



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 12:23 AM EDT

PDB ID : 7UVZ / pdb_00007uvz
EMDB ID : EMD-26821
Title : A. baumannii ribosome-Streptothricin-D complex: 70S with E-site tRNA
Authors : Morgan, C.E.; Yu, E.W.
Deposited on : 2022-05-02
Resolution : 2.21 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

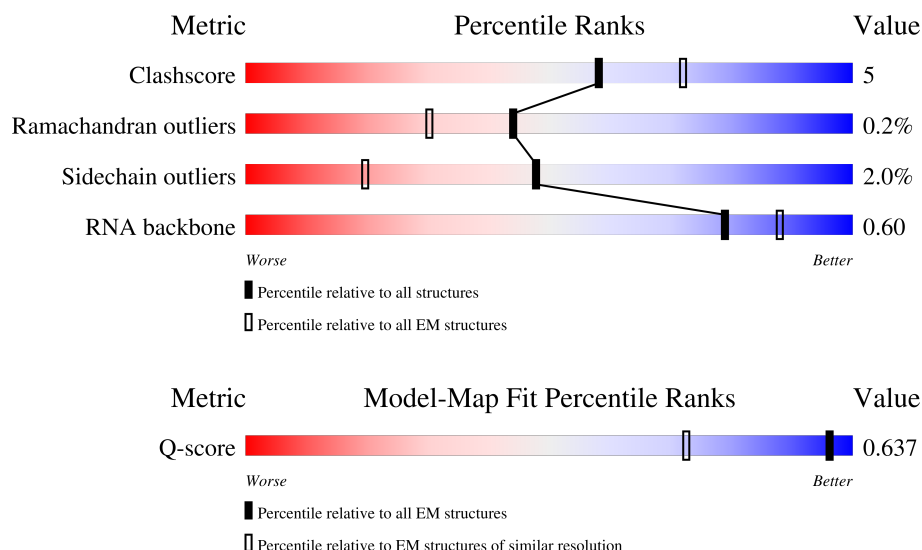
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.21 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	3231 (1.71 - 2.71)

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	51	
2	1	44	
3	2	64	

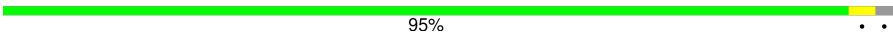
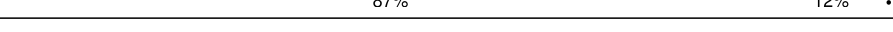
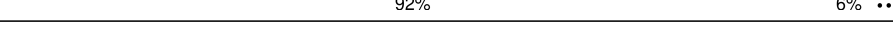
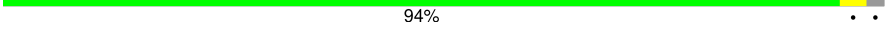
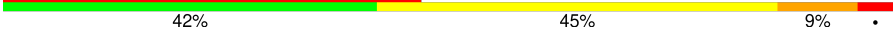
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Mol	Chain	Length	Quality of chain
4	3	38	
5	A	2918	
6	B	115	
7	C	274	
8	D	212	
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	

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Mol	Chain	Length	Quality of chain
29	Y	58	 95% . .
30	Z	61	 82% 7% 11%
31	a	1544	 67% 29% . .
32	b	250	 80% 66% 22% 10%
33	c	250	 76% 10% 14%
34	d	208	 6% 73% 27%
35	e	165	 82% 12% 6%
36	f	127	 68% 14% 18%
37	g	156	 18% 71% 15% 13%
38	h	131	 89% 10% .
39	i	128	 89% 9% . .
40	j	103	 7% 86% 11% .
41	k	128	 70% 20% 9%
42	l	124	 5% 79% 17% . .
43	m	118	 85% 13% .
44	n	101	 87% 12% .
45	o	89	 92% 6% . .
46	p	101	 76% 5% 19%
47	q	85	 80% 13% 7%
48	r	75	 61% 7% 31%
49	s	91	 82% 8% 10%
50	t	88	 94% . .
51	u	71	 58% 66% 21% 11%
52	v	77	 47% 42% 45% 9%
53	w	3	 33% 67%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 138943 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 L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2730	Total	C	N	O	P	0	0
			58566	26143	10721	18972	2730		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	272	Total	C	N	O	S	0	0
			2111	1302	436	365	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	200	Total	C	N	O	S	0	0
			1516	952	281	278	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	174	Total	C	N	O	S	0	0
			1370	871	243	248	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	144	Total	C	N	O		0	0
			1071	663	213	195			

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total	C	N	O	S	0	0
			1087	687	210	185	5		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	116	Total	C	N	O	S	0	0
			873	537	176	158	2		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	117	Total	C	N	O		0	0
			919	578	177	164			

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total	C	N	O	S	0	0
			807	506	155	143	3		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total	C	N	O	S	0	0
			826	514	158	150	4		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	91	Total	C	N	O	S	0	0
			710	452	128	129	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	103	Total	C	N	O	S	0	0
			766	476	142	148			

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total	C	N	O	S	0	0
			760	477	143	139	1		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	76	Total	C	N	O	S	0	0
			577	358	111	106	2		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	77	Total	C	N	O	S	0	0
			632	395	130	105	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	60	Total	C	N	O	S	0	0
			486	302	93	90	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	57	Total	C	N	O	S	0	0
			455	281	87	84	3		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	54	Total	C	N	O	S	0	0
			447	265	100	81	1		

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1528	Total	C	N	O	P	0	0
			32782	14631	5994	10630	1527		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	225	Total	C	N	O	S	0	0
			1769	1110	328	325	6		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	104	Total	C	N	O	S	0	0
			867	546	158	159	4		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	136	Total	C	N	O	S	0	0
			1073	671	201	194	7		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	126	Total	C	N	O	S	0	0
			991	618	197	175	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			862	535	167	159	1		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	82	Total	C	N	O	S	0	0
			644	403	128	112	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	52	Total	C	N	O	0	0
			426	273	74	79		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			646	412	125	107	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	86	Total	C	N	O	S	0	0
			663	409	139	113	2		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	63	Total	C	N	O	S	0	0
			522	327	105	89	1		

- Molecule 52 is a RNA chain called tRNA-met.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	v	77	Total	C	N	O	P	S	0	0
			1636	733	291	535	76	1		

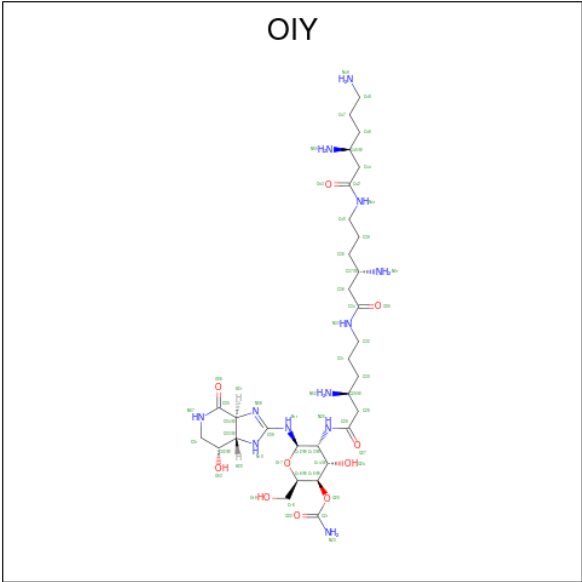
- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total	Zn	0
			1	1	

- Molecule 55 is Streptothricin D (CCD ID: OIY) (formula: C₃₁H₅₈N₁₂O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
55	A	1	Total	C	N	O	0
			31	16	7	8	
55	A	1	Total	C	N	O	0
			53	31	12	10	
55	A	1	Total	C	N	O	0
			40	22	9	9	
55	A	1	Total	C	N	O	0
			47	27	10	10	
55	A	1	Total	C	N	O	0
			53	31	12	10	
55	A	1	Total	C	N	O	0
			35	19	8	8	
55	N	1	Total	C	N	O	0
			35	19	8	8	
55	a	1	Total	C	N	O	0
			35	19	8	8	
55	a	1	Total	C	N	O	0
			53	31	12	10	
55	a	1	Total	C	N	O	0
			53	31	12	10	
55	a	1	Total	C	N	O	0
			35	19	8	8	

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

Mol	Chain	Residues	Atoms		AltConf
56	A	1	Total	Mg	0
			1	1	

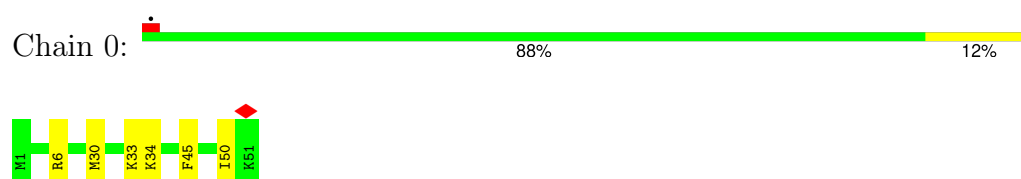
- Molecule 57 is water.

Mol	Chain	Residues	Atoms		AltConf
57	A	4	Total 4	O 4	0
57	R	1	Total 1	O 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 L33

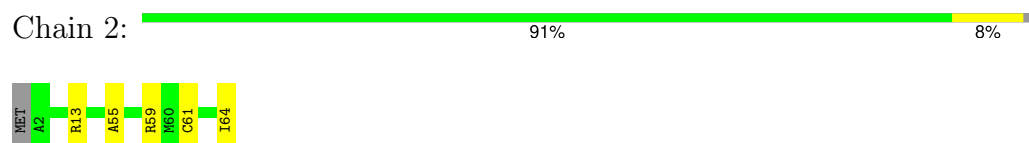


- Molecule 2: 50S ribosomal protein L34

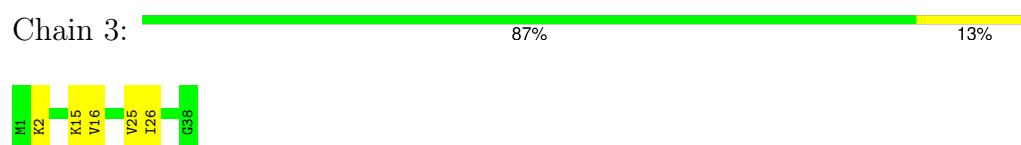


There are no outlier residues recorded for this chain.

