	C	81	GLN
10	A	54	ASP
10	A	219	ASN
20	K	72	ASN
28	S	37	LYS
56	x	49	GLU
11	B	216	ASN
15	F	20	THR
20	K	57	LYS
33	a	128	ILE
38	f	12	LEU
56	x	59	ALA
14	E	169	VAL
15	F	12	LEU

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Mol	Chain	Res	Type
21	L	123	SER
14	E	148	LYS
18	I	100	VAL
19	J	114	CYS
24	O	47	LYS
56	x	18	SER
21	L	116	VAL
11	B	46	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	0	41/41 (100%)	41 (100%)	0	100	100
2	1	51/51 (100%)	51 (100%)	0	100	100
3	2	35/35 (100%)	34 (97%)	1 (3%)	37	67
10	A	238/262 (91%)	238 (100%)	0	100	100
11	B	195/232 (84%)	193 (99%)	2 (1%)	68	81
12	C	182/183 (100%)	180 (99%)	2 (1%)	65	80
13	D	125/178 (70%)	125 (100%)	0	100	100
14	E	165/196 (84%)	163 (99%)	2 (1%)	63	79
15	F	132/132 (100%)	131 (99%)	1 (1%)	73	83
16	G	123/124 (99%)	121 (98%)	2 (2%)	55	76
17	H	112/115 (97%)	112 (100%)	0	100	100
18	I	97/99 (98%)	96 (99%)	1 (1%)	68	81
19	J	91/97 (94%)	91 (100%)	0	100	100
20	K	117/120 (98%)	116 (99%)	1 (1%)	70	82
21	L	104/105 (99%)	104 (100%)	0	100	100
22	M	47/48 (98%)	47 (100%)	0	100	100
23	N	77/78 (99%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	O	76/82 (93%)	76 (100%)	0	100	100
25	P	75/75 (100%)	74 (99%)	1 (1%)	61	79
26	Q	62/94 (66%)	61 (98%)	1 (2%)	55	76
27	R	76/77 (99%)	76 (100%)	0	100	100
28	S	71/77 (92%)	70 (99%)	1 (1%)	59	78
29	T	55/56 (98%)	55 (100%)	0	100	100
30	X	27/406 (7%)	27 (100%)	0	100	100
32	Z	2/2 (100%)	2 (100%)	0	100	100
33	a	241/243 (99%)	239 (99%)	2 (1%)	73	83
34	b	188/233 (81%)	186 (99%)	2 (1%)	65	80
35	c	183/184 (100%)	181 (99%)	2 (1%)	65	80
36	d	153/154 (99%)	153 (100%)	0	100	100
37	e	153/159 (96%)	152 (99%)	1 (1%)	76	84
38	f	133/134 (99%)	131 (98%)	2 (2%)	57	77
39	g	100/129 (78%)	100 (100%)	0	100	100
40	h	102/110 (93%)	102 (100%)	0	100	100
41	i	126/128 (98%)	123 (98%)	3 (2%)	43	70
42	j	103/103 (100%)	103 (100%)	0	100	100
43	k	125/126 (99%)	123 (98%)	2 (2%)	55	76
44	l	113/115 (98%)	112 (99%)	1 (1%)	70	82
45	m	105/109 (96%)	105 (100%)	0	100	100
46	n	99/99 (100%)	99 (100%)	0	100	100
47	o	104/105 (99%)	103 (99%)	1 (1%)	68	81
48	p	104/108 (96%)	104 (100%)	0	100	100
49	q	90/91 (99%)	89 (99%)	1 (1%)	65	80
50	r	118/132 (89%)	118 (100%)	0	100	100
51	s	84/208 (40%)	81 (96%)	3 (4%)	31	62
52	t	96/96 (100%)	95 (99%)	1 (1%)	68	81
53	u	70/85 (82%)	70 (100%)	0	100	100
54	v	59/60 (98%)	59 (100%)	0	100	100
55	w	97/98 (99%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	x	85/86 (99%)	82 (96%)	3 (4%)	32	62
57	y	48/49 (98%)	48 (100%)	0	100	100
58	z	47/50 (94%)	46 (98%)	1 (2%)	47	72
All	All	5302/6159 (86%)	5262 (99%)	40 (1%)	70	83

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	4	ARG
11	B	15	ASN
11	B	82	ASN
12	C	79	LEU
12	C	188	PRO
14	E	31	ASN
14	E	43	LYS
15	F	121	ASN
16	G	81	ILE
16	G	109	ASN
18	I	14	ILE
20	K	30	LEU
25	P	79	LYS
26	Q	40	TYR
28	S	35	PHE
33	a	70	ASP
33	a	141	ILE
34	b	74	ASN
34	b	100	ASN
35	c	7	ILE
35	c	208	GLU
37	e	7	ARG
38	f	8	ASP
38	f	84	HIS
41	i	20	ILE
41	i	62	SER
41	i	146	SER
43	k	99	ILE
43	k	139	VAL
44	l	63	LYS
47	o	33	VAL
49	q	75	SER
51	s	12	LEU

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Mol	Chain	Res	Type
51	s	24	THR
51	s	84	THR
52	t	92	VAL
56	x	6	HIS
56	x	27	SER
56	x	91	HIS
58	z	12	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	20	HIS
3	2	36	GLN
10	A	55	HIS
10	A	81	GLN
10	A	192	ASN
10	A	221	GLN
11	B	6	ASN
11	B	150	ASN
11	B	231	ASN
12	C	70	GLN
12	C	88	ASN
14	E	101	ASN
14	E	123	ASN
15	F	67	ASN
16	G	56	ASN
16	G	109	ASN
17	H	62	ASN
19	J	111	HIS
19	J	112	ASN
25	P	32	HIS
28	S	24	GLN
28	S	40	ASN
28	S	50	GLN
28	S	63	ASN
29	T	30	GLN
29	T	58	ASN
33	a	15	HIS
33	a	57	HIS
33	a	262	HIS
34	b	66	GLN
34	b	73	ASN

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Mol	Chain	Res	Type
34	b	171	HIS
35	c	126	HIS
38	f	96	GLN
41	i	80	HIS
41	i	134	ASN
41	i	138	GLN
43	k	67	ASN
43	k	125	HIS
45	m	77	GLN
47	o	7	GLN
48	p	8	GLN
48	p	40	GLN
48	p	71	GLN
48	p	106	ASN
50	r	7	GLN
52	t	109	ASN
54	v	6	GLN
54	v	16	ASN
55	w	42	HIS
56	x	91	HIS
56	x	98	ASN
57	y	4	GLN
58	z	24	ASN
58	z	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	Y	20/21 (95%)	14 (70%)	4 (20%)
4	3	2892/2907 (99%)	522 (18%)	22 (0%)
5	4	107/108 (99%)	29 (27%)	0
6	5	1506/1520 (99%)	255 (16%)	9 (0%)
7	6	75/76 (98%)	30 (40%)	6 (8%)
8	7	74/75 (98%)	20 (27%)	2 (2%)
9	8	75/76 (98%)	23 (30%)	0
All	All	4749/4783 (99%)	893 (18%)	43 (0%)

All (893) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	3	11	U

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Mol	Chain	Res	Type
4	3	12	A
4	3	13	C
4	3	14	U
4	3	28	G
4	3	37	G
4	3	48	G
4	3	64	U
4	3	65	A
4	3	73	A
4	3	76	A
4	3	77	G
4	3	102	A
4	3	103	G
4	3	119	A
4	3	121	U
4	3	126	C
4	3	132	G
4	3	141	A
4	3	142	A
4	3	163	A
4	3	180	A
4	3	184	A
4	3	187	C
4	3	200	A
4	3	203	A
4	3	219	G
4	3	220	A
4	3	225	A
4	3	226	A
4	3	232	A
4	3	234	G
4	3	237	A
4	3	245	U
4	3	246	G
4	3	252	G
4	3	269	A
4	3	276	A
4	3	284	U
4	3	287	G
4	3	295	U
4	3	296	U
4	3	297	G

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Mol	Chain	Res	Type
4	3	298	U
4	3	299	A
4	3	309	A
4	3	310	U
4	3	311	G
4	3	315	A
4	3	316	C
4	3	317	U
4	3	319	G
4	3	325	G
4	3	336	C
4	3	345	A
4	3	363	G
4	3	364	A
4	3	365	U
4	3	402	A
4	3	409	A
4	3	410	G
4	3	411	U
4	3	418	G
4	3	419	A
4	3	424	G
4	3	425	U
4	3	426	U
4	3	432	G
4	3	437	A
4	3	440	C
4	3	460	G
4	3	483	A
4	3	517	G
4	3	539	U
4	3	540	A
4	3	548	A
4	3	562	C
4	3	565	C
4	3	566	G
4	3	567	U
4	3	573	A
4	3	581	A
4	3	583	U
4	3	596	G
4	3	598	G

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Mol	Chain	Res	Type
4	3	607	U
4	3	608	A
4	3	610	G
4	3	620	G
4	3	636	U
4	3	637	U
4	3	638	A
4	3	648	G
4	3	649	A
4	3	650	G
4	3	663	A
4	3	670	G
4	3	673	A
4	3	681	A
4	3	682	A
4	3	689	U
4	3	691	G
4	3	705	A
4	3	712	A
4	3	716	G
4	3	721	G
4	3	722	C
4	3	765	A
4	3	775	C
4	3	782	U
4	3	792	G
4	3	797	U
4	3	800	C
4	3	810	G
4	3	811	G
4	3	817	A
4	3	819	U
4	3	820	U
4	3	824	A
4	3	828	A
4	3	829	A
4	3	840	G
4	3	846	U
4	3	847	C
4	3	854	A
4	3	862	U
4	3	881	A

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Mol	Chain	Res	Type
4	3	882	C
4	3	883	A
4	3	901	C
4	3	902	U
4	3	904	C
4	3	906	G
4	3	918	G
4	3	924	C
4	3	926	U
4	3	927	A
4	3	928	G
4	3	930	C
4	3	932	U
4	3	934	C
4	3	935	U
4	3	936	G
4	3	944	U
4	3	947	A
4	3	949	C
4	3	951	C
4	3	952	U
4	3	953	G
4	3	970	U
4	3	981	A
4	3	982	G
4	3	994	U
4	3	997	G
4	3	998	C
4	3	1008	A
4	3	1010	G
4	3	1016	A
4	3	1019	A
4	3	1026	A
4	3	1032	A
4	3	1039	G
4	3	1045	A
4	3	1049	U
4	3	1058	U
4	3	1060	G
4	3	1061	A
4	3	1068	U
4	3	1074	A

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Mol	Chain	Res	Type
4	3	1080	A
4	3	1082	A
4	3	1084	C
4	3	1095	U
4	3	1096	U
4	3	1097	G
4	3	1098	G
4	3	1099	C
4	3	1102	A
4	3	1104	A
4	3	1105	A
4	3	1106	G
4	3	1107	C
4	3	1110	C
4	3	1111	C
4	3	1113	U
4	3	1114	C
4	3	1115	G
4	3	1120	A
4	3	1122	G
4	3	1123	A
4	3	1125	U
4	3	1130	A
4	3	1132	C
4	3	1138	A
4	3	1144	C
4	3	1145	G
4	3	1146	A
4	3	1147	G
4	3	1165	U
4	3	1167	U
4	3	1168	A
4	3	1170	C
4	3	1176	U
4	3	1177	A
4	3	1178	A
4	3	1204	A
4	3	1208	A
4	3	1209	U
4	3	1210	A
4	3	1212	C
4	3	1215	G

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Mol	Chain	Res	Type
4	3	1234	U
4	3	1235	U
4	3	1236	G
4	3	1242	G
4	3	1246	U
4	3	1250	A
4	3	1251	G
4	3	1253	G
4	3	1256	A
4	3	1257	G
4	3	1266	G
4	3	1268	U
4	3	1280	G
4	3	1281	A
4	3	1283	A
4	3	1285	U
4	3	1286	G
4	3	1292	A
4	3	1301	G
4	3	1304	U
4	3	1313	G
4	3	1325	C
4	3	1328	A
4	3	1329	U
4	3	1330	U
4	3	1369	U
4	3	1378	C
4	3	1380	U
4	3	1388	G
4	3	1393	A
4	3	1406	A
4	3	1407	U
4	3	1412	A
4	3	1423	A
4	3	1424	U
4	3	1431	A
4	3	1444	C
4	3	1445	U
4	3	1446	G
4	3	1448	U
4	3	1456	C
4	3	1463	G

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Mol	Chain	Res	Type
4	3	1467	U
4	3	1480	A
4	3	1481	U
4	3	1483	G
4	3	1486	U
4	3	1487	U
4	3	1502	A
4	3	1504	G
4	3	1508	G
4	3	1510	A
4	3	1513	A
4	3	1514	U
4	3	1515	A
4	3	1519	A
4	3	1522	U
4	3	1534	A
4	3	1535	A
4	3	1541	A
4	3	1546	U
4	3	1550	G
4	3	1569	A
4	3	1570	A
4	3	1571	G
4	3	1580	G
4	3	1582	G
4	3	1584	U
4	3	1585	A
4	3	1588	A
4	3	1589	A
4	3	1603	A
4	3	1612	U
4	3	1617	U
4	3	1618	U
4	3	1619	A
4	3	1641	A
4	3	1642	G
4	3	1643	A
4	3	1644	A
4	3	1645	C
4	3	1650	A
4	3	1651	C
4	3	1661	A

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Mol	Chain	Res	Type
4	3	1668	G
4	3	1680	A
4	3	1681	G
4	3	1682	C
4	3	1694	A
4	3	1708	G
4	3	1727	U
4	3	1737	G
4	3	1748	U
4	3	1749	A
4	3	1764	U
4	3	1769	A
4	3	1770	A
4	3	1771	C
4	3	1780	A
4	3	1789	C
4	3	1791	A
4	3	1807	C
4	3	1808	C
4	3	1809	A
4	3	1816	A
4	3	1823	U
4	3	1836	A
4	3	1854	A
4	3	1855	A
4	3	1866	G
4	3	1869	G
4	3	1878	A
4	3	1886	C
4	3	1910	G
4	3	1913	G
4	3	1920	A
4	3	1936	G
4	3	1937	G
4	3	1938	U
4	3	1943	A
4	3	1944	A
4	3	1962	U
4	3	1974	U
4	3	1977	A
4	3	1978	U
4	3	1979	G

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Mol	Chain	Res	Type
4	3	1998	U
4	3	1999	G
4	3	2000	U
4	3	2004	G
4	3	2028	G
4	3	2030	A
4	3	2038	A
4	3	2040	A
4	3	2041	C
4	3	2042	A
4	3	2050	G
4	3	2057	C
4	3	2062	C
4	3	2063	G
4	3	2067	A
4	3	2068	G
4	3	2069	A
4	3	2076	G
4	3	2084	A
4	3	2099	U
4	3	2100	G
4	3	2106	G
4	3	2108	C
4	3	2110	U
4	3	2111	U
4	3	2112	A
4	3	2114	C
4	3	2115	A
4	3	2116	U
4	3	2117	G
4	3	2118	U
4	3	2119	A
4	3	2123	A
4	3	2124	A
4	3	2125	U
4	3	2126	A
4	3	2130	A
4	3	2131	G
4	3	2133	A
4	3	2134	G
4	3	2139	C
4	3	2140	G

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Mol	Chain	Res	Type
4	3	2144	C
4	3	2150	C
4	3	2152	C
4	3	2153	U
4	3	2154	A
4	3	2157	A
4	3	2164	G
4	3	2166	U
4	3	2169	G
4	3	2170	A
4	3	2173	G
4	3	2175	U
4	3	2180	U
4	3	2181	A
4	3	2182	C
4	3	2183	U
4	3	2184	A
4	3	2185	C
4	3	2193	U
4	3	2194	G
4	3	2195	U
4	3	2198	G
4	3	2199	C
4	3	2200	U
4	3	2201	G
4	3	2202	U
4	3	2207	A
4	3	2211	G
4	3	2212	U
4	3	2219	U
4	3	2220	A
4	3	2221	U
4	3	2227	U
4	3	2228	U
4	3	2233	A
4	3	2246	G
4	3	2247	G
4	3	2259	OMG
4	3	2274	A
4	3	2276	A
4	3	2287	G
4	3	2291	U

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Mol	Chain	Res	Type
4	3	2295	A
4	3	2298	G
4	3	2305	C
4	3	2311	G
4	3	2313	U
4	3	2316	G
4	3	2319	A
4	3	2327	U
4	3	2329	G
4	3	2333	G
4	3	2335	A
4	3	2336	A
4	3	2342	U
4	3	2343	A
4	3	2344	A
4	3	2353	G
4	3	2355	C
4	3	2358	U
4	3	2366	A
4	3	2391	G
4	3	2393	C
4	3	2397	G
4	3	2410	C
4	3	2411	C
4	3	2414	U
4	3	2422	G
4	3	2431	U
4	3	2433	A
4	3	2437	G
4	3	2438	A
4	3	2443	A
4	3	2449	U
4	3	2456	A
4	3	2477	A
4	3	2481	U
4	3	2482	U
4	3	2483	C
4	3	2484	A
4	3	2486	A
4	3	2488	C
4	3	2499	U
4	3	2510	G

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Mol	Chain	Res	Type
4	3	2512	U
4	3	2513	G
4	3	2521	A
4	3	2526	A
4	3	2537	G
4	3	2543	G
4	3	2574	A
4	3	2575	G
4	3	2580	A
4	3	2585	A
4	3	2593	U
4	3	2594	C
4	3	2605	G
4	3	2610	A
4	3	2617	U
4	3	2618	C
4	3	2621	U
4	3	2623	U
4	3	2637	A
4	3	2638	G
4	3	2654	U
4	3	2668	A
4	3	2669	G
4	3	2697	C
4	3	2698	U
4	3	2722	G
4	3	2734	C
4	3	2737	G
4	3	2741	A
4	3	2752	G
4	3	2756	A
4	3	2760	C
4	3	2764	U
4	3	2765	A
4	3	2773	A
4	3	2786	A
4	3	2798	A
4	3	2799	U
4	3	2804	C
4	3	2806	A
4	3	2807	G
4	3	2808	A

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Mol	Chain	Res	Type
4	3	2810	A
4	3	2813	A
4	3	2822	C
4	3	2824	A
4	3	2829	G
4	3	2839	A
4	3	2853	U
4	3	2862	U
4	3	2863	G
4	3	2871	G
4	3	2876	G
4	3	2884	C
4	3	2887	A
4	3	2888	U
4	3	2895	A
4	3	2896	G
4	3	2899	C
5	4	9	C
5	4	10	C
5	4	11	A
5	4	13	G
5	4	14	U
5	4	22	G
5	4	23	A
5	4	28	C
5	4	33	U
5	4	35	C
5	4	39	U
5	4	41	C
5	4	48	A
5	4	49	G
5	4	54	U
5	4	56	A
5	4	60	C
5	4	64	G
5	4	65	G
5	4	80	G
5	4	82	U
5	4	83	U
5	4	84	C
5	4	85	A
5	4	88	G

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Mol	Chain	Res	Type
5	4	89	A
5	4	99	A
5	4	106	A
5	4	108	C
6	5	6	C
6	5	10	G
6	5	33	A
6	5	40	G
6	5	48	C
6	5	49	C
6	5	52	A
6	5	57	U
6	5	61	A
6	5	106	C
6	5	114	C
6	5	115	A
6	5	117	U
6	5	120	A
6	5	149	G
6	5	154	G
6	5	163	G
6	5	167	A
6	5	171	A
6	5	173	U
6	5	176	G
6	5	180	C
6	5	182	C
6	5	185	G
6	5	186	A
6	5	189	C
6	5	190	A
6	5	197	A
6	5	198	A
6	5	199	A
6	5	220	U
6	5	223	G
6	5	239	A
6	5	241	C
6	5	243	G
6	5	247	G
6	5	262	G
6	5	263	C

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Mol	Chain	Res	Type
6	5	269	A
6	5	275	A
6	5	285	G
6	5	301	G
6	5	302	A
6	5	324	C
6	5	325	A
6	5	326	C
6	5	328	G
6	5	341	C
6	5	342	G
6	5	344	G
6	5	347	G
6	5	348	C
6	5	350	G
6	5	359	A
6	5	363	U
6	5	368	C
6	5	369	A
6	5	370	A
6	5	374	G
6	5	380	G
6	5	383	U
6	5	394	U
6	5	408	U
6	5	416	U
6	5	418	U
6	5	419	A
6	5	422	A
6	5	425	G
6	5	426	U
6	5	447	G
6	5	449	A
6	5	450	U
6	5	452	A
6	5	461	G
6	5	462	G
6	5	464	A
6	5	468	G
6	5	470	U
6	5	475	U
6	5	476	U

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Mol	Chain	Res	Type
6	5	477	U
6	5	481	U
6	5	482	G
6	5	488	U
6	5	489	U
6	5	493	A
6	5	494	A
6	5	495	U
6	5	507	A
6	5	509	C
6	5	510	U
6	5	516	C
6	5	517	C
6	5	522	G
6	5	525	7MG
6	5	530	A
6	5	531	A
6	5	545	A
6	5	557	A
6	5	560	U
6	5	562	U
6	5	570	A
6	5	571	A
6	5	574	C
6	5	575	A
6	5	579	G
6	5	586	G
6	5	594	A
6	5	595	G
6	5	628	A
6	5	650	A
6	5	661	G
6	5	662	G
6	5	683	G
6	5	700	G
6	5	715	A
6	5	719	G
6	5	720	U
6	5	721	G
6	5	728	G
6	5	745	U
6	5	752	G

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Mol	Chain	Res	Type
6	5	768	G
6	5	790	U
6	5	791	A
6	5	811	A
6	5	812	A
6	5	814	C
6	5	818	A
6	5	825	A
6	5	829	G
6	5	836	C
6	5	838	A
6	5	839	U
6	5	867	A
6	5	883	A
6	5	885	U
6	5	908	A
6	5	910	C
6	5	911	G
6	5	921	G
6	5	922	G
6	5	929	C
6	5	930	A
6	5	955	U
6	5	964	A
6	5	970	A
6	5	971	A
6	5	972	A
6	5	982	A
6	5	987	U
6	5	988	G
6	5	989	A
6	5	994	C
6	5	995	U
6	5	996	U
6	5	997	G
6	5	998	G
6	5	999	C
6	5	1000	A
6	5	1002	A
6	5	1007	U
6	5	1009	G
6	5	1015	U

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Mol	Chain	Res	Type
6	5	1018	U
6	5	1019	G
6	5	1020	G
6	5	1022	G
6	5	1023	G
6	5	1024	U
6	5	1025	U
6	5	1027	A
6	5	1028	C
6	5	1029	C
6	5	1030	G
6	5	1032	G
6	5	1034	G
6	5	1036	C
6	5	1044	G
6	5	1047	U
6	5	1056	U
6	5	1072	G
6	5	1076	U
6	5	1078	G
6	5	1083	A
6	5	1085	G
6	5	1086	U
6	5	1092	A
6	5	1118	A
6	5	1121	U
6	5	1122	U
6	5	1123	G
6	5	1124	U
6	5	1134	C
6	5	1135	U
6	5	1141	U
6	5	1142	G
6	5	1158	A
6	5	1159	A
6	5	1170	C
6	5	1171	A
6	5	1172	A
6	5	1188	A
6	5	1189	U
6	5	1202	A
6	5	1203	A