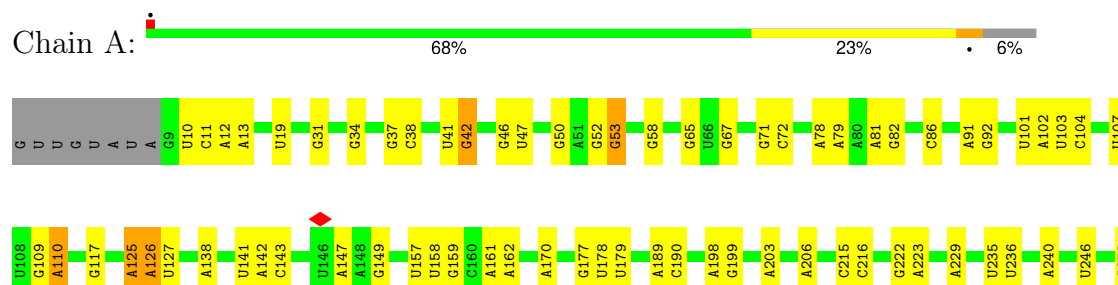
- Molecule 3: 50S ribosomal protein L35



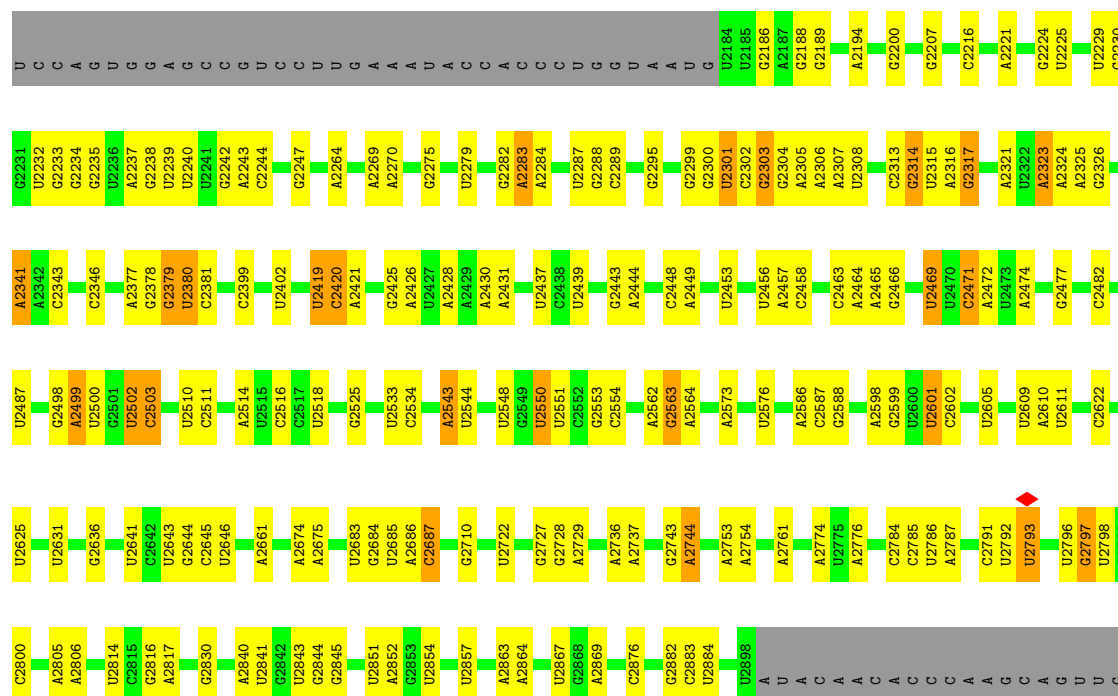
- Molecule 4: 50S ribosomal protein L36



- Molecule 5: 23S ribosomal RNA







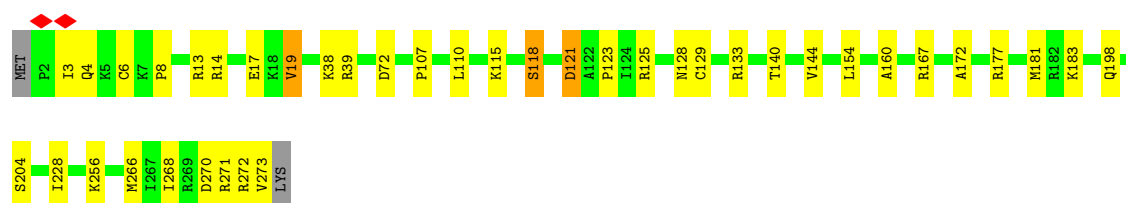
- Molecule 6: 5s ribosomal RNA

Chain B: 76% 20% .



- Molecule 7: 50S ribosomal protein L2

Chain C: 85% 14% ..



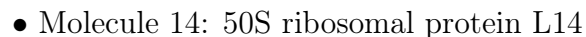
- Molecule 8: 50S ribosomal protein L3

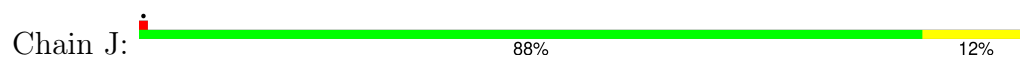
Chain D: 92% 7% .



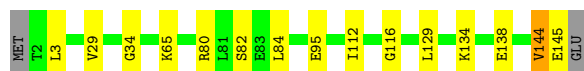
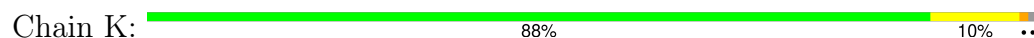
- Molecule 9: 50S ribosomal protein L4

Chain E: 92% 8%

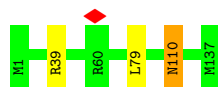




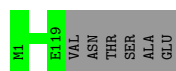
- Molecule 15: 50S ribosomal protein L15



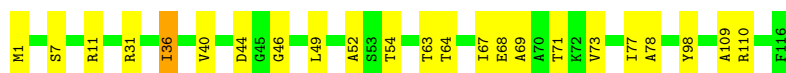
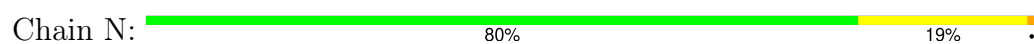
- Molecule 16: 50S ribosomal protein L16



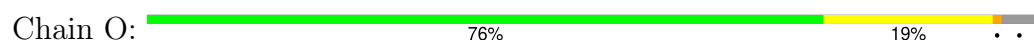
- Molecule 17: 50S ribosomal protein L17



- Molecule 18: 50S ribosomal protein L18



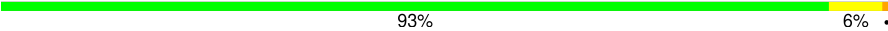
- Molecule 19: 50S ribosomal protein L19



- Molecule 20: 50S ribosomal protein L20



- Molecule 21: 50S ribosomal protein L21

Chain Q:  93% 6%



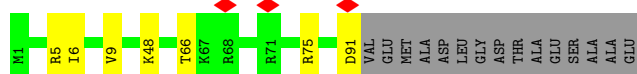
- Molecule 22: 50S ribosomal protein L22

Chain R:  90% 10%



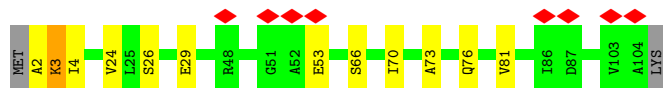
- Molecule 23: 50S ribosomal protein L23

Chain S:  79% 7% 14%



- Molecule 24: 50S ribosomal protein L24

Chain T:  8% 87% 10%



- Molecule 25: 50S ribosomal protein L25

Chain U:  90% 9%

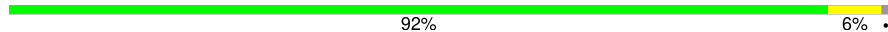


- Molecule 26: 50S ribosomal protein L27

Chain V:  85% 5% 11%

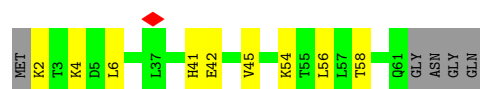
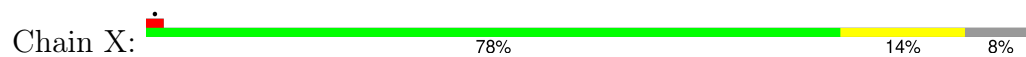


- Molecule 27: 50S ribosomal protein L28

Chain W:  92% 6%



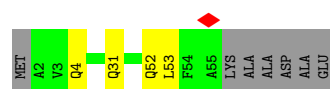
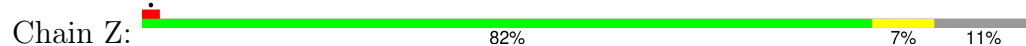
- Molecule 28: 50S ribosomal protein L29



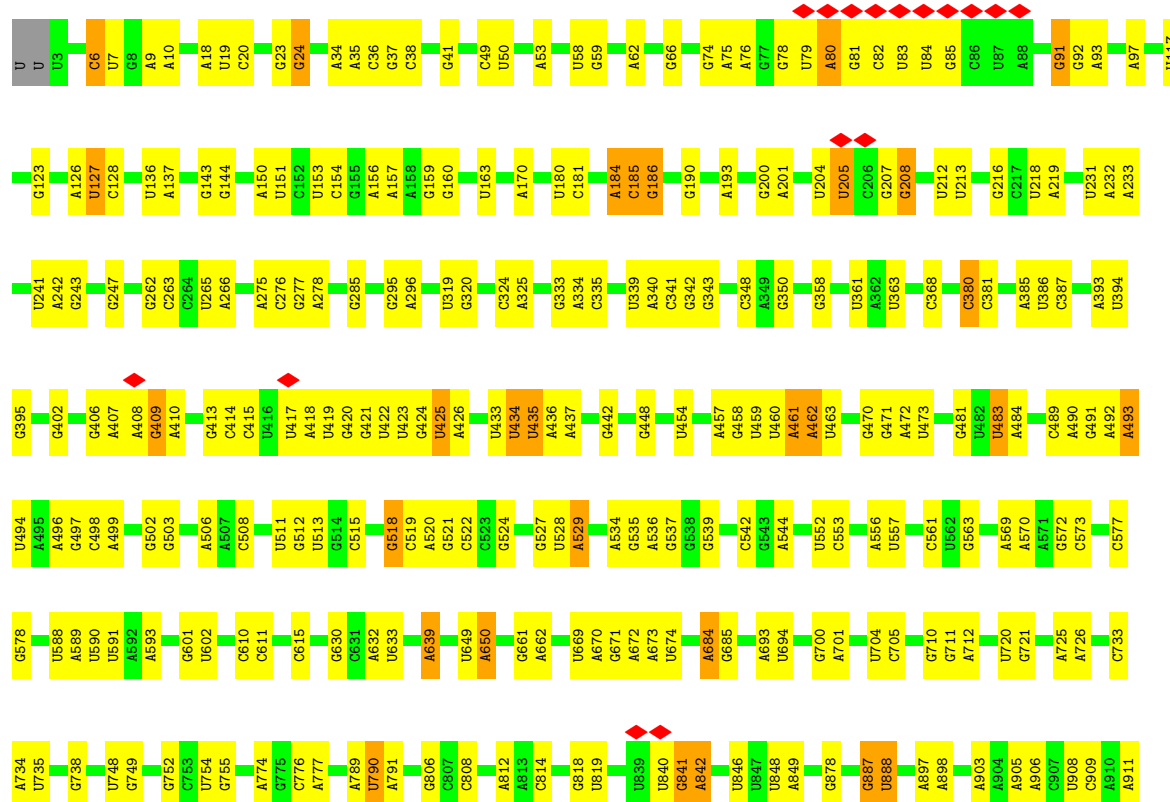
- Molecule 29: 50S ribosomal protein L30

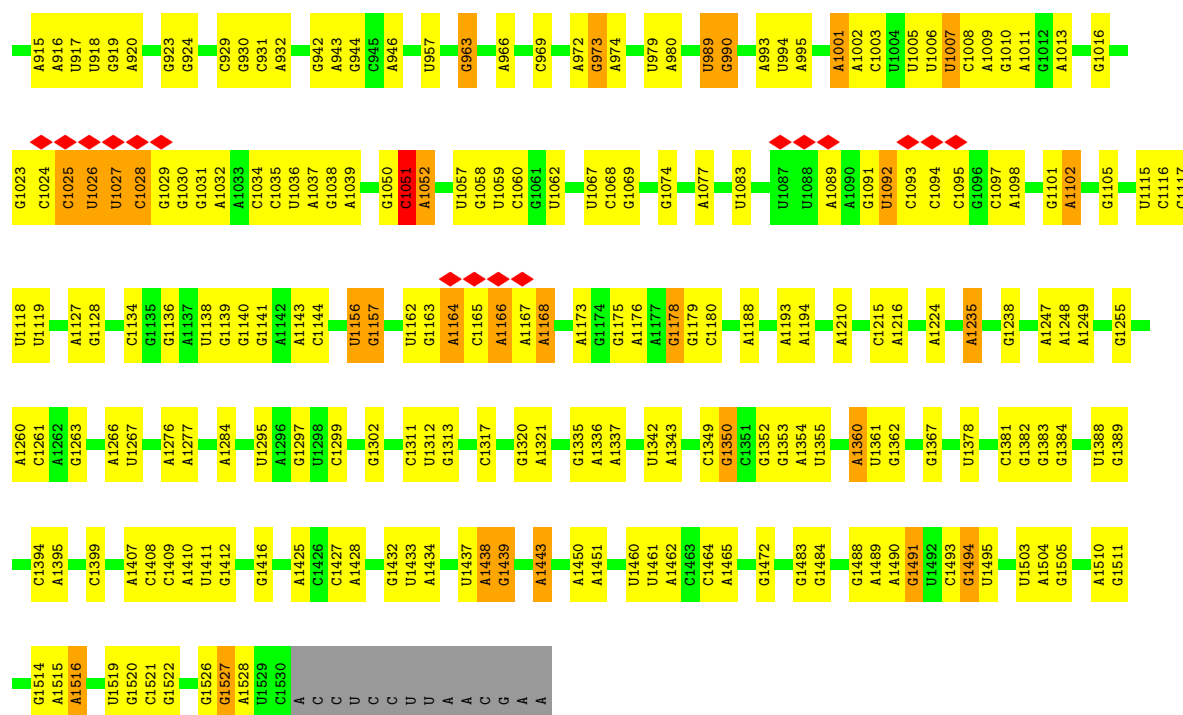


- Molecule 30: 50S ribosomal protein L32



- Molecule 31: 16s Ribosomal RNA

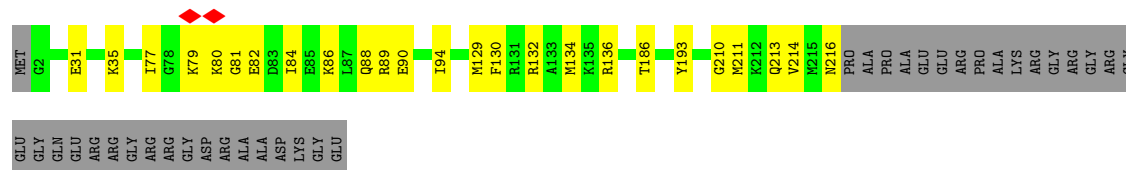
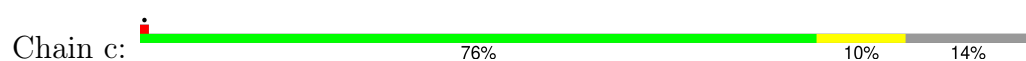




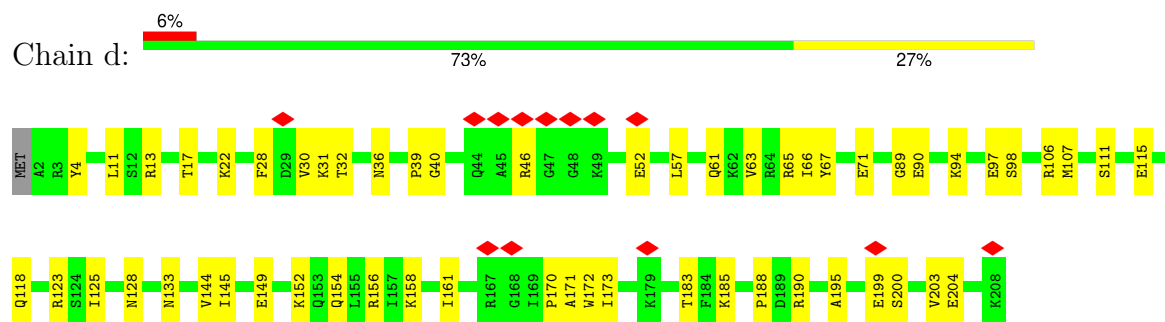
• Molecule 32: 30S ribosomal protein S2



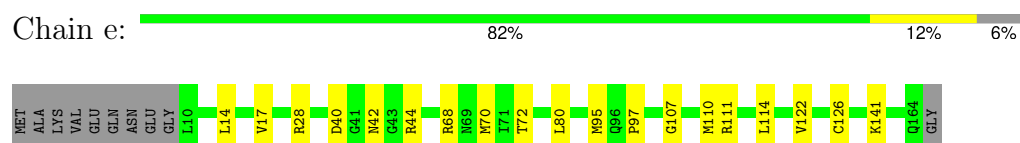
• Molecule 33: 30S ribosomal protein S3



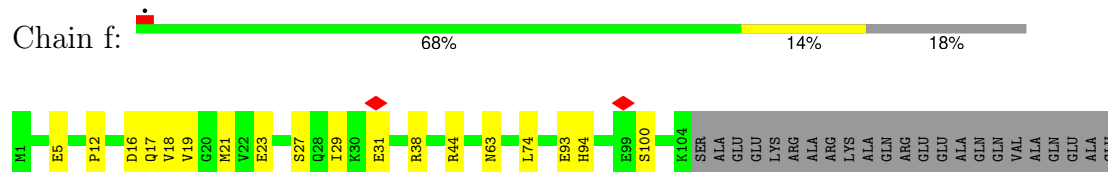
- Molecule 34: 30S ribosomal protein S4



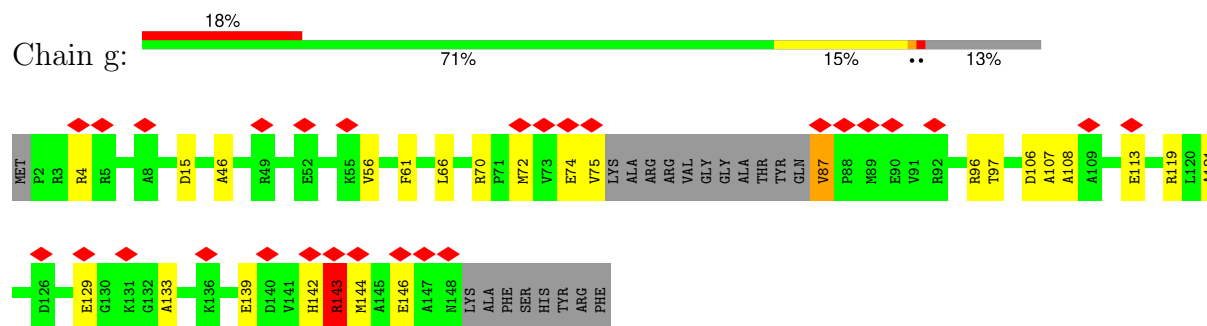
- Molecule 35: 30S ribosomal protein S5



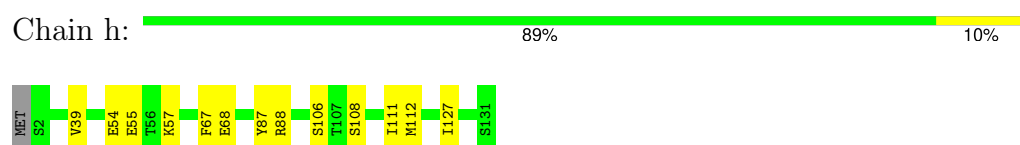
- Molecule 36: 30S ribosomal protein S6



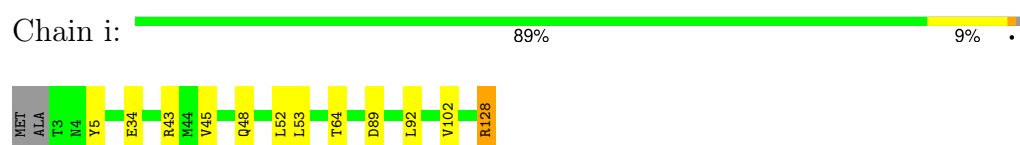
- Molecule 37: 30S ribosomal protein S7



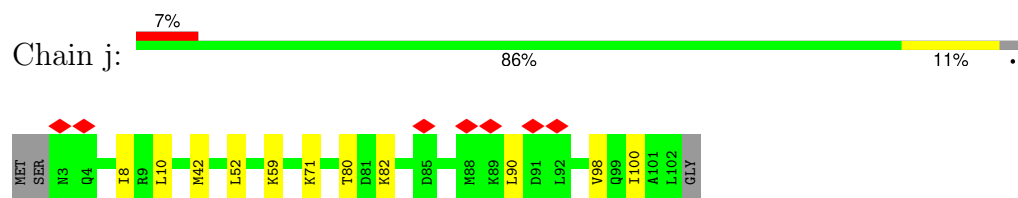
- Molecule 38: 30S ribosomal protein S8



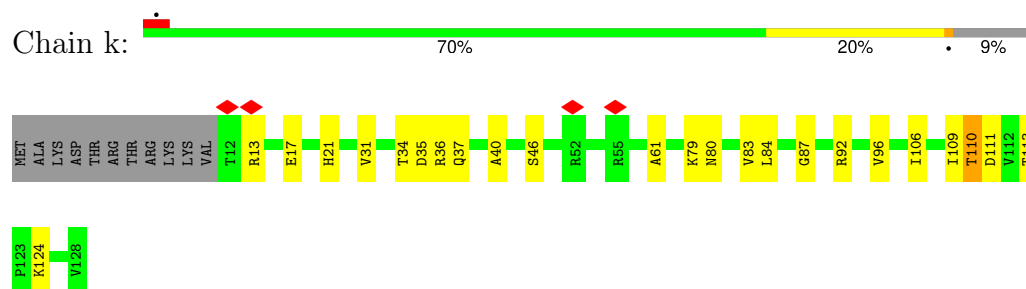
- Molecule 39: 30S ribosomal protein S9



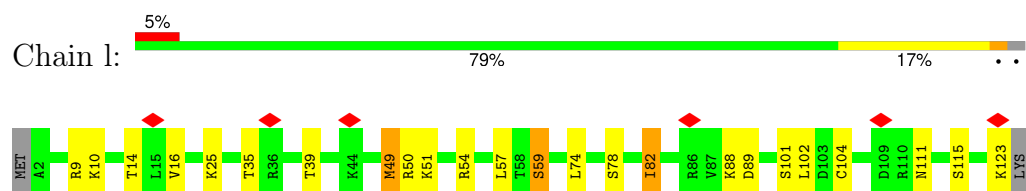
- Molecule 40: 30S ribosomal protein S10