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Mol	Chain	Res	Type
6	5	1213	A
6	5	1215	U
6	5	1231	U
6	5	1232	C
6	5	1233	G
6	5	1235	C
6	5	1255	A
6	5	1260	U
6	5	1271	U
6	5	1273	A
6	5	1274	G
6	5	1276	U
6	5	1279	G
6	5	1291	C
6	5	1294	U
6	5	1296	C
6	5	1297	G
6	5	1306	A
6	5	1312	G
6	5	1320	A
6	5	1321	G
6	5	1337	U
6	5	1338	A
6	5	1339	U
6	5	1343	G
6	5	1345	G
6	5	1372	C
6	5	1373	A
6	5	1397	G
6	5	1417	U
6	5	1426	U
6	5	1427	U
6	5	1428	A
6	5	1429	G
6	5	1462	G
6	5	1466	U
6	5	1467	A
6	5	1469	G
6	5	1472	G
6	5	1478	A
6	5	1480	G
6	5	1481	U

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Mol	Chain	Res	Type
6	5	1482	A
6	5	1492	G
6	5	1494	MA6
6	5	1504	G
6	5	1505	G
6	5	1510	C
6	5	1511	C
7	6	2	G
7	6	6	U
7	6	9	A
7	6	11	C
7	6	13	C
7	6	14	A
7	6	15	A
7	6	16	C
7	6	17	U
7	6	18	G
7	6	19	A
7	6	20	U
7	6	21	A
7	6	22	G
7	6	35	G
7	6	37	A
7	6	44	A
7	6	45	G
7	6	46	G
7	6	47	U
7	6	54	U
7	6	55	U
7	6	57	G
7	6	59	G
7	6	61	C
7	6	70	U
7	6	71	C
7	6	72	C
7	6	75	C
7	6	76	A
8	7	4	U
8	7	11	U
8	7	13	U
8	7	15	G
8	7	16	U

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Mol	Chain	Res	Type
8	7	17	G
8	7	19	A
8	7	20	U
8	7	21	A
8	7	22	A
8	7	34	G
8	7	44	G
8	7	46	U
8	7	47	U
8	7	48	G
8	7	51	G
8	7	57	A
8	7	71	C
8	7	73	C
8	7	75	A
9	8	3	A
9	8	9	A
9	8	10	G
9	8	15	G
9	8	16	U
9	8	17	U
9	8	18	G
9	8	19	G
9	8	20	U
9	8	21	A
9	8	30	G
9	8	31	A
9	8	41	A
9	8	46	G
9	8	47	U
9	8	48	C
9	8	58	A
9	8	60	C
9	8	71	G
9	8	73	A
9	8	74	C
9	8	75	C
9	8	76	A
31	Y	36	U
31	Y	37	G
31	Y	40	G
31	Y	42	U

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Mol	Chain	Res	Type
31	Y	43	A
31	Y	46	G
31	Y	47	U
31	Y	49	U
31	Y	50	U
31	Y	51	C
31	Y	52	A
31	Y	53	A
31	Y	54	A
31	Y	55	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	3	315	A
4	3	410	G
4	3	881	A
4	3	901	C
4	3	1124	G
4	3	1209	U
4	3	1352	G
4	3	1583	G
4	3	1618	U
4	3	2115	A
4	3	2116	U
4	3	2117	G
4	3	2129	U
4	3	2130	A
4	3	2152	C
4	3	2165	A
4	3	2169	G
4	3	2182	C
4	3	2183	U
4	3	2184	A
4	3	2194	G
4	3	2764	U
6	5	196	G
6	5	571	A
6	5	994	C
6	5	995	U
6	5	1024	U
6	5	1123	G

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Mol	Chain	Res	Type
6	5	1158	A
6	5	1273	A
6	5	1338	A
7	6	17	U
7	6	18	G
7	6	46	G
7	6	54	U
7	6	58	A
7	6	71	C
8	7	10	G
8	7	46	U
31	Y	42	U
31	Y	49	U
31	Y	51	C
31	Y	54	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	B8T	5	1377	6	19,22,23	3.32	8 (42%)	25,31,34	0.85	1 (4%)
6	7MG	5	525	6	23,26,27	3.62	11 (47%)	27,39,42	2.17	9 (33%)
6	MA6	5	1493	6	23,26,27	1.40	3 (13%)	33,38,41	3.24	14 (42%)
4	2MA	3	2511	4,62	22,25,26	4.12	10 (45%)	32,37,40	3.53	12 (37%)
6	MA6	5	1494	6	23,26,27	1.41	3 (13%)	33,38,41	3.25	14 (42%)
6	5MC	5	1375	6	19,22,23	4.56	8 (42%)	26,32,35	1.02	2 (7%)
4	OMG	3	2259	4,8,62	23,26,27	2.60	7 (30%)	32,38,41	2.43	10 (31%)
4	1MG	3	783	4	23,26,27	3.01	6 (26%)	33,39,42	2.34	8 (24%)

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
6	B8T	5	1377	6	-	2/7/27/28	0/2/2/2
6	7MG	5	525	6	-	2/7/37/38	0/3/3/3
6	MA6	5	1493	6	-	0/11/29/30	0/3/3/3
4	2MA	3	2511	4,62	-	1/7/25/26	0/3/3/3
6	MA6	5	1494	6	-	3/11/29/30	0/3/3/3
6	5MC	5	1375	6	-	0/7/25/26	0/2/2/2
4	OMG	3	2259	4,8,62	-	3/9/27/28	0/3/3/3
4	1MG	3	783	4	-	0/7/25/26	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	2511	2MA	C4-N3	11.92	1.49	1.34
6	5	1375	5MC	C6-C5	9.97	1.50	1.34
6	5	1375	5MC	C5-C4	9.27	1.51	1.44
6	5	525	7MG	C8-N9	8.72	1.51	1.45
4	3	783	1MG	C2-N3	8.50	1.47	1.33
4	3	2511	2MA	C2-N3	8.07	1.47	1.34
6	5	1375	5MC	C4-N3	7.94	1.46	1.34
4	3	2511	2MA	C6-N1	7.47	1.45	1.35
6	5	1377	B8T	C4-N3	7.47	1.45	1.32
4	3	2259	OMG	C2-N2	7.28	1.51	1.34
6	5	525	7MG	C5-N7	7.24	1.44	1.35
6	5	1375	5MC	C2-N3	7.19	1.50	1.36
4	3	783	1MG	C4-N3	6.72	1.49	1.34
6	5	1377	B8T	C2-N3	6.60	1.49	1.36
4	3	783	1MG	C2-N2	6.52	1.45	1.34
4	3	2511	2MA	C2-N1	6.45	1.45	1.34
4	3	2259	OMG	C4-N3	6.17	1.48	1.34
6	5	1377	B8T	C6-C5	6.10	1.49	1.35
6	5	525	7MG	C2-N3	5.82	1.47	1.33
6	5	1375	5MC	C4-N4	5.80	1.49	1.34
6	5	525	7MG	C4-N3	5.77	1.47	1.34
6	5	1375	5MC	C6-N1	5.62	1.47	1.38
4	3	2511	2MA	C5-C6	5.30	1.55	1.41
6	5	525	7MG	C4-N9	5.21	1.44	1.37
4	3	2259	OMG	C2-N3	5.16	1.45	1.33
6	5	525	7MG	C2-N2	4.82	1.45	1.34
6	5	1375	5MC	C2-N1	4.80	1.50	1.40
6	5	1377	B8T	C4-N4	4.64	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	1377	B8T	C2-N1	4.40	1.49	1.40
6	5	1493	MA6	C6-N6	4.21	1.48	1.36
6	5	1494	MA6	C6-N6	4.14	1.48	1.36
4	3	783	1MG	C2-N1	4.09	1.44	1.37
6	5	525	7MG	C2-N1	3.92	1.47	1.37
4	3	2511	2MA	C5-N7	-3.70	1.32	1.39
6	5	1377	B8T	C5-C4	3.70	1.49	1.41
6	5	525	7MG	C5-C6	3.68	1.52	1.43
6	5	525	7MG	C6-N1	3.49	1.45	1.38
4	3	783	1MG	C5-C6	3.49	1.54	1.45
4	3	2259	OMG	C2-N1	3.40	1.45	1.37
4	3	2511	2MA	C8-N7	3.35	1.38	1.31
6	5	1377	B8T	C6-N1	3.14	1.45	1.38
6	5	1377	B8T	O2-C2	-2.65	1.18	1.23
4	3	783	1MG	C5-N7	-2.63	1.33	1.39
6	5	525	7MG	O6-C6	-2.43	1.18	1.23
6	5	1494	MA6	C5-C4	-2.37	1.34	1.39
4	3	2259	OMG	C5-C6	2.36	1.53	1.44
6	5	1494	MA6	C5-N7	-2.34	1.34	1.39
6	5	1493	MA6	C5-C4	-2.30	1.35	1.39
6	5	1493	MA6	C5-N7	-2.29	1.34	1.39
6	5	1375	5MC	O2-C2	-2.18	1.19	1.23
4	3	2511	2MA	C6-N6	-2.14	1.28	1.34
4	3	2511	2MA	C4-N9	-2.12	1.33	1.37
4	3	2259	OMG	C8-N7	2.07	1.38	1.32
6	5	525	7MG	C5-C4	2.03	1.44	1.37
4	3	2259	OMG	O2'-CM2	-2.03	1.35	1.42
4	3	2511	2MA	C8-N9	-2.01	1.34	1.37