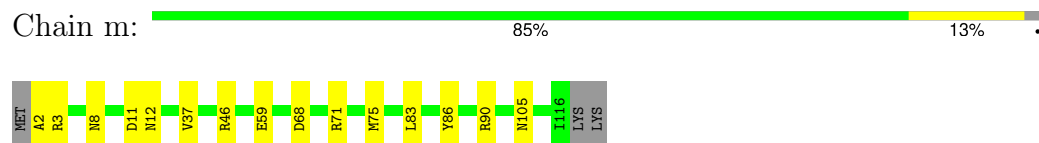
- Molecule 41: 30S ribosomal protein S11



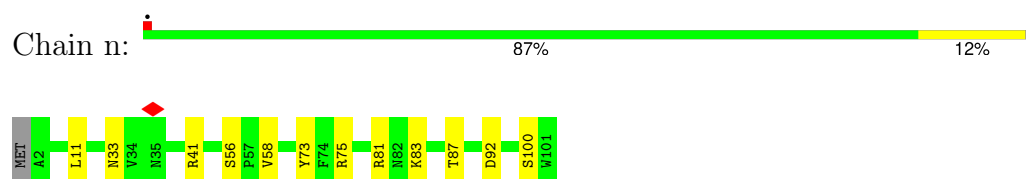
- Molecule 42: 30S ribosomal protein S12



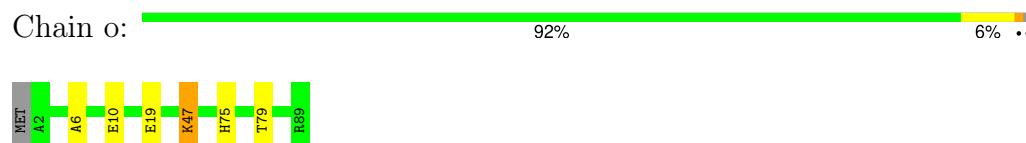
- Molecule 43: 30S ribosomal protein S13



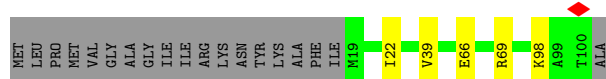
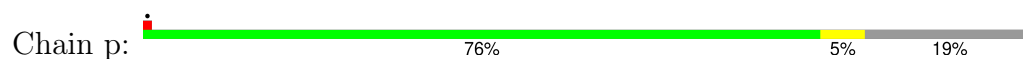
- Molecule 44: 30S ribosomal protein S14



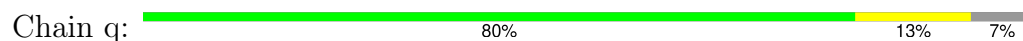
- Molecule 45: 30S ribosomal protein S15



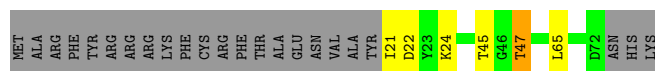
- Molecule 46: 30S ribosomal protein S16



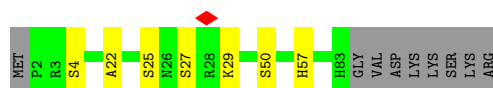
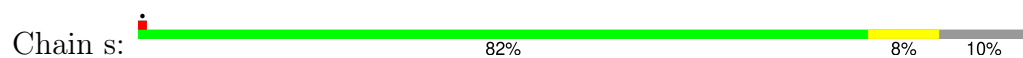
- Molecule 47: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S18



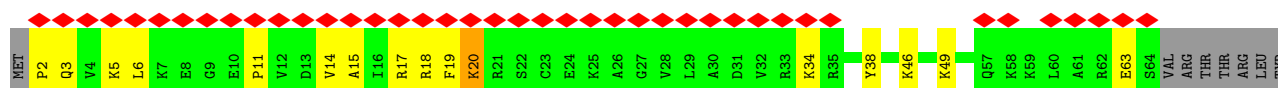
- Molecule 49: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S20

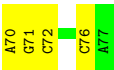


- Molecule 51: 30S ribosomal protein S21



- Molecule 52: tRNA-met





● Molecule 53: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	451971	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.975	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	460.80002, 460.80002, 460.80002	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.72, 0.72, 0.72	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 4OC, OMU, 6MZ, H2U, 3TD, OMG, PSU, 2MG, 5MU, 2MA, 4SU, 5MC, MA6, OIY, 7MG, UR3

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	0.14	0/434	0.32	0/573
2	1	0.14	0/367	0.34	0/481
3	2	0.16	0/515	0.37	0/678
4	3	0.18	0/296	0.40	0/389
5	A	0.19	0/65229	0.30	0/101736
6	B	0.15	0/2739	0.29	0/4266
7	C	0.17	0/2152	0.38	0/2891
8	D	0.16	0/1590	0.34	0/2142
9	E	0.15	0/1537	0.34	0/2073
10	F	0.19	0/1390	0.51	0/1863
11	G	0.17	0/1337	0.42	0/1807
12	H	0.19	0/461	0.54	0/616
13	I	0.17	0/1151	0.40	2/1551 (0.1%)
14	J	0.16	0/956	0.36	0/1286
15	K	0.15	0/1079	0.35	0/1439
16	L	0.16	0/1104	0.37	0/1475
17	M	0.17	0/956	0.37	0/1282
18	N	0.15	0/881	0.40	0/1177
19	O	0.17	0/931	0.35	0/1249
20	P	0.17	0/947	0.31	0/1262
21	Q	0.16	0/818	0.33	0/1094
22	R	0.15	0/831	0.32	0/1113
23	S	0.14	0/716	0.29	0/957
24	T	0.15	0/770	0.36	0/1034
25	U	0.14	0/770	0.38	0/1036
26	V	0.17	0/585	0.35	0/783
27	W	0.16	0/642	0.34	0/856
28	X	0.15	0/487	0.36	0/646
29	Y	0.16	0/460	0.29	0/614
30	Z	0.16	0/453	0.37	0/604
31	a	0.17	0/36476	0.28	1/56895 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.18	0/1799	0.49	2/2429 (0.1%)
33	c	0.16	0/1714	0.38	0/2304
34	d	0.15	0/1653	0.37	0/2213
35	e	0.16	0/1141	0.38	0/1537
36	f	0.15	0/882	0.40	0/1189
37	g	0.19	0/1087	0.50	2/1456 (0.1%)
38	h	0.16	0/993	0.34	0/1331
39	i	0.16	0/1002	0.34	0/1339
40	j	0.17	0/811	0.34	0/1096
41	k	0.15	0/878	0.37	0/1189
42	l	0.18	0/958	0.47	0/1284
43	m	0.15	0/913	0.38	0/1226
44	n	0.16	0/803	0.32	0/1071
45	o	0.17	0/715	0.34	0/958
46	p	0.16	0/655	0.35	0/879
47	q	0.16	0/628	0.35	0/847
48	r	0.17	0/432	0.41	0/583
49	s	0.17	0/664	0.37	0/897
50	t	0.19	0/669	0.29	0/892
51	u	0.22	0/528	0.56	1/697 (0.1%)
52	v	0.16	0/1739	0.29	0/2709
53	w	0.09	0/72	0.19	0/110
All	All	0.17	0/149796	0.32	8/224104 (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
21	Q	0	1
32	b	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1051	C	C2'-C3'-O3'	7.68	121.03	109.50
32	b	115	ARG	CG-CD-NE	-7.50	95.49	112.00
51	u	20	LYS	N-CA-CB	6.18	119.82	110.30
32	b	115	ARG	N-CA-CB	5.96	120.42	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	143	ARG	CB-CG-CD	5.63	124.24	111.30
37	g	143	ARG	CG-CD-NE	5.35	123.76	112.00
13	I	78	THR	CA-C-N	-5.10	112.20	122.55
13	I	78	THR	C-N-CA	-5.10	112.20	122.55

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	Q	51	ALA	Peptide
32	b	92	PRO	Peptide

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	427	0	462	3	0
2	1	363	0	401	0	0
3	2	509	0	566	3	0
4	3	295	0	326	4	0
5	A	58566	0	29452	318	0
6	B	2450	0	1241	18	0
7	C	2111	0	2176	25	0
8	D	1572	0	1610	8	0
9	E	1516	0	1569	10	0
10	F	1370	0	1420	49	0
11	G	1318	0	1373	25	0
12	H	458	0	480	10	0
13	I	1125	0	1148	11	0
14	J	946	0	1007	11	0
15	K	1071	0	1141	11	0
16	L	1087	0	1162	2	0
17	M	942	0	987	0	0
18	N	873	0	917	15	0
19	O	919	0	973	15	0
20	P	934	0	997	5	0
21	Q	807	0	842	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	R	826	0	894	7	0
23	S	710	0	768	3	0
24	T	766	0	816	7	0
25	U	760	0	783	5	0
26	V	577	0	580	2	0
27	W	632	0	667	2	0
28	X	486	0	528	8	0
29	Y	455	0	476	1	0
30	Z	447	0	435	3	0
31	a	32782	0	16508	268	0
32	b	1769	0	1787	49	0
33	c	1690	0	1774	19	0
34	d	1631	0	1691	37	0
35	e	1129	0	1174	14	0
36	f	867	0	868	11	0
37	g	1073	0	1118	20	0
38	h	985	0	1047	9	0
39	i	991	0	1048	7	0
40	j	801	0	832	7	0
41	k	862	0	877	20	0
42	l	945	0	998	16	0
43	m	903	0	962	11	0
44	n	792	0	833	8	0
45	o	705	0	712	4	0
46	p	644	0	655	3	0
47	q	621	0	665	6	0
48	r	426	0	447	5	0
49	s	646	0	663	5	0
50	t	663	0	715	2	0
51	u	522	0	565	14	0
52	v	1636	0	835	27	0
53	w	65	0	33	3	0
54	3	1	0	0	0	0
55	A	259	0	0	3	0
55	N	35	0	0	1	0
55	a	176	0	0	3	0
56	A	1	0	0	0	0
57	A	4	0	0	0	0
57	R	1	0	0	0	0
All	All	138943	0	93004	1075	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 5.