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	2511	2MA	C1'-N9-C8	-12.44	99.48	127.09
4	3	2511	2MA	C4-N9-C1'	10.79	151.88	126.63
6	5	1494	MA6	N1-C6-N6	-10.46	104.11	116.86
6	5	1493	MA6	N1-C6-N6	-10.43	104.15	116.86
6	5	1494	MA6	C5-C6-N6	6.85	136.18	125.33
6	5	1493	MA6	C5-C6-N6	6.85	136.17	125.33
4	3	783	1MG	C1'-N9-C4	-6.84	106.27	126.49
4	3	2259	OMG	C1'-N9-C8	-6.84	107.31	126.73
4	3	783	1MG	C1'-N9-C8	6.44	145.03	126.73
4	3	2511	2MA	C5-C4-N3	-5.83	121.03	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1494	MA6	N1-C2-N3	-5.64	120.04	128.58
4	3	2259	OMG	C1'-N9-C4	5.63	143.12	126.49
6	5	1493	MA6	N1-C2-N3	-5.58	120.13	128.58
6	5	1494	MA6	C1'-N9-C8	-5.25	115.44	127.09
6	5	1493	MA6	C1'-N9-C8	-5.24	115.47	127.09
4	3	783	1MG	C5-C4-N3	-5.11	120.25	128.39
6	5	525	7MG	C5-C6-N1	5.00	119.73	110.94
6	5	1493	MA6	C5-C4-N3	-4.78	120.13	126.72
4	3	2511	2MA	N9-C8-N7	-4.70	107.27	113.94
6	5	525	7MG	C2-N3-C4	4.70	120.39	112.30
6	5	1494	MA6	C5-C4-N3	-4.69	120.25	126.72
4	3	2259	OMG	C5-C4-N3	-4.57	121.12	128.39
6	5	1494	MA6	N9-C8-N7	-4.42	107.66	113.94
4	3	2259	OMG	C2-N3-C4	4.35	119.78	112.30
6	5	1493	MA6	N9-C8-N7	-4.26	107.90	113.94
6	5	1493	MA6	C4-N9-C1'	4.15	136.33	126.63
6	5	525	7MG	C5-C4-N3	-4.14	120.36	128.13
6	5	1494	MA6	C4-N9-C1'	4.08	136.18	126.63
6	5	1493	MA6	C4-C5-C6	3.93	119.97	115.91
6	5	1494	MA6	C4-C5-C6	3.78	119.82	115.91
6	5	525	7MG	C4-C5-N7	3.73	109.79	105.38
4	3	783	1MG	C2-N3-C4	3.62	120.12	111.98
4	3	2259	OMG	N9-C8-N7	-3.55	106.81	113.40
6	5	1494	MA6	C2-N1-C6	3.43	120.20	111.83
6	5	1493	MA6	C2-N1-C6	3.40	120.13	111.83
6	5	1494	MA6	C2-N3-C4	3.34	119.98	111.83
6	5	1493	MA6	C2-N3-C4	3.32	119.95	111.83
4	3	2511	2MA	N3-C2-N1	-3.27	119.99	125.77
4	3	783	1MG	N9-C8-N7	-3.15	107.55	113.40
6	5	525	7MG	C5-C4-N9	3.15	110.37	106.33
4	3	783	1MG	N9-C4-N3	3.15	132.25	125.95
4	3	2511	2MA	C5-N7-C8	3.04	108.23	103.45
6	5	1494	MA6	C5-N7-C8	2.97	108.11	103.45
4	3	2511	2MA	N3-C4-N9	2.96	130.74	126.99
4	3	2259	OMG	C2-N1-C6	-2.95	119.75	125.11
6	5	1493	MA6	C5-N7-C8	2.93	108.06	103.45
6	5	1375	5MC	C5-C6-N1	-2.87	120.20	123.31
6	5	525	7MG	C2-N1-C6	-2.83	119.98	125.11
6	5	525	7MG	O6-C6-C5	-2.82	120.69	127.62
6	5	1493	MA6	N3-C4-N9	2.79	131.91	127.17
4	3	2259	OMG	N9-C4-N3	2.76	131.47	125.95
4	3	2511	2MA	C4-N9-C8	2.76	108.63	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1494	MA6	N3-C4-N9	2.75	131.85	127.17
4	3	783	1MG	C5-C6-N1	2.69	120.00	115.02
4	3	2259	OMG	C5-C6-N1	2.66	120.02	113.25
4	3	2511	2MA	CM2-C2-N1	2.64	121.08	117.13
6	5	525	7MG	N9-C4-N3	2.60	129.27	125.46
4	3	2511	2MA	C4-C5-N7	-2.56	107.65	110.58
6	5	1377	B8T	C6-C5-C4	2.54	120.06	117.00
6	5	1494	MA6	C4-N9-C8	2.51	108.38	105.74
4	3	2259	OMG	O6-C6-C5	-2.43	120.13	126.53
6	5	1493	MA6	C4-C5-N7	-2.35	107.89	110.58
6	5	1493	MA6	C4-N9-C8	2.34	108.19	105.74
4	3	2259	OMG	C8-N7-C5	2.30	108.36	104.26
6	5	1494	MA6	C4-C5-N7	-2.30	107.95	110.58
6	5	525	7MG	N9-C8-N7	2.30	106.63	103.37
4	3	2511	2MA	C5-C4-N9	2.21	108.22	105.81
4	3	783	1MG	C8-N7-C5	2.20	108.17	104.26
4	3	2511	2MA	N6-C6-N1	2.19	119.98	117.03
6	5	1375	5MC	CM5-C5-C6	-2.17	119.91	122.85

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	3	2259	OMG	O4'-C4'-C5'-O5'
4	3	2259	OMG	C1'-C2'-O2'-CM2
6	5	525	7MG	O4'-C4'-C5'-O5'
6	5	1494	MA6	O4'-C4'-C5'-O5'
4	3	2259	OMG	C3'-C4'-C5'-O5'
6	5	525	7MG	C3'-C4'-C5'-O5'
6	5	1494	MA6	C3'-C4'-C5'-O5'
6	5	1377	B8T	O4'-C4'-C5'-O5'
6	5	1494	MA6	C5-C6-N6-C10
4	3	2511	2MA	C4'-C5'-O5'-P
6	5	1377	B8T	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	5	1493	MA6	1	0
4	3	783	1MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 367 ligands modelled in this entry, 331 are monoatomic - leaving 36 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	$\# Z > 2$
65	SPD	3	3234	-	9,9,9	0.32	0	8,8,8	0.85	0
65	SPD	3	3245	-	9,9,9	0.32	0	8,8,8	0.82	0
64	SPM	3	3248	-	13,13,13	0.35	0	12,12,12	0.88	0
66	N2P	3	3242	-	6,6,6	0.25	0	5,5,5	0.63	0
65	SPD	5	1603	-	9,9,9	0.30	0	8,8,8	0.79	0
66	N2P	5	1602	-	6,6,6	0.25	0	5,5,5	0.62	0
63	PUT	3	3224	-	5,5,5	0.24	0	4,4,4	0.51	0
65	SPD	3	3235	-	9,9,9	0.32	0	8,8,8	0.82	0
65	SPD	3	3233	-	9,9,9	0.32	0	8,8,8	0.77	0
65	SPD	3	3232	-	9,9,9	0.31	0	8,8,8	0.87	0
63	PUT	5	1604	-	5,5,5	0.25	0	4,4,4	0.52	0
65	SPD	3	3238	-	9,9,9	0.32	0	8,8,8	0.87	0
67	LYS	8	103	9	7,8,9	0.87	0	3,8,10	0.30	0
65	SPD	3	3229	-	9,9,9	0.32	0	8,8,8	0.79	0
65	SPD	3	3239	-	9,9,9	0.32	0	8,8,8	0.85	0
60	CLM	3	3001	-	20,20,20	0.69	1 (5%)	23,27,27	0.62	0
65	SPD	3	3247	-	9,9,9	0.31	0	8,8,8	0.87	0
66	N2P	3	3243	-	6,6,6	0.23	0	5,5,5	0.61	0
65	SPD	3	3231	-	9,9,9	0.34	0	8,8,8	0.74	0
63	PUT	3	3230	-	5,5,5	0.24	0	4,4,4	0.49	0
63	PUT	3	3241	-	5,5,5	0.25	0	4,4,4	0.52	0
65	SPD	3	3228	-	9,9,9	0.32	0	8,8,8	0.85	0
64	SPM	b	303	-	13,13,13	0.17	0	12,12,12	0.31	0
65	SPD	3	3227	-	9,9,9	0.32	0	8,8,8	0.86	0
63	PUT	3	3223	-	5,5,5	0.24	0	4,4,4	0.52	0
65	SPD	3	3236	-	9,9,9	0.32	0	8,8,8	0.92	0
65	SPD	3	3237	-	9,9,9	0.32	0	8,8,8	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
64	SPM	3	3226	-	13,13,13	0.35	0	12,12,12	0.90	0
65	SPD	5	1601	-	9,9,9	0.35	0	8,8,8	0.77	0
63	PUT	3	3222	-	5,5,5	0.23	0	4,4,4	0.54	0
65	SPD	3	3249	-	9,9,9	0.18	0	8,8,8	0.18	0
64	SPM	3	3240	-	13,13,13	0.35	0	12,12,12	0.91	0
65	SPD	3	3244	-	9,9,9	0.32	0	8,8,8	0.88	0
66	N2P	3	3246	-	6,6,6	0.24	0	5,5,5	0.65	0
63	PUT	3	3221	-	5,5,5	0.23	0	4,4,4	0.53	0
63	PUT	3	3225	-	5,5,5	0.24	0	4,4,4	0.50	0

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
65	SPD	3	3234	-	-	0/7/7/7	-
65	SPD	3	3245	-	-	1/7/7/7	-
64	SPM	3	3248	-	-	2/11/11/11	-
66	N2P	3	3242	-	-	1/4/4/4	-
65	SPD	5	1603	-	-	1/7/7/7	-
66	N2P	5	1602	-	-	3/4/4/4	-
63	PUT	3	3224	-	-	1/3/3/3	-
65	SPD	3	3235	-	-	0/7/7/7	-
65	SPD	3	3233	-	-	2/7/7/7	-
65	SPD	3	3232	-	-	0/7/7/7	-
63	PUT	5	1604	-	-	0/3/3/3	-
65	SPD	3	3238	-	-	2/7/7/7	-
67	LYS	8	103	9	-	3/6/7/9	-
65	SPD	3	3229	-	-	0/7/7/7	-
65	SPD	3	3239	-	-	0/7/7/7	-
60	CLM	3	3001	-	-	2/20/22/22	0/1/1/1
65	SPD	3	3247	-	-	0/7/7/7	-
66	N2P	3	3243	-	-	2/4/4/4	-
65	SPD	3	3231	-	-	1/7/7/7	-
63	PUT	3	3230	-	-	0/3/3/3	-
63	PUT	3	3241	-	-	0/3/3/3	-
65	SPD	3	3228	-	-	1/7/7/7	-
64	SPM	b	303	-	-	2/11/11/11	-
65	SPD	3	3227	-	-	0/7/7/7	-
63	PUT	3	3223	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	SPD	3	3236	-	-	1/7/7/7	-
65	SPD	3	3237	-	-	0/7/7/7	-
64	SPM	3	3226	-	-	4/11/11/11	-
65	SPD	5	1601	-	-	1/7/7/7	-
63	PUT	3	3222	-	-	0/3/3/3	-
65	SPD	3	3249	-	-	0/7/7/7	-
64	SPM	3	3240	-	-	2/11/11/11	-
65	SPD	3	3244	-	-	0/7/7/7	-
66	N2P	3	3246	-	-	1/4/4/4	-
63	PUT	3	3221	-	-	0/3/3/3	-
63	PUT	3	3225	-	-	0/3/3/3	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	3	3001	CLM	C1-C2	-2.11	1.49	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
67	8	103	LYS	O-C-CA-CB
67	8	103	LYS	C-CA-CB-CG
65	5	1603	SPD	C8-C7-N6-C5
66	5	1602	N2P	C2-C3-C4-C5
66	3	3242	N2P	C2-C3-C4-C5
65	3	3228	SPD	N6-C7-C8-C9
60	3	3001	CLM	C5-C3-N2-C2
64	3	3240	SPM	C7-C6-N5-C4
64	3	3226	SPM	C7-C8-C9-N10
66	3	3246	N2P	C2-C3-C4-C5
66	3	3243	N2P	C2-C3-C4-C5
64	3	3248	SPM	C6-C7-C8-C9
65	3	3233	SPD	C8-C7-N6-C5
64	3	3226	SPM	C7-C6-N5-C4
67	8	103	LYS	N-CA-CB-CG
66	5	1602	N2P	C3-C4-C5-N1
65	3	3231	SPD	N1-C2-C3-C4
65	3	3238	SPD	C8-C7-N6-C5
65	3	3236	SPD	C8-C7-N6-C5

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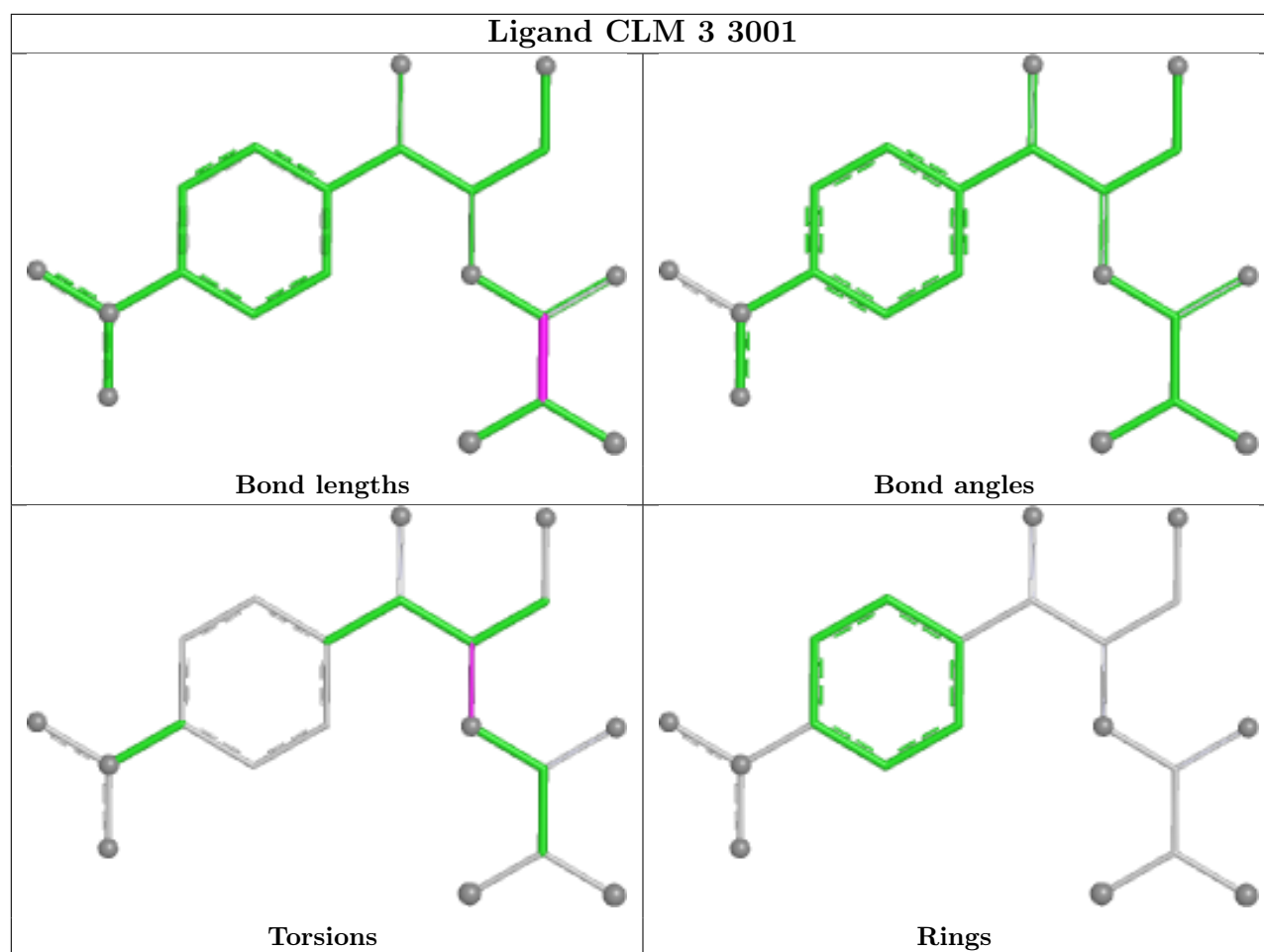
Mol	Chain	Res	Type	Atoms
63	3	3224	PUT	C1-C2-C3-C4
60	3	3001	CLM	C4-C3-N2-C2
66	3	3243	N2P	C3-C4-C5-N1
66	5	1602	N2P	NE2-C1-C2-C3
64	b	303	SPM	C3-C4-N5-C6
64	3	3226	SPM	N10-C11-C12-C13
64	3	3240	SPM	N10-C11-C12-C13
65	5	1601	SPD	N1-C2-C3-C4
64	b	303	SPM	C7-C6-N5-C4
65	3	3238	SPD	C2-C3-C4-C5
65	3	3233	SPD	C4-C5-N6-C7
64	3	3226	SPM	C6-C7-C8-C9
64	3	3248	SPM	C7-C8-C9-N10
65	3	3245	SPD	C3-C4-C5-N6

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	3	3248	SPM	1	0
65	5	1603	SPD	1	0
63	3	3224	PUT	1	0
60	3	3001	CLM	4	0
65	3	3247	SPD	1	0
63	3	3230	PUT	1	0
64	3	3226	SPM	4	0
65	3	3249	SPD	3	0
64	3	3240	SPM	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

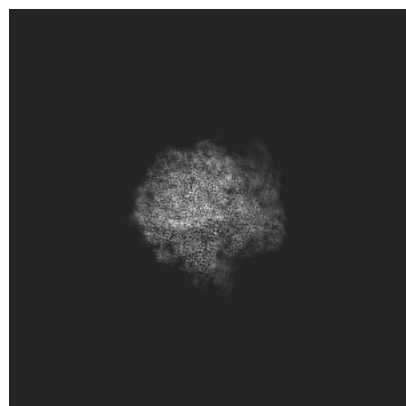
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17132. These allow visual inspection of the internal detail of the map and identification of artifacts.

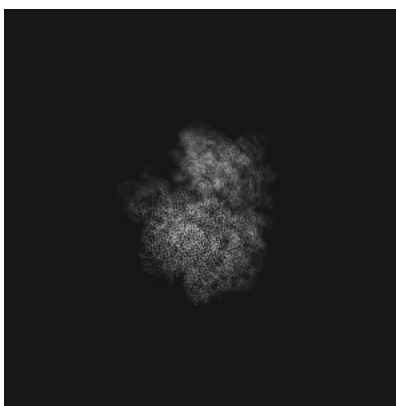
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

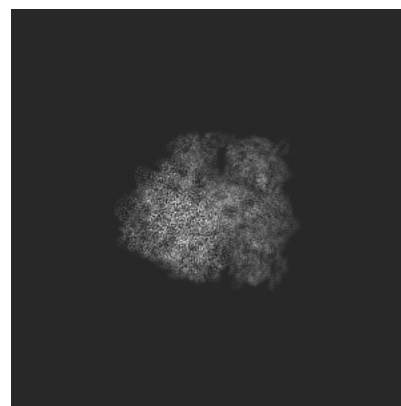
6.1.1 Primary map



X

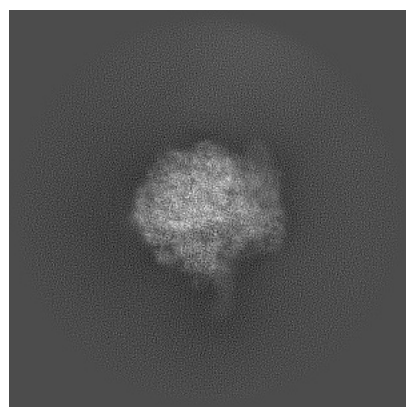


Y

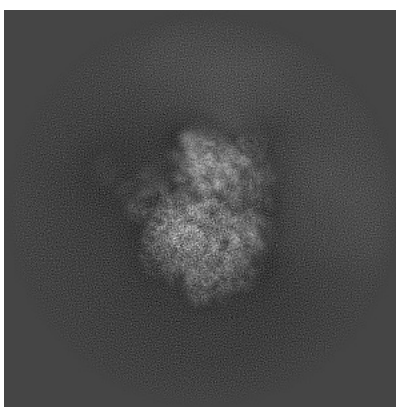


Z

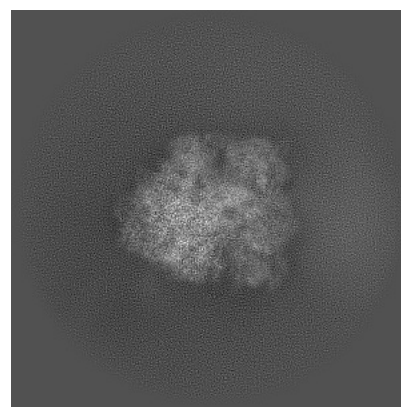
6.1.2 Raw map



X



Y

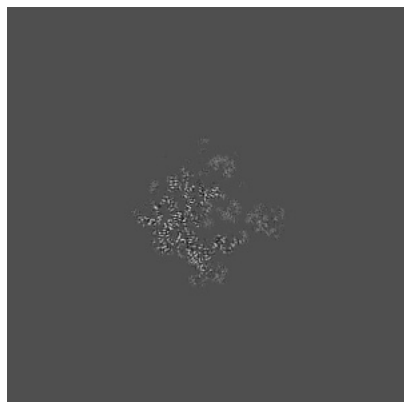


Z

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

6.2 Central slices [i](#)

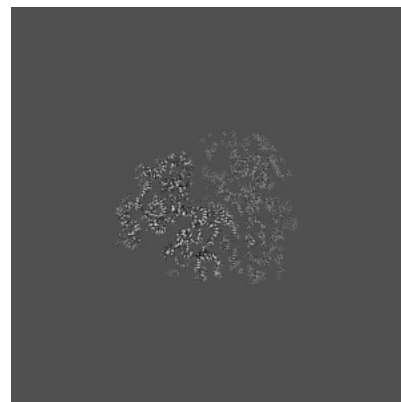
6.2.1 Primary map



X Index: 211

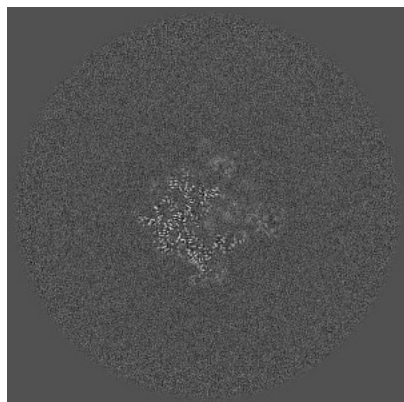


Y Index: 211

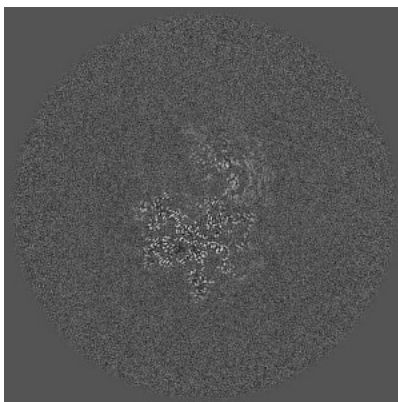


Z Index: 211

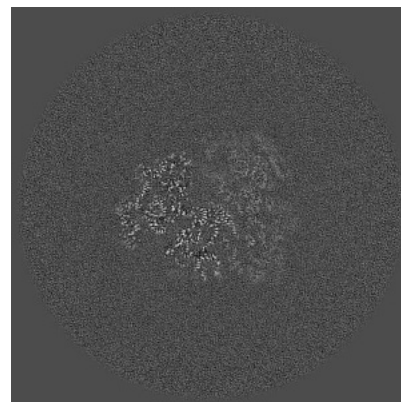
6.2.2 Raw map



X Index: 211



Y Index: 211



Z Index: 211

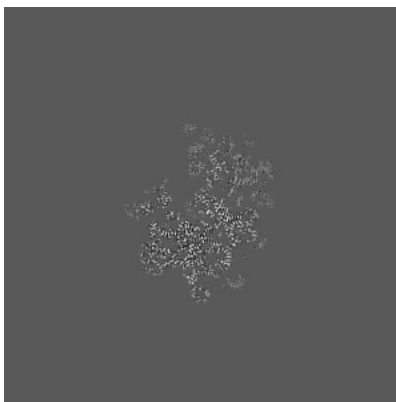
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