All (1075) 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)
32:b:111:GLN:O	32:b:115:ARG:NH1	1.88	1.06
37:g:139:GLU:HA	37:g:143:ARG:HH21	1.25	1.00
31:a:1007:U:H3	31:a:1016:G:H1	1.15	0.94
52:v:27:A:H61	52:v:45:G:H1	1.17	0.91
5:A:2093:U:H3	5:A:2188:G:H1	1.15	0.88
5:A:279:U:H3	5:A:366:G:H1	1.23	0.86
32:b:115:ARG:HH11	32:b:115:ARG:H	1.22	0.86
31:a:454:U:H3	31:a:470:G:H1	1.26	0.84
37:g:72:MET:HA	37:g:96:ARG:HE	1.43	0.84
5:A:2840:A:HO2'	19:O:2:SER:N	1.79	0.81
5:A:1044:G:O2'	5:A:1108:A:N6	2.13	0.80
52:v:27:A:N6	52:v:45:G:H1	1.79	0.80
34:d:11:LEU:HD22	34:d:65:ARG:HE	1.45	0.80
23:S:66:THR:HG22	23:S:75:ARG:HG3	1.64	0.79
11:G:98:VAL:HG23	11:G:125:THR:HG23	1.66	0.77
32:b:112:SER:HA	32:b:115:ARG:HH12	1.48	0.77
5:A:279:U:O2	5:A:366:G:N2	2.18	0.77
10:F:44:ALA:HB2	10:F:80:ARG:HH12	1.49	0.76
10:F:78:LYS:HE3	10:F:78:LYS:HA	1.65	0.76
34:d:154:GLN:H	34:d:158:LYS:HZ1	1.35	0.75
31:a:74:G:H1	31:a:93:A:H61	1.33	0.75
31:a:75:A:H61	31:a:92:G:H1	1.33	0.75
15:K:134:LYS:NZ	15:K:138:GLU:OE2	2.20	0.74
51:u:6:LEU:HD22	51:u:15:ALA:HB1	1.70	0.73
52:v:27:A:N1	52:v:45:G:N2	2.35	0.73
18:N:1:MET:N	55:N:201:OIY:O06	2.22	0.72
32:b:10:ASP:OD1	32:b:10:ASP:N	2.20	0.71
5:A:2469:U:OP1	5:A:2471:C:N4	2.22	0.71
35:e:110:MET:HE2	35:e:126:CYS:SG	2.32	0.70
31:a:661:G:H22	31:a:738:G:H1	1.40	0.70
5:A:1908:A:O2'	31:a:1491:G:O2'	2.10	0.69
12:H:45:ALA:O	12:H:49:ALA:CB	2.40	0.69
41:k:34:THR:HG22	41:k:40:ALA:HA	1.75	0.69
37:g:74:GLU:HG2	37:g:75:VAL:HG12	1.72	0.69
47:q:18:MET:HG3	47:q:21:SER:HB2	1.74	0.69
11:G:44:LYS:HE3	11:G:44:LYS:HA	1.75	0.69
16:L:110:ASN:OD1	16:L:110:ASN:N	2.26	0.68
10:F:31:ILE:HD11	10:F:34:ILE:HD11	1.75	0.68
5:A:2287:U:H2'	5:A:2288:G:C8	2.28	0.68
34:d:170:PRO:HG2	34:d:173:ILE:HD12	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:135:GLU:HB3	32:b:139:ARG:NH2	2.10	0.67
34:d:190:ARG:HH22	34:d:195:ALA:HA	1.59	0.67
42:l:39:THR:HG21	42:l:49:MET:HG3	1.77	0.67
5:A:1932:A:OP2	5:A:1958:C:N4	2.28	0.67
34:d:36:ASN:HA	34:d:46:ARG:HE	1.60	0.67
37:g:139:GLU:HA	37:g:143:ARG:NH2	2.04	0.66
52:v:35:C:H42	53:w:3:G:H1	1.43	0.66
5:A:1908:A:HO2'	31:a:1491:G:HO2'	1.43	0.66
37:g:113:GLU:O	37:g:119:ARG:NH1	2.28	0.66
10:F:170:MET:SD	10:F:175:PHE:HB3	2.36	0.66
32:b:143:MET:HE2	32:b:143:MET:HA	1.77	0.66
31:a:710:G:H2'	31:a:711:G:C8	2.31	0.66
5:A:1595:A:H5''	5:A:1596:A:H5'	1.78	0.66
31:a:1036:U:H2'	31:a:1037:A:H8	1.60	0.65
10:F:12:LEU:HD12	10:F:172:ALA:HB1	1.79	0.65
11:G:86:LYS:O	11:G:165:SER:OG	2.14	0.65
31:a:471:G:H2'	31:a:472:A:C8	2.31	0.65
51:u:17:ARG:O	51:u:20:LYS:HD3	1.96	0.65
31:a:1394:C:OP2	35:e:28:ARG:NH2	2.25	0.65
10:F:5:LYS:HG2	10:F:6:ALA:H	1.61	0.64
5:A:854:G:H2'	5:A:855:G:C8	2.32	0.64
31:a:841:G:H1'	31:a:842:A:C8	2.33	0.64
41:k:109:ILE:HG12	51:u:19:PHE:CD1	2.32	0.64
7:C:271:ARG:NE	7:C:273:VAL:HG12	2.14	0.63
41:k:17:GLU:OE1	41:k:80:ASN:ND2	2.31	0.63
31:a:943:A:H2'	31:a:944:G:C8	2.33	0.63
11:G:17:VAL:HG11	11:G:50:LEU:HD21	1.81	0.63
31:a:498:C:H2'	31:a:499:A:H8	1.64	0.63
5:A:2324:A:H2'	5:A:2325:A:C8	2.33	0.62
10:F:120:LYS:HG3	10:F:121:SER:H	1.63	0.62
46:p:22:ILE:HG12	46:p:39:VAL:HG22	1.82	0.62
52:v:18:G:H21	52:v:59:A:H5'	1.65	0.62
40:j:80:THR:HG22	40:j:82:LYS:H	1.64	0.62
5:A:1605:G:H5''	5:A:1606:A:H5'	1.79	0.62
31:a:1067:U:H3	31:a:1102:A:H61	1.48	0.62
5:A:2753:A:N1	11:G:67:THR:HG21	2.15	0.62
5:A:2095:U:H3	5:A:2186:G:H1	1.46	0.62
10:F:34:ILE:HD13	10:F:96:MET:HB2	1.82	0.62
41:k:96:VAL:HG21	41:k:109:ILE:HD12	1.82	0.62
36:f:12:PRO:O	36:f:44:ARG:NH2	2.33	0.62
5:A:2315:U:O2'	5:A:2317:G:N7	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:49:LEU:HD12	10:F:148:ARG:HE	1.65	0.61
32:b:164:PHE:HA	32:b:186:ILE:O	2.00	0.61
31:a:423:U:OP2	31:a:424:G:O2'	2.13	0.61
31:a:670:A:H2'	31:a:671:G:C8	2.35	0.61
5:A:1717:G:O2'	5:A:1735:A:N6	2.33	0.61
5:A:2308:U:H5'	10:F:85:ILE:HD11	1.82	0.61
24:T:53:GLU:OE2	24:T:53:GLU:N	2.33	0.61
10:F:101:ASP:OD1	10:F:102:ARG:N	2.33	0.61
12:H:45:ALA:O	12:H:49:ALA:HB2	2.00	0.61
31:a:1162:U:H3	31:a:1168:A:H61	1.47	0.61
43:m:3:ARG:NH1	43:m:8:ASN:OD1	2.34	0.61
31:a:143:G:H2'	31:a:144:G:C8	2.36	0.61
48:r:45:THR:OG1	48:r:47:THR:OG1	2.18	0.61
5:A:2063:G:H1	5:A:2439:U:H3	1.49	0.60
10:F:80:ARG:HE	10:F:83:TRP:CD1	2.18	0.60
32:b:115:ARG:NH1	32:b:115:ARG:H	1.95	0.60
52:v:52:A:H61	52:v:64:C:H42	1.49	0.60
34:d:52:GLU:OE2	34:d:52:GLU:N	2.34	0.60
31:a:1527:G:O6	51:u:46:LYS:NZ	2.34	0.60
32:b:186:ILE:HG12	32:b:200:TYR:HB2	1.83	0.60
5:A:1108:A:H8	5:A:1109:G:H1'	1.66	0.60
5:A:2313:C:H2'	5:A:2314:G:C8	2.35	0.60
31:a:994:U:H2'	31:a:995:A:H8	1.65	0.60
10:F:14:ALA:O	10:F:18:GLU:HG3	2.00	0.60
11:G:30:LYS:NZ	11:G:81:GLU:O	2.33	0.60
27:W:34:HIS:NE2	27:W:56:MET:HE3	2.17	0.60
5:A:1036:A:O3'	25:U:49:ARG:NH2	2.35	0.59
31:a:1175:G:N2	31:a:1178:G:OP2	2.27	0.59
5:A:1464:A:H2'	5:A:1465:A:C8	2.38	0.59
25:U:68:LYS:HG2	25:U:73:VAL:HG22	1.85	0.59
5:A:579:C:H2'	5:A:580:A:C8	2.37	0.59
13:I:114:LEU:HG	13:I:118:MET:HE3	1.85	0.59
5:A:284:U:H3	5:A:360:A:H62	1.47	0.59
5:A:2060:C:H2'	5:A:2061:C:C6	2.37	0.59
31:a:1353:G:H2'	31:a:1354:A:C8	2.37	0.59
31:a:231:U:H2'	31:a:232:A:H8	1.68	0.59
31:a:1320:G:H2'	31:a:1321:A:C8	2.37	0.59
5:A:1792:U:H2'	5:A:1793:C:C6	2.38	0.58
31:a:498:C:H2'	31:a:499:A:C8	2.38	0.58
31:a:1383:G:H2'	31:a:1384:G:H8	1.67	0.58
49:s:22:ALA:O	49:s:25:SER:O	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1052:A:OP2	55:a:1604:OIY:N52	2.36	0.58
34:d:144:VAL:HG22	34:d:183:THR:HG22	1.85	0.58
10:F:27:GLU:N	10:F:27:GLU:OE2	2.36	0.58
49:s:22:ALA:O	49:s:25:SER:C	2.47	0.58
31:a:733:C:H2'	31:a:734:A:H8	1.68	0.58
32:b:75:LYS:HD2	32:b:167:ASP:HB2	1.85	0.58
6:B:87:A:OP2	16:L:39:ARG:NE	2.34	0.58
9:E:170:ASP:OD1	9:E:171:ALA:N	2.36	0.58
11:G:63:MET:O	11:G:67:THR:HG23	2.03	0.58
31:a:733:C:H2'	31:a:734:A:C8	2.39	0.58
31:a:1001:A:C5	31:a:1023:G:H1'	2.39	0.58
5:A:2300:G:H22	5:A:2308:U:H3	1.51	0.58
5:A:2325:A:H2'	5:A:2326:G:C8	2.39	0.58
32:b:79:SER:OG	32:b:95:ASP:OD1	2.19	0.57
33:c:79:LYS:HD2	33:c:80:LYS:N	2.18	0.57
5:A:579:C:H2'	5:A:580:A:H8	1.69	0.57
5:A:1749:G:N2	5:A:1752:G:OP2	2.33	0.57