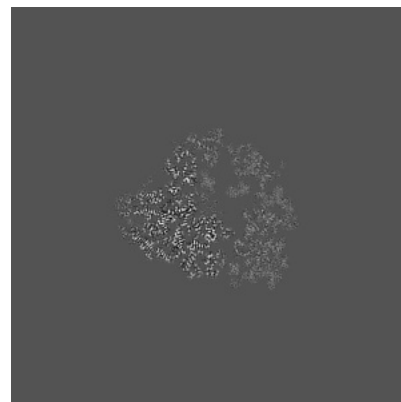
6.3.1 Primary map



X Index: 182

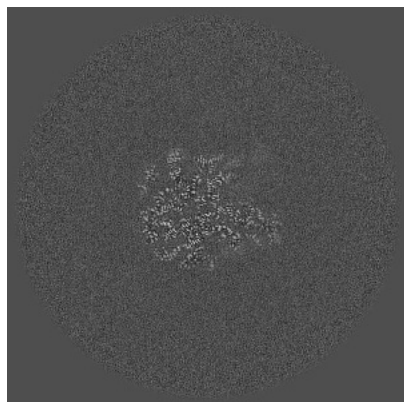


Y Index: 204

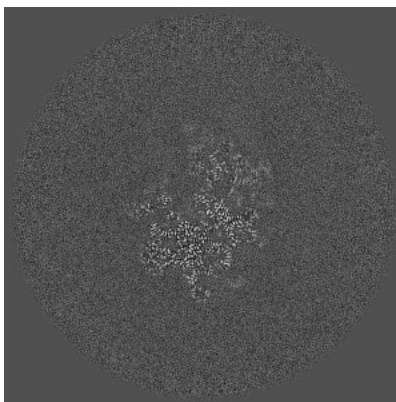


Z Index: 199

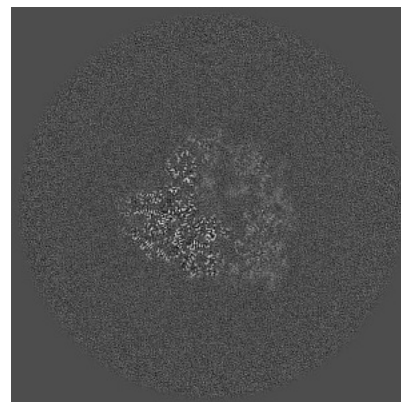
6.3.2 Raw map



X Index: 185



Y Index: 204

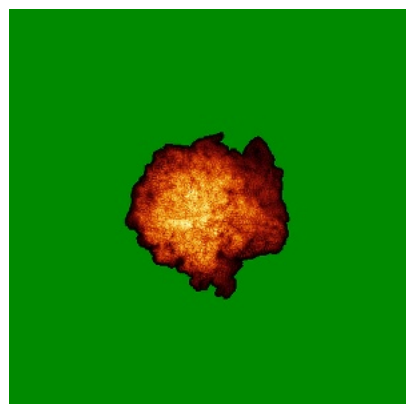


Z Index: 199

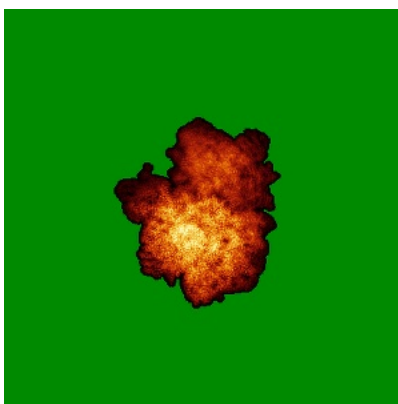
The images above show the largest variance slices of the map in three orthogonal directions.

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

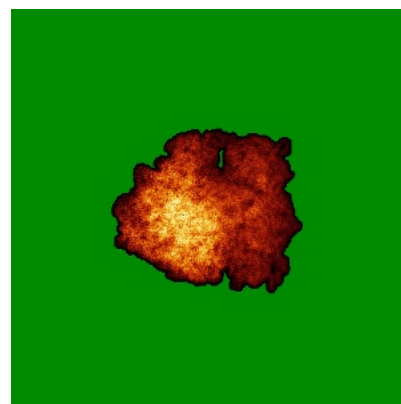
6.4.1 Primary map



X

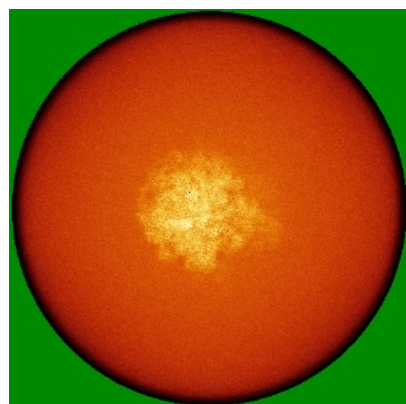


Y

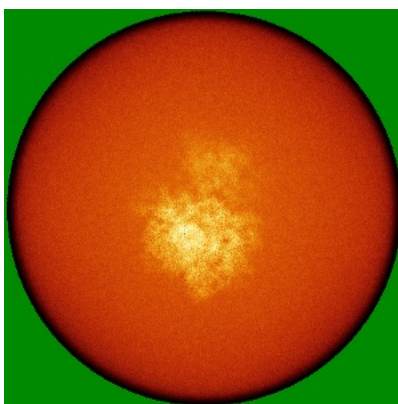


Z

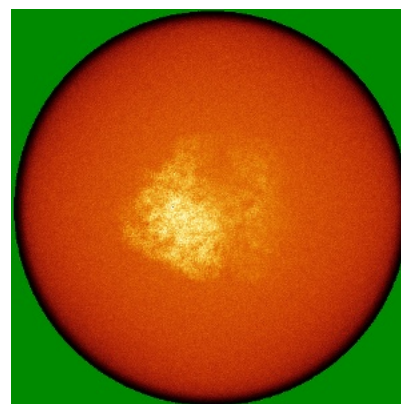
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



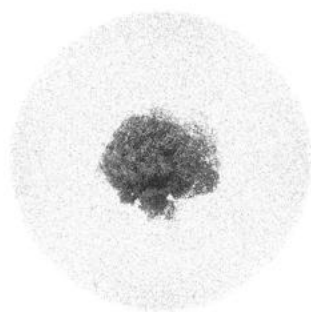
Y



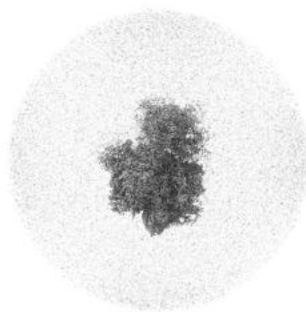
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

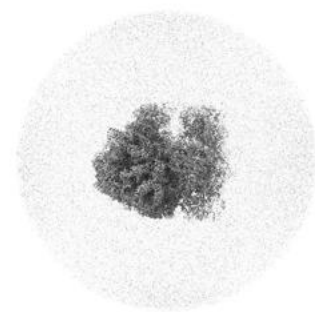
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

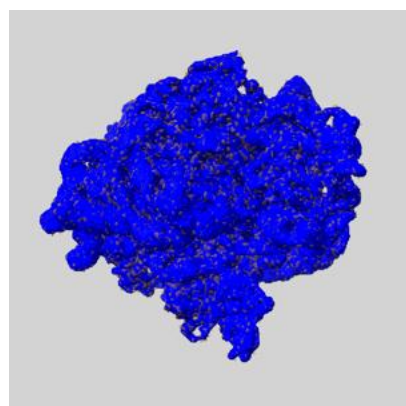
6.6 Mask visualisation [i](#)

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

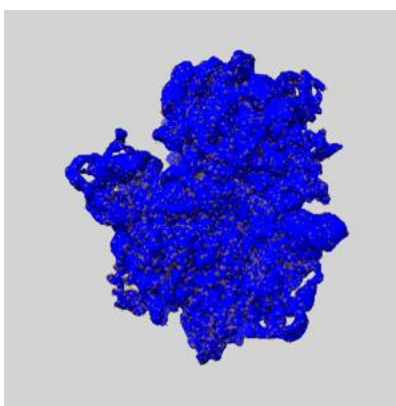
A mask typically either:

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

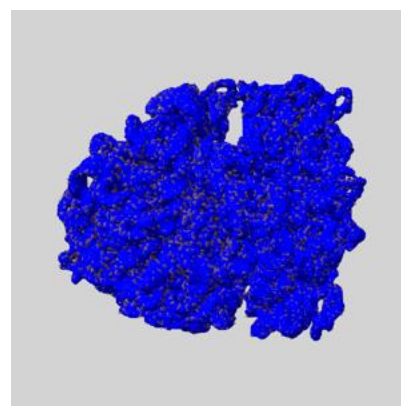
6.6.1 emd_17132_msk_1.map [i](#)