19:O:30:VAL:HG22	19:O:47:GLU:HB2	1.86	0.57
31:a:806:G:OP1	45:o:47:LYS:NZ	2.36	0.57
5:A:1185:G:H5'	15:K:34:GLY:HA2	1.86	0.57
5:A:1523:A:H2'	5:A:1524:A:C8	2.40	0.57
6:B:11:A:O2'	6:B:13:A:OP2	2.21	0.57
11:G:13:ASN:OD1	11:G:14:GLY:N	2.36	0.57
40:j:10:LEU:HD22	40:j:98:VAL:HG22	1.87	0.57
5:A:368:C:H4'	5:A:369:G:O5'	2.03	0.57
31:a:74:G:H1	31:a:93:A:N6	2.02	0.57
31:a:265:U:H2'	31:a:266:A:C8	2.39	0.57
31:a:711:G:H2'	31:a:712:A:C8	2.39	0.57
32:b:112:SER:CA	32:b:115:ARG:HH12	2.14	0.57
31:a:919:G:H2'	31:a:920:A:C8	2.40	0.57
43:m:2:ALA:N	43:m:11:ASP:OD1	2.38	0.57
5:A:2465:A:N6	5:A:2477:G:O2'	2.38	0.57
9:E:14:SER:N	9:E:196:GLU:OE2	2.38	0.57
31:a:75:A:N6	31:a:92:G:H1	2.00	0.57
5:A:591:U:H2'	5:A:592:U:C6	2.40	0.57
5:A:2067:A:H2'	5:A:2068:C:C6	2.39	0.57
31:a:1024:C:H2'	31:a:1025:C:C6	2.40	0.56
31:a:1263:G:N2	31:a:1266:A:OP2	2.36	0.56
5:A:71:G:H2'	5:A:72:C:H6	1.70	0.56
5:A:831:A:H2'	5:A:832:G:C8	2.40	0.56
5:A:2082:U:H2'	5:A:2083:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:82:SER:HB3	15:K:116:GLY:HA3	1.86	0.56
19:O:94:ASP:OD2	19:O:114:ARG:NH2	2.38	0.56
36:f:27:SER:O	36:f:31:GLU:HG3	2.05	0.56
31:a:789:A:H4'	31:a:790:U:O5'	2.06	0.56
52:v:40:U:H2'	52:v:41:G:H8	1.70	0.56
5:A:2587:C:H2'	5:A:2588:G:H8	1.70	0.56
6:B:28:C:H1'	6:B:55:A:H61	1.70	0.56
10:F:4:LEU:C	10:F:5:LYS:HD3	2.30	0.56
36:f:38:ARG:HB3	36:f:63:ASN:HB2	1.87	0.56
11:G:11:VAL:HG13	11:G:15:VAL:HG22	1.88	0.56
31:a:19:U:H2'	31:a:20:C:C6	2.41	0.56
10:F:144:ASP:OD1	43:m:71:ARG:NH1	2.38	0.56
34:d:36:ASN:HA	34:d:46:ARG:NE	2.21	0.56
35:e:14:LEU:HD11	35:e:17:VAL:HG23	1.87	0.56
38:h:106:SER:HB2	38:h:127:ILE:HD11	1.88	0.56
5:A:52:G:H5''	5:A:53:G:H5'	1.87	0.55
5:A:1827:G:OP1	55:A:3001:OIY:N11	2.39	0.55
7:C:6:CYS:SG	7:C:13:ARG:NH1	2.78	0.55
11:G:84:GLU:HA	11:G:133:LEU:O	2.07	0.55
5:A:2744:A:H1'	11:G:67:THR:HG22	1.87	0.55
10:F:136:ILE:O	10:F:137:VAL:HG22	2.07	0.55
7:C:4:GLN:OE1	7:C:4:GLN:N	2.25	0.55
19:O:8:VAL:O	19:O:12:GLU:HG3	2.06	0.55
20:P:43:GLY:HA3	21:Q:75:ILE:HD12	1.89	0.55
5:A:1182:G:H5'	21:Q:83:TYR:CE1	2.42	0.55
5:A:2543:A:H2'	5:A:2544:U:C6	2.41	0.55
5:A:2843:U:H2'	5:A:2844:G:O4'	2.06	0.55
36:f:16:ASP:OD1	36:f:17:GLN:NE2	2.39	0.55
5:A:365:U:H4'	5:A:366:G:O5'	2.06	0.55
6:B:57:A:H4'	18:N:1:MET:HB3	1.88	0.55
34:d:94:LYS:O	34:d:98:SER:OG	2.20	0.55
5:A:71:G:H2'	5:A:72:C:C6	2.42	0.55
18:N:69:ALA:O	18:N:73:VAL:HG23	2.07	0.55
40:j:8:ILE:HG12	40:j:100:ILE:HG12	1.88	0.55
5:A:280:A:H2'	5:A:281:A:C8	2.41	0.55
10:F:170:MET:HE1	10:F:177:PHE:C	2.32	0.55
21:Q:52:PRO:HB2	21:Q:53:VAL:HG12	1.89	0.55
5:A:1792:U:H2'	5:A:1793:C:H6	1.72	0.54
5:A:1798:A:H2'	5:A:1799:A:C8	2.42	0.54
11:G:166:ASP:OD1	11:G:166:ASP:N	2.38	0.54
22:R:95:ARG:HH11	22:R:95:ARG:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1383:G:H2'	31:a:1384:G:C8	2.42	0.54
34:d:90:GLU:HG3	34:d:190:ARG:HB2	1.89	0.54
19:O:36:LYS:HE3	19:O:36:LYS:HA	1.89	0.54
31:a:649:U:O4	31:a:749:G:O2'	2.22	0.54
34:d:89:GLY:HA3	34:d:199:GLU:HG3	1.89	0.54
5:A:12:A:H2'	5:A:13:A:C8	2.42	0.54
11:G:43:LEU:HD11	11:G:50:LEU:HB3	1.89	0.54
39:i:53:LEU:HD21	39:i:92:LEU:HD13	1.90	0.54
12:H:45:ALA:O	12:H:49:ALA:HB3	2.07	0.54
21:Q:75:ILE:HG12	21:Q:86:GLN:HG2	1.90	0.54
29:Y:5:LYS:HZ3	29:Y:36:GLU:HG3	1.73	0.54
34:d:118:GLN:HG2	34:d:156:ARG:HH22	1.73	0.54
42:l:74:LEU:HD11	42:l:104:CYS:SG	2.48	0.54
5:A:358:A:H2'	5:A:359:U:C6	2.44	0.53
5:A:740:G:H2'	5:A:741:U:C6	2.42	0.53
5:A:1910:C:H3'	5:A:1911:3TD:H6	1.89	0.53
6:B:11:A:N1	6:B:67:G:O2'	2.37	0.53
31:a:1010:G:N2	31:a:1013:A:OP2	2.26	0.53
5:A:1634:G:H2'	5:A:1635:A:C8	2.43	0.53
32:b:6:VAL:HG21	32:b:52:LEU:HD13	1.90	0.53
39:i:128:ARG:HH11	39:i:128:ARG:HB3	1.74	0.53
43:m:86:TYR:O	43:m:90:ARG:HG2	2.07	0.53
31:a:1027:U:H3'	31:a:1028:C:H4'	1.89	0.53
31:a:231:U:H2'	31:a:232:A:C8	2.43	0.53
32:b:111:GLN:O	32:b:114:ASN:HB2	2.08	0.53
5:A:1530:A:H3'	5:A:1531:C:H4'	1.90	0.53
5:A:1885:A:H2'	5:A:1886:A:C8	2.44	0.53
5:A:2093:U:O2	5:A:2188:G:N2	2.30	0.53
5:A:2282:G:H4'	5:A:2283:A:O4'	2.08	0.53
31:a:1001:A:C6	31:a:1023:G:H1'	2.44	0.53
32:b:115:ARG:HD3	32:b:115:ARG:N	2.23	0.53
5:A:2844:G:O2'	5:A:2864:A:N6	2.41	0.53
31:a:929:C:H2'	31:a:930:G:C8	2.43	0.53
31:a:1409:C:H2'	31:a:1410:A:C8	2.43	0.53
5:A:846:U:H2'	5:A:847:A:C8	2.44	0.53
13:I:77:HIS:ND1	13:I:78:THR:O	2.42	0.53
36:f:18:VAL:HA	36:f:21:MET:HE3	1.91	0.53
5:A:606:A:H2'	5:A:607:A:C8	2.44	0.53
5:A:2323:A:H2'	5:A:2324:A:C8	2.43	0.53
7:C:115:LYS:O	7:C:125:ARG:NH1	2.41	0.53
31:a:1215:C:H2'	31:a:1216:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2674:A:H2'	5:A:2675:A:C8	2.44	0.52
31:a:973:G:OP2	31:a:1355:U:O2'	2.27	0.52
32:b:102:MET:HE2	32:b:102:MET:HA	1.91	0.52
5:A:347:A:H1'	5:A:348:A:H2	1.74	0.52
5:A:2587:C:H2'	5:A:2588:G:C8	2.44	0.52
6:B:86:U:H4'	6:B:87:A:O5'	2.09	0.52
11:G:11:VAL:HG23	11:G:50:LEU:HD11	1.91	0.52
31:a:1038:G:H2'	31:a:1039:A:H8	1.74	0.52
31:a:1074:G:N2	31:a:1077:A:OP2	2.39	0.52
34:d:123:ARG:HG3	34:d:133:ASN:HB3	1.91	0.52
5:A:2743:G:OP1	11:G:74:ASN:ND2	2.39	0.52
7:C:4:GLN:H	7:C:4:GLN:CD	2.16	0.52
11:G:123:ALA:HA	11:G:132:ILE:O	2.09	0.52
5:A:308:U:H2'	5:A:309:G:O4'	2.10	0.52
18:N:31:ARG:HG3	18:N:36:ILE:HD12	1.90	0.52
11:G:164:TYR:HB2	11:G:167:GLU:HB2	1.91	0.52
22:R:95:ARG:HB3	22:R:95:ARG:NH1	2.24	0.52
31:a:1438:A:O2'	31:a:1439:G:O5'	2.28	0.52
5:A:846:U:H2'	5:A:847:A:H8	1.73	0.52
5:A:2242:G:H2'	5:A:2243:A:C8	2.45	0.52
5:A:2533:U:H2'	5:A:2534:C:C6	2.44	0.52
31:a:725:A:H2'	31:a:726:A:C8	2.45	0.52
31:a:1156:U:H3'	32:b:134:ARG:HH21	1.75	0.52
5:A:2242:G:H2'	5:A:2243:A:H8	1.75	0.52
32:b:68:LYS:HZ2	32:b:70:LEU:HA	1.74	0.52
32:b:144:GLU:O	32:b:148:ARG:HG2	2.10	0.52
51:u:5:LYS:O	51:u:18:ARG:NH1	2.43	0.52
5:A:161:A:H2'	5:A:162:A:C8	2.45	0.52
36:f:38:ARG:NH1	36:f:100:SER:HB3	2.24	0.52
6:B:52:G:H21	10:F:26:MET:HE2	1.75	0.52
7:C:121:ASP:OD1	7:C:121:ASP:N	2.32	0.52
37:g:113:GLU:OE1	37:g:113:GLU:N	2.43	0.52
41:k:110:THR:HB	51:u:3:GLN:H	1.75	0.52
5:A:1523:A:H2'	5:A:1524:A:H8	1.73	0.51
10:F:80:ARG:HD3	10:F:80:ARG:N	2.25	0.51
31:a:58:U:H2'	31:a:59:G:C8	2.45	0.51
31:a:409:G:N2	31:a:425:U:OP2	2.21	0.51