X



Y

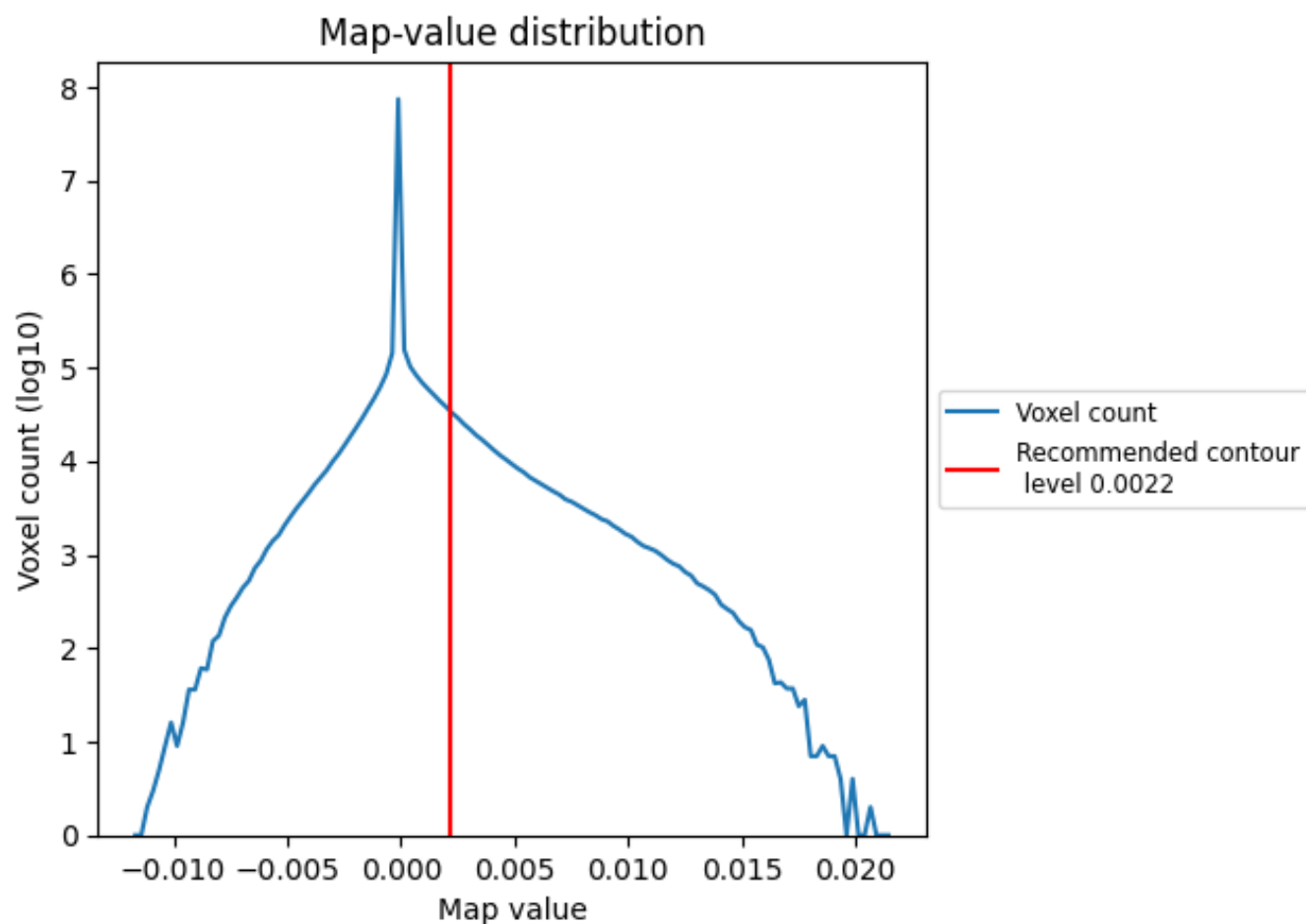


Z

7 Map analysis [i](#)

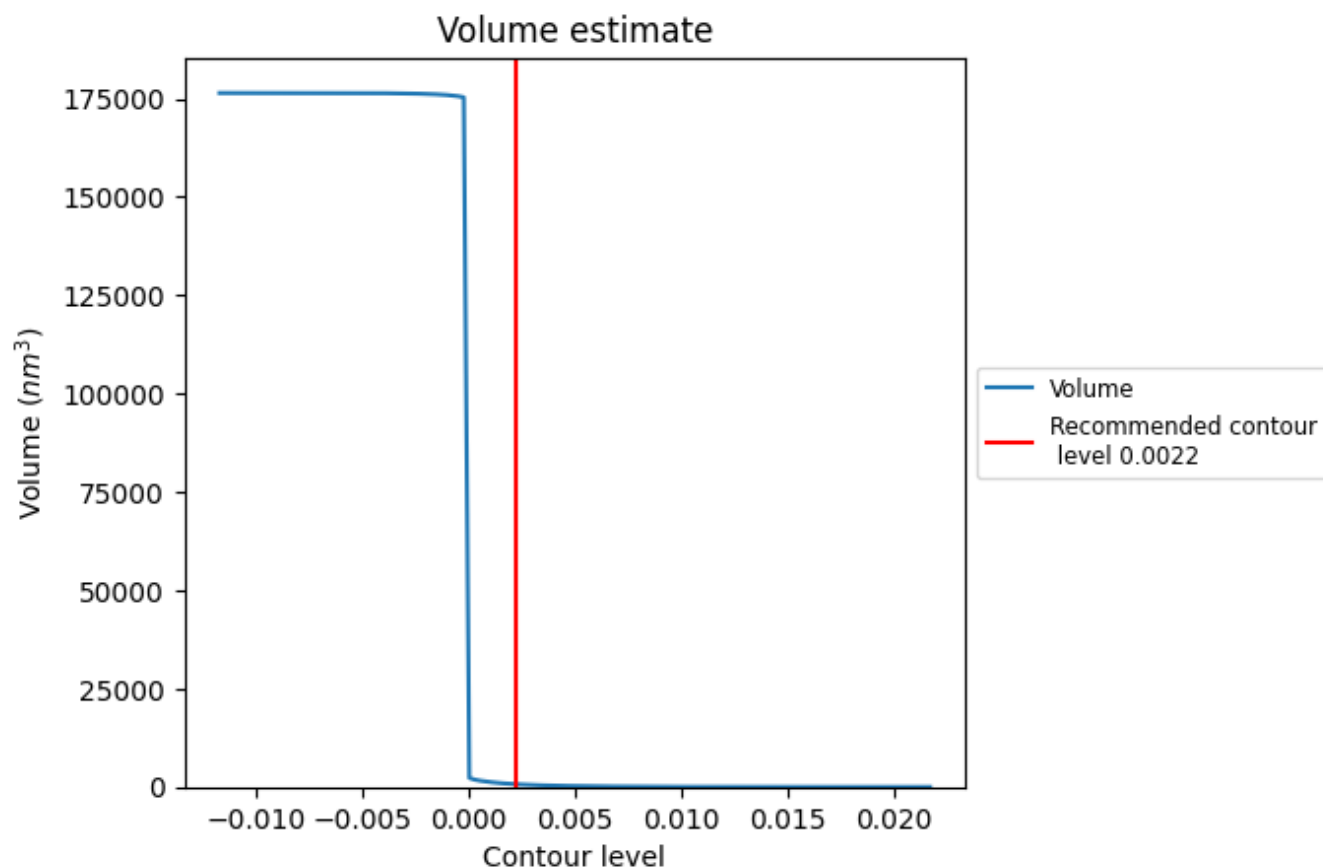
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

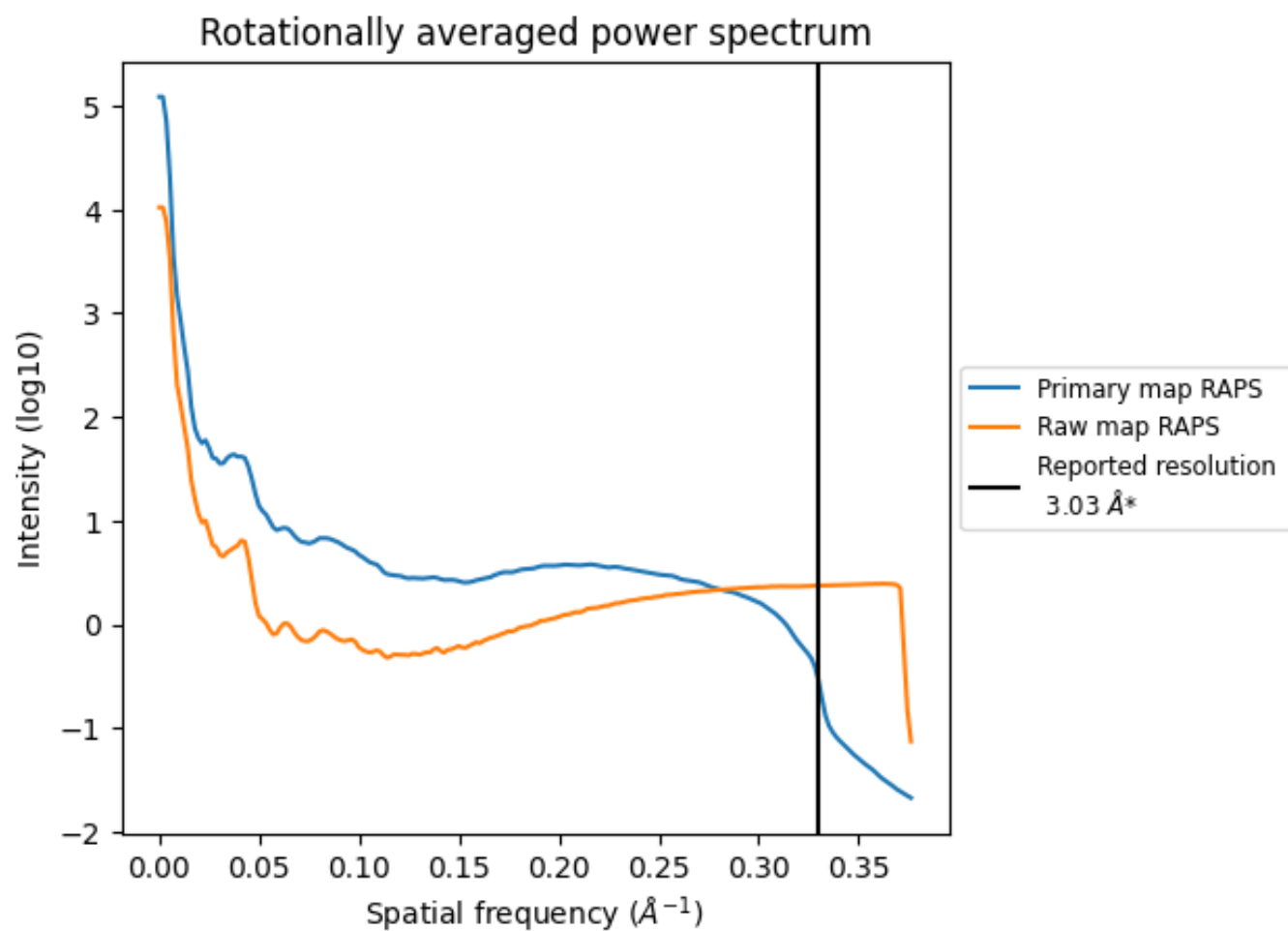
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 710 nm^3 ; this corresponds to an approximate mass of 642 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

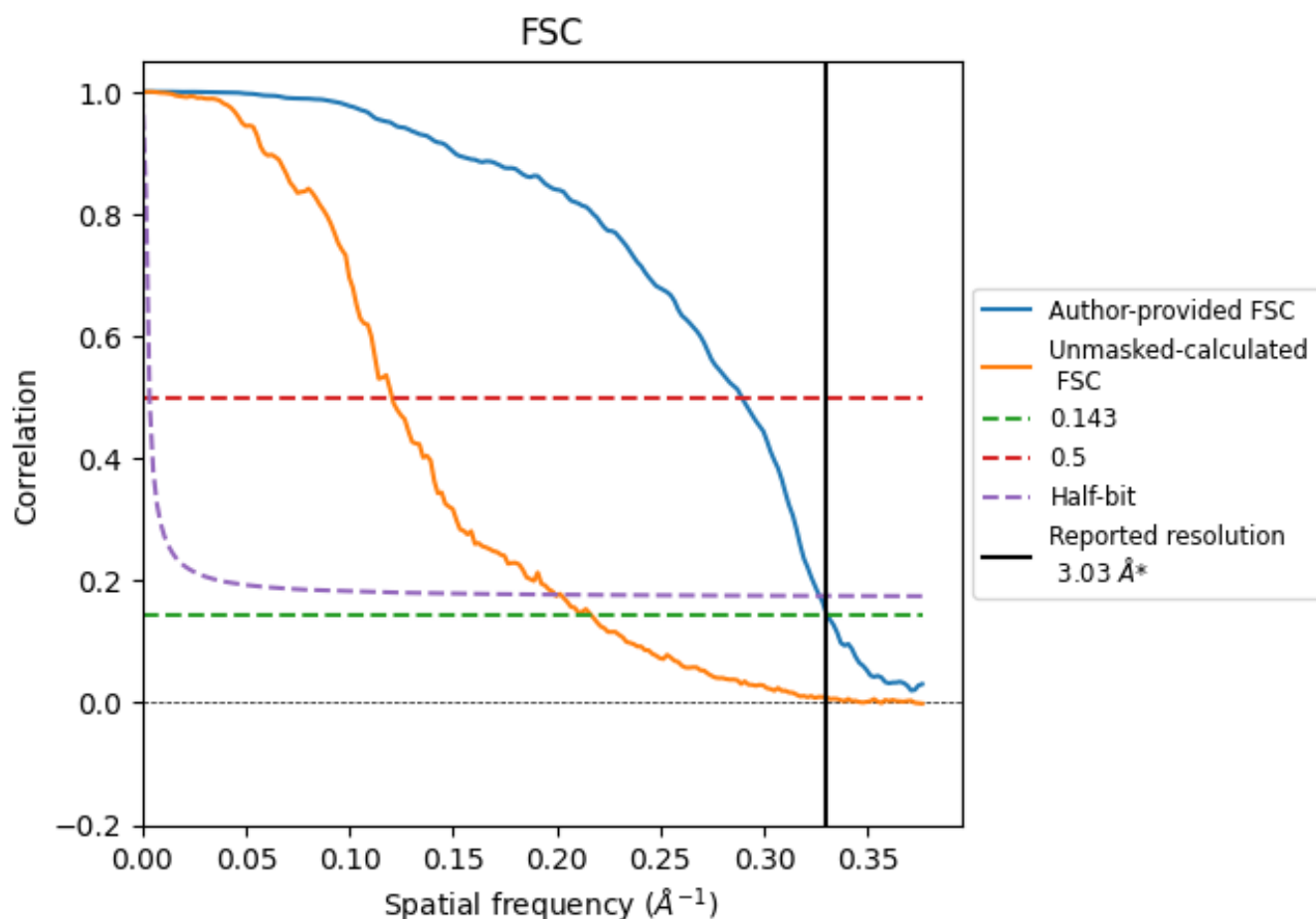


*Reported resolution corresponds to spatial frequency of 0.330 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.330 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

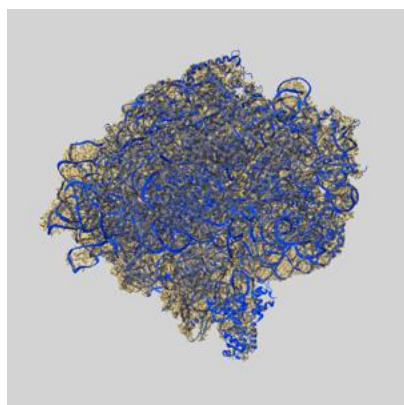
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.02	3.46	3.06
Unmasked-calculated*	4.61	8.30	5.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.61 differs from the reported value 3.03 by more than 10 %

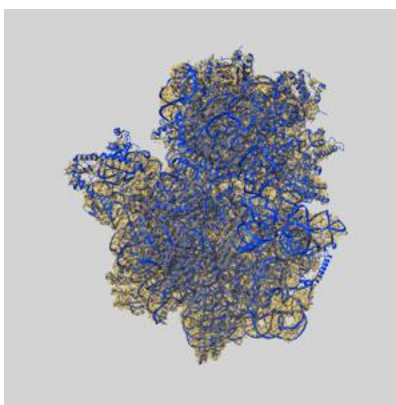
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17132 and PDB model 8P7X. Per-residue inclusion information can be found in section [3](#) on page [21](#).