5:A:1563:C:O2	5:A:1564:A:O2'	2.29	0.51
5:A:1794:U:OP2	7:C:273:VAL:HB	2.11	0.51
10:F:110:ARG:HB3	10:F:137:VAL:HG12	1.93	0.51
32:b:135:GLU:HB3	32:b:139:ARG:HH22	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:158:LYS:HE2	34:d:158:LYS:H	1.75	0.51
37:g:143:ARG:HA	37:g:146:GLU:OE2	2.11	0.51
5:A:1568:A:H2'	5:A:1569:A:C8	2.45	0.51
42:l:35:THR:N	42:l:54:ARG:O	2.44	0.51
5:A:288:U:H2'	5:A:289:G:H8	1.75	0.51
5:A:637:U:H2'	5:A:638:C:C6	2.45	0.51
5:A:1520:A:H2'	5:A:1521:G:C8	2.46	0.51
31:a:265:U:H2'	31:a:266:A:H8	1.75	0.51
31:a:1311:C:H2'	31:a:1312:U:C6	2.45	0.51
37:g:142:HIS:HB3	37:g:143:ARG:CZ	2.40	0.51
39:i:34:GLU:HA	39:i:43:ARG:HH11	1.76	0.51
42:l:57:LEU:HD11	42:l:82:ILE:HD11	1.92	0.51
13:I:34:ARG:HG3	13:I:39:LYS:HB2	1.93	0.51
5:A:2060:C:H2'	5:A:2061:C:H6	1.75	0.51
5:A:2308:U:O3'	10:F:68:THR:HG21	2.11	0.51
6:B:13:A:O3'	6:B:14:G:H8	1.94	0.51
10:F:91:LEU:HD23	10:F:96:MET:HA	1.91	0.51
5:A:287:G:H2'	5:A:288:U:C6	2.46	0.51
12:H:8:ARG:HB2	12:H:14:LYS:HD2	1.92	0.51
34:d:28:PHE:O	34:d:32:THR:HG22	2.10	0.51
42:l:25:LYS:HE3	42:l:59:SER:HB3	1.92	0.51
44:n:33:ASN:O	44:n:41:ARG:NH1	2.43	0.51
14:J:97:ARG:NH1	31:a:335:C:OP2	2.44	0.51
31:a:207:G:O2'	31:a:208:G:O4'	2.20	0.51
5:A:413:C:H2'	5:A:414:A:C8	2.46	0.51
5:A:2301:U:C2	10:F:151:GLY:HA3	2.46	0.51
19:O:86:LYS:HG2	19:O:88:GLU:OE1	2.11	0.51
5:A:2314:G:H2'	5:A:2315:U:O4'	2.11	0.50
10:F:175:PHE:CG	10:F:176:PRO:HD2	2.46	0.50
31:a:127:U:H2'	31:a:128:C:C6	2.46	0.50
31:a:610:C:H2'	31:a:611:C:C6	2.45	0.50
31:a:946:A:N7	43:m:105:ASN:ND2	2.58	0.50
45:o:19:GLU:HA	45:o:19:GLU:OE2	2.11	0.50
52:v:20:H2U:H2'	52:v:20:H2U:O2	2.11	0.50
5:A:286:U:H2'	5:A:287:G:C8	2.47	0.50
5:A:1176:U:H2'	5:A:1177:A:C8	2.46	0.50
5:A:1589:C:H2'	5:A:1590:A:C8	2.46	0.50
5:A:1790:A:H2'	5:A:1791:C:H6	1.76	0.50
49:s:27:SER:OG	49:s:29:LYS:HG2	2.11	0.50
5:A:1471:U:H2'	5:A:1472:A:H8	1.77	0.50
5:A:2070:U:H2'	5:A:2071:U:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:490:A:H2'	31:a:491:G:C8	2.46	0.50
32:b:88:ARG:NH2	32:b:221:ASP:OD1	2.37	0.50
5:A:830:U:H2'	5:A:831:A:C8	2.47	0.50
5:A:1849:A:H2'	5:A:1850:A:C8	2.46	0.50
9:E:86:ALA:O	9:E:87:ARG:NH1	2.43	0.50
5:A:2518:U:O2'	5:A:2643:U:OP1	2.23	0.50
31:a:232:A:H2'	31:a:233:A:C8	2.46	0.50
31:a:534:A:H2'	31:a:535:G:H8	1.77	0.50
31:a:1002:A:C5	31:a:1003:C:H1'	2.47	0.50
31:a:1438:A:O2'	31:a:1439:G:H8	1.95	0.50
43:m:71:ARG:HG3	43:m:71:ARG:HH11	1.77	0.50
11:G:25:GLU:OE1	11:G:32:THR:HG23	2.12	0.50
52:v:69:U:H2'	52:v:70:A:C8	2.47	0.50
52:v:71:G:H2'	52:v:72:C:C6	2.46	0.50
31:a:1025:C:H2'	31:a:1026:U:C6	2.47	0.50
5:A:1471:U:H2'	5:A:1472:A:C8	2.47	0.50
31:a:58:U:H2'	31:a:59:G:H8	1.75	0.50
35:e:107:GLY:O	35:e:111:ARG:HB2	2.11	0.50
31:a:969:C:OP2	40:j:59:LYS:NZ	2.33	0.49
31:a:1089:A:OP2	37:g:4:ARG:NH1	2.41	0.49
31:a:1360:A:O2'	31:a:1362:G:N7	2.42	0.49
32:b:33:ILE:HG22	32:b:35:GLY:H	1.76	0.49
7:C:72:ASP:OD1	7:C:118:SER:OG	2.30	0.49
31:a:1092:U:H2'	31:a:1093:C:C6	2.47	0.49
31:a:1460:U:H2'	31:a:1461:U:H6	1.77	0.49
5:A:2287:U:H2'	5:A:2288:G:H8	1.75	0.49
5:A:2553:G:H2'	5:A:2554:C:C6	2.47	0.49
10:F:44:ALA:HA	10:F:47:LYS:NZ	2.28	0.49
31:a:989:U:H4'	31:a:990:G:O5'	2.12	0.49
32:b:68:LYS:HE3	32:b:92:PRO:HG2	1.93	0.49
5:A:830:U:H2'	5:A:831:A:H8	1.77	0.49
5:A:1025:A:H2'	5:A:1026:A:C8	2.47	0.49
5:A:1790:A:H2'	5:A:1791:C:C6	2.47	0.49
18:N:98:TYR:OH	18:N:110:ARG:NH2	2.45	0.49
31:a:943:A:H2'	31:a:944:G:H8	1.77	0.49
31:a:1464:C:H2'	31:a:1465:A:H8	1.77	0.49
40:j:52:LEU:HB2	44:n:81:ARG:HD2	1.95	0.49
41:k:13:ARG:NH2	41:k:35:ASP:OD2	2.41	0.49
5:A:655:U:H2'	5:A:656:U:C6	2.47	0.49
14:J:38:ILE:HD11	14:J:111:PHE:HZ	1.78	0.49
31:a:1381:C:H2'	31:a:1382:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1382:G:H2'	31:a:1383:G:H8	1.77	0.49
34:d:61:GLN:HB3	34:d:65:ARG:NH1	2.26	0.49
6:B:46:U:H2'	6:B:47:C:C6	2.47	0.49
31:a:536:A:H2'	31:a:537:G:C8	2.47	0.49
55:a:1602:OIY:O53	35:e:141:LYS:HE2	2.12	0.49
37:g:87:VAL:N	37:g:144:MET:HE3	2.28	0.49
5:A:418:U:H2'	5:A:419:C:C6	2.47	0.49
5:A:2792:U:O2'	5:A:2793:U:H5''	2.12	0.49
11:G:42:GLU:OE2	11:G:43:LEU:N	2.45	0.49
32:b:68:LYS:NZ	32:b:70:LEU:HA	2.28	0.49
43:m:71:ARG:O	43:m:75:MET:HG2	2.12	0.49
5:A:578:U:H2'	5:A:579:C:C6	2.46	0.49
7:C:17:GLU:HB2	7:C:204:SER:HB3	1.95	0.49
31:a:529:A:OP1	33:c:193:TYR:OH	2.29	0.49
31:a:887:G:H4'	31:a:888:U:O5'	2.11	0.49
31:a:1388:U:H2'	31:a:1389:G:C8	2.48	0.49
34:d:171:ALA:O	34:d:185:LYS:NZ	2.42	0.49
5:A:1348:A:H2'	5:A:1349:A:C8	2.48	0.49
18:N:7:SER:O	18:N:11:ARG:HG3	2.12	0.49
5:A:1311:A:H2'	5:A:1312:G:H8	1.78	0.49
28:X:54:LYS:O	28:X:58:THR:HG22	2.13	0.49
31:a:1247:A:H2'	31:a:1248:A:C8	2.47	0.49
41:k:36:ARG:O	41:k:37:GLN:HB2	2.13	0.49
5:A:2188:G:H2'	5:A:2189:G:H8	1.78	0.48
31:a:669:U:H2'	31:a:670:A:C8	2.48	0.48
31:a:1313:G:H4'	44:n:58:VAL:HG11	1.94	0.48
32:b:92:PRO:HA	32:b:93:TYR:CD2	2.48	0.48
36:f:5:GLU:OE2	48:r:24:LYS:NZ	2.45	0.48
3:2:55:ALA:O	3:2:59:ARG:HG3	2.12	0.48
5:A:286:U:H2'	5:A:287:G:H8	1.77	0.48
5:A:495:G:N7	55:A:3005:OIY:N49	2.61	0.48
5:A:574:U:H2'	5:A:575:G:C8	2.48	0.48
5:A:862:G:H2'	5:A:863:C:C6	2.47	0.48
31:a:78:G:H2'	31:a:79:U:C6	2.48	0.48
31:a:942:G:C2	31:a:943:A:C8	3.01	0.48
31:a:1008:C:H2'	31:a:1009:A:H8	1.77	0.48
31:a:1438:A:O2'	31:a:1439:G:C8	2.65	0.48
42:l:101:SER:OG	42:l:102:LEU:N	2.46	0.48
5:A:811:U:H2'	5:A:812:C:H6	1.77	0.48
5:A:1193:U:H2'	5:A:1194:U:C6	2.48	0.48
10:F:17:GLN:NE2	10:F:22:ILE:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:80:ALA:HB3	25:U:94:ASP:HB2	1.96	0.48
31:a:499:A:OP1	42:l:115:SER:OG	2.20	0.48
31:a:1411:U:H2'	31:a:1412:G:H8	1.77	0.48
34:d:149:GLU:HA	34:d:152:LYS:HG3	1.95	0.48
34:d:154:GLN:O	34:d:158:LYS:HE2	2.13	0.48
46:p:98:LYS:HB2	46:p:98:LYS:NZ	2.28	0.48
5:A:19:U:O2	5:A:2622:C:H4'	2.13	0.48
5:A:2341:A:N3	5:A:2377:A:H2'	2.28	0.48
5:A:2469:U:H2'	5:A:2469:U:O2	2.14	0.48
19:O:91:ARG:NH1	19:O:115:GLU:HB2	2.29	0.48
31:a:1059:U:H2'	31:a:1060:C:C6	2.48	0.48
34:d:200:SER:O	34:d:204:GLU:HG2	2.12	0.48
39:i:45:VAL:HA	39:i:48:GLN:HG3	1.95	0.48
41:k:111:ASP:H	51:u:2:PRO:HG2	1.78	0.48
43:m:3:ARG:HH11	43:m:3:ARG:HB2	1.78	0.48