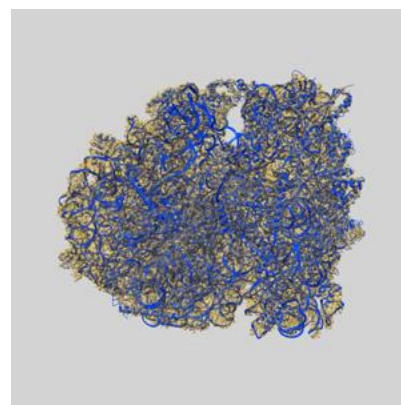
9.1 Map-model overlay [i](#)



X



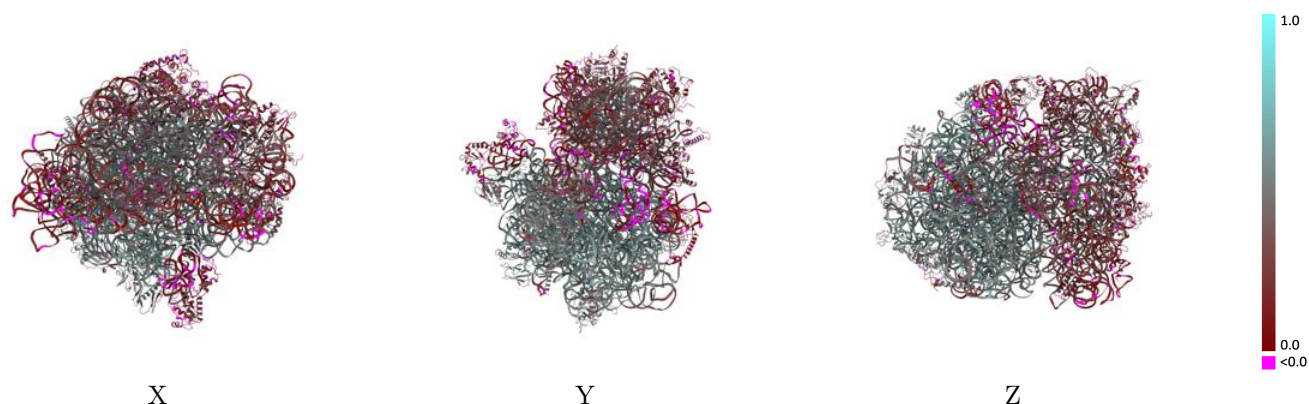
Y



Z

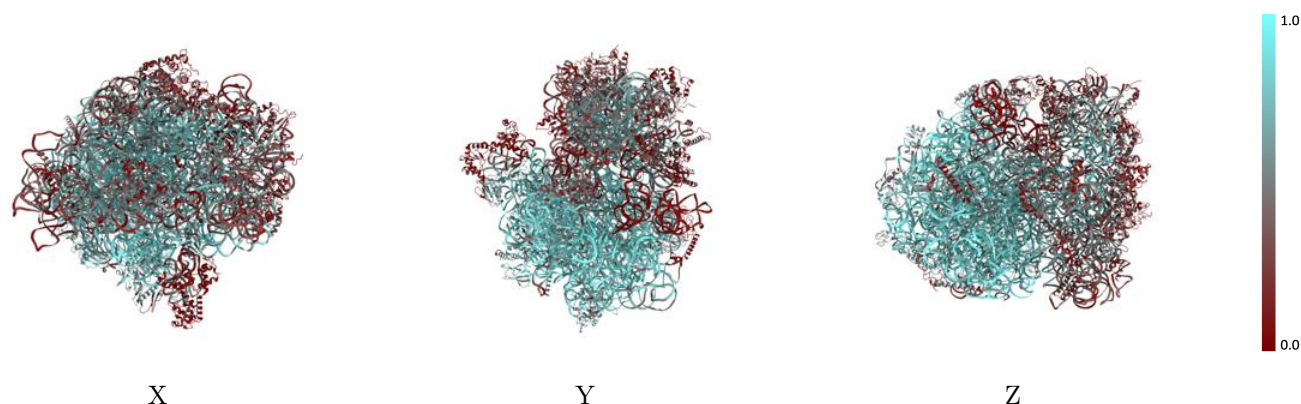
The images above show the 3D surface view of the map at the recommended contour level 0.0022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



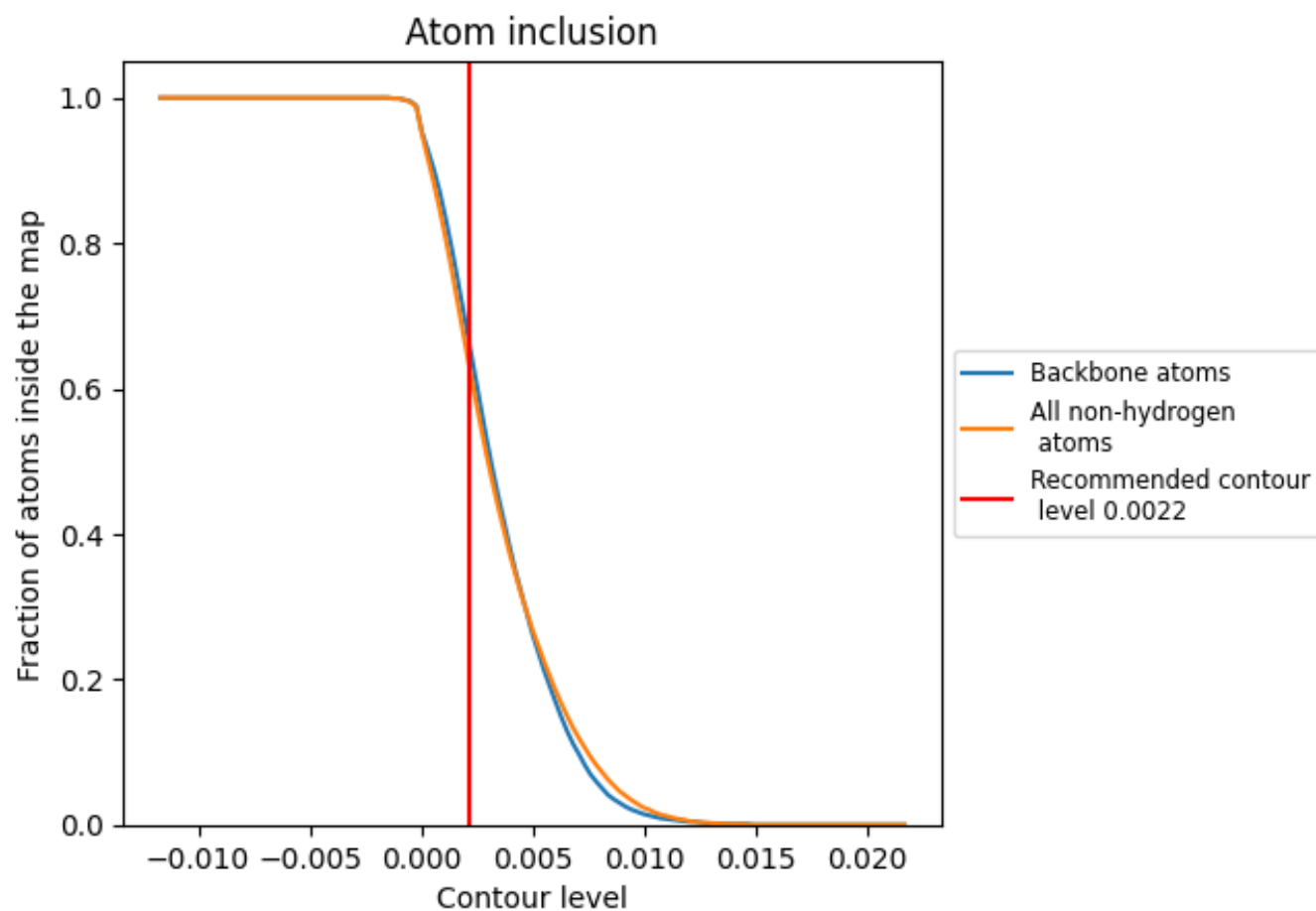
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6250	 0.4120
0	 0.7390	 0.5420
1	 0.7000	 0.5460
2	 0.7070	 0.5340
3	 0.8280	 0.5150
4	 0.7390	 0.4420
5	 0.5710	 0.3220
6	 0.0210	 0.0020
7	 0.5260	 0.3410
8	 0.2850	 0.2860
A	 0.2370	 0.2030
B	 0.3660	 0.3460
C	 0.1850	 0.1980
D	 0.4190	 0.3590
E	 0.1760	 0.1810
F	 0.1790	 0.2280
G	 0.3020	 0.2960
H	 0.2360	 0.2410
I	 0.2570	 0.2710
J	 0.2360	 0.2450
K	 0.4300	 0.3510
L	 0.1700	 0.1900
M	 0.3880	 0.3510
N	 0.2750	 0.2470
O	 0.2220	 0.1900
P	 0.1950	 0.1980
Q	 0.2400	 0.2100
R	 0.1470	 0.1980
S	 0.2400	 0.2080
T	 0.2940	 0.2930
X	 0.0170	 0.1100
Y	 0.3770	 0.3210
Z	 0.0700	 0.1600
a	 0.6990	 0.5260
b	 0.6870	 0.5170



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Chain	Atom inclusion	Q-score
c	 0.6560	 0.4900
d	 0.3530	 0.3310
e	 0.4920	 0.4340
f	 0.1300	 0.1140
g	 0.0820	 0.1300
h	 0.0260	 0.0700
i	 0.7010	 0.5140
j	 0.6700	 0.5200
k	 0.6430	 0.4890
l	 0.7100	 0.5230
m	 0.7040	 0.5300
n	 0.5760	 0.4810
o	 0.6550	 0.5000
p	 0.6840	 0.5400
q	 0.6910	 0.5180
r	 0.7020	 0.5280
s	 0.6390	 0.4880
t	 0.4990	 0.4120
u	 0.6550	 0.5070
v	 0.6470	 0.5030
w	 0.5020	 0.4290
x	 0.1260	 0.1760
y	 0.7210	 0.5340
z	 0.6830	 0.5260