5:A:1464:A:H2'	5:A:1465:A:H8	1.77	0.48
5:A:2463:C:H2'	5:A:2464:A:O4'	2.13	0.48
6:B:49:G:H2'	6:B:50:A:C8	2.49	0.48
7:C:118:SER:HB2	7:C:129:CYS:HB3	1.95	0.48
8:D:6:VAL:HG11	8:D:79:LEU:HD11	1.96	0.48
20:P:58:ARG:HA	20:P:61:TRP:CE3	2.48	0.48
31:a:36:C:H2'	31:a:37:G:H8	1.78	0.48
31:a:386:U:H2'	31:a:387:C:C6	2.49	0.48
30:Z:52:GLN:OE1	30:Z:53:LEU:N	2.47	0.48
31:a:339:U:O2'	31:a:342:G:O6	2.27	0.48
31:a:552:U:H2'	31:a:553:C:C6	2.48	0.48
31:a:888:U:OP2	31:a:903:A:N6	2.47	0.48
34:d:13:ARG:NH2	34:d:39:PRO:HA	2.28	0.48
52:v:10:G:N2	52:v:27:A:H1'	2.28	0.48
37:g:106:ASP:OD1	37:g:106:ASP:N	2.47	0.48
37:g:113:GLU:HB2	37:g:119:ARG:HG3	1.96	0.48
5:A:1127:U:O2'	5:A:1128:G:H2'	2.13	0.48
5:A:2644:G:N7	55:A:3006:OIY:N52	2.61	0.48
31:a:536:A:OP1	42:l:111:ASN:ND2	2.41	0.48
31:a:905:A:H2'	31:a:906:A:H8	1.79	0.48
33:c:130:PHE:HD1	33:c:134:MET:HE2	1.79	0.48
34:d:97:GLU:OE1	34:d:106:ARG:NH1	2.47	0.48
5:A:1531:C:O2'	5:A:1533:U:O4	2.25	0.48
5:A:1917:G:H2'	5:A:1918:G:H8	1.78	0.48
6:B:64:A:H61	6:B:104:U:H2'	1.79	0.48
21:Q:37:ASP:OD1	21:Q:37:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1038:G:H2'	31:a:1039:A:C8	2.48	0.48
31:a:1349:C:H2'	31:a:1350:G:C8	2.48	0.48
31:a:1382:G:H2'	31:a:1383:G:C8	2.49	0.48
31:a:1433:U:H2'	31:a:1434:A:H8	1.79	0.48
5:A:199:G:O2'	5:A:675:A:N1	2.43	0.47
5:A:2563:G:H2'	5:A:2564:A:C8	2.49	0.47
31:a:333:G:H2'	31:a:334:A:C8	2.48	0.47
31:a:385:A:H3'	31:a:386:U:H6	1.79	0.47
31:a:588:U:H2'	31:a:589:A:C8	2.48	0.47
31:a:1510:A:H2'	31:a:1511:G:C8	2.49	0.47
5:A:811:U:H2'	5:A:812:C:C6	2.49	0.47
12:H:8:ARG:HH12	12:H:10:LYS:HD2	1.79	0.47
31:a:76:A:H61	31:a:91:G:H1	1.61	0.47
32:b:61:GLN:HB3	32:b:65:LYS:NZ	2.29	0.47
5:A:1481:U:H2'	5:A:1482:C:C6	2.49	0.47
5:A:2611:U:C2	30:Z:4:GLN:HA	2.50	0.47
11:G:124:GLU:HG3	11:G:132:ILE:HB	1.96	0.47
24:T:73:ALA:O	24:T:76:GLN:NE2	2.46	0.47
5:A:34:G:N2	5:A:511:G:H1'	2.28	0.47
5:A:1025:A:N3	5:A:2482:C:O2'	2.46	0.47
5:A:1243:G:C4	9:E:82:LYS:HE2	2.49	0.47
5:A:1481:U:H2'	5:A:1482:C:H6	1.78	0.47
5:A:2324:A:H2'	5:A:2325:A:H8	1.78	0.47
5:A:2586:A:H2'	5:A:2587:C:H6	1.80	0.47
9:E:194:LYS:HE2	9:E:194:LYS:HB3	1.70	0.47
10:F:141:ILE:HG12	10:F:145:LYS:HB2	1.96	0.47
28:X:41:HIS:O	28:X:45:VAL:HG23	2.14	0.47
31:a:406:G:OP2	34:d:31:LYS:NZ	2.39	0.47
31:a:1460:U:H2'	31:a:1461:U:C6	2.49	0.47
31:a:1461:U:H2'	31:a:1462:A:H8	1.79	0.47
37:g:129:GLU:N	37:g:129:GLU:OE1	2.47	0.47
5:A:992:C:H41	13:I:1:MET:HE3	1.79	0.47
5:A:2502:U:O2'	5:A:2503:C:OP1	2.30	0.47
5:A:2510:U:H2'	5:A:2511:C:C6	2.50	0.47
7:C:181:MET:HE2	7:C:268:ILE:HD11	1.97	0.47
23:S:5:ARG:O	23:S:9:VAL:HG23	2.14	0.47
31:a:461:A:H2'	31:a:462:A:C8	2.50	0.47
31:a:777:A:H5''	41:k:124:LYS:HD2	1.95	0.47
39:i:89:ASP:HB3	39:i:92:LEU:HG	1.96	0.47
5:A:413:C:H2'	5:A:414:A:H8	1.80	0.47
5:A:1503:C:H4'	5:A:1505:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1680:G:H2'	5:A:1681:U:C6	2.49	0.47
5:A:2239:U:H2'	5:A:2240:U:C6	2.49	0.47
7:C:271:ARG:CZ	7:C:273:VAL:HG12	2.44	0.47
14:J:17:ARG:HG3	14:J:17:ARG:HH11	1.79	0.47
31:a:242:A:C2	31:a:278:A:C5	3.02	0.47
5:A:287:G:H2'	5:A:288:U:H6	1.80	0.47
5:A:580:A:H2'	5:A:581:G:C8	2.50	0.47
5:A:1104:G:H2'	5:A:1105:U:C2	2.50	0.47
5:A:1381:A:H2'	5:A:1382:U:C6	2.50	0.47
7:C:133:ARG:HB3	7:C:133:ARG:NH1	2.30	0.47
10:F:120:LYS:NZ	10:F:122:PHE:H	2.12	0.47
10:F:120:LYS:HZ1	10:F:122:PHE:H	1.62	0.47
19:O:2:SER:O	19:O:2:SER:OG	2.25	0.47
31:a:669:U:H2'	31:a:670:A:H8	1.79	0.47
31:a:908:U:H2'	31:a:909:C:C6	2.50	0.47
31:a:1235:A:H2	31:a:1238:G:N3	2.13	0.47
32:b:134:ARG:HD3	32:b:137:LEU:HD21	1.96	0.47
48:r:21:ILE:N	48:r:21:ILE:HD12	2.30	0.47
51:u:11:PRO:HD2	51:u:14:VAL:HB	1.96	0.47
5:A:157:U:H2'	5:A:158:U:C6	2.50	0.47
5:A:279:U:H2'	5:A:364:A:C6	2.49	0.47
5:A:1025:A:N6	5:A:1122:G:H2'	2.30	0.47
5:A:2419:U:H4'	5:A:2420:C:O5'	2.15	0.47
24:T:4:ILE:HD13	24:T:70:ILE:HG23	1.97	0.47
31:a:1464:C:H2'	31:a:1465:A:C8	2.49	0.47
32:b:58:PHE:HD2	32:b:186:ILE:HD11	1.80	0.47
32:b:134:ARG:O	32:b:137:LEU:HG	2.14	0.47
39:i:128:ARG:NH1	52:v:36:A:OP1	2.48	0.47
5:A:288:U:H2'	5:A:289:G:C8	2.50	0.47
10:F:65:PRO:HA	10:F:89:VAL:HG22	1.96	0.47
31:a:433:U:O2'	31:a:434:U:H5'	2.15	0.47
41:k:46:SER:HB3	41:k:61:ALA:HB1	1.97	0.47
42:l:123:LYS:HE2	42:l:123:LYS:HA	1.95	0.47
4:3:16:VAL:HG22	4:3:25:VAL:HG22	1.96	0.47
5:A:568:G:H2'	5:A:2026:6MZ:N7	2.30	0.47
5:A:908:A:H2'	5:A:909:A:C8	2.49	0.47
5:A:1111:C:H2'	5:A:1112:G:C8	2.50	0.47
5:A:2645:C:H2'	5:A:2646:U:H6	1.79	0.47
7:C:183:LYS:NZ	7:C:266:MET:HA	2.30	0.47
31:a:394:U:H2'	31:a:395:G:H8	1.80	0.47
31:a:1311:C:H2'	31:a:1312:U:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:29:C:H2'	52:v:30:G:H8	1.79	0.47
5:A:110:A:OP2	5:A:110:A:H8	1.97	0.46
5:A:740:G:H2'	5:A:741:U:H6	1.80	0.46
6:B:46:U:H2'	6:B:47:C:H6	1.80	0.46
8:D:20:GLY:HA3	19:O:83:VAL:HG23	1.96	0.46
20:P:86:ALA:HB2	20:P:116:ALA:HB2	1.97	0.46
5:A:1311:A:H2'	5:A:1312:G:C8	2.51	0.46
8:D:33:ASN:N	8:D:33:ASN:HD22	2.12	0.46
10:F:54:VAL:HG13	10:F:65:PRO:HG2	1.96	0.46
37:g:56:VAL:HG11	37:g:61:PHE:HD2	1.81	0.46
5:A:831:A:H2'	5:A:832:G:H8	1.79	0.46
5:A:1172:U:O2'	5:A:1173:G:O4'	2.27	0.46
10:F:56:ASP:O	10:F:60:ILE:HD12	2.15	0.46
31:a:212:U:H2'	31:a:213:U:C6	2.49	0.46
31:a:671:G:H2'	31:a:672:A:H8	1.80	0.46
31:a:748:U:H2'	31:a:749:G:O4'	2.16	0.46
41:k:122:PRO:HD2	51:u:38:TYR:HB2	1.98	0.46
5:A:701:U:H2'	5:A:702:G:O4'	2.15	0.46
5:A:944:A:H2'	5:A:945:C:C6	2.50	0.46
5:A:2224:G:H2'	5:A:2225:U:C6	2.51	0.46
5:A:2229:U:H2'	5:A:2230:G:C8	2.50	0.46
9:E:110:GLU:HB3	15:K:3:LEU:HD22	1.97	0.46
31:a:671:G:H21	41:k:117:HIS:HB2	1.80	0.46
5:A:478:A:N3	5:A:480:G:H5''	2.30	0.46
5:A:782:G:H5'	5:A:783:G:OP1	2.16	0.46
12:H:13:GLY:O	12:H:14:LYS:HD3	2.16	0.46
31:a:35:A:H2'	31:a:36:C:H6	1.81	0.46
31:a:184:A:H3'	31:a:185:C:O2	2.16	0.46
31:a:472:A:H2'	31:a:473:U:C6	2.50	0.46
38:h:87:TYR:O	38:h:88:ARG:NH1	2.48	0.46
27:W:70:ASP:O	27:W:74:GLN:HG3	2.15	0.46
31:a:200:G:H2'	31:a:201:A:H8	1.80	0.46
31:a:435:U:C2	31:a:436:A:C8	3.04	0.46
31:a:1488:G:H2'	31:a:1489:A:C8	2.51	0.46
44:n:83:LYS:HA	44:n:83:LYS:HD3	1.62	0.46
5:A:2533:U:H2'	5:A:2534:C:H6	1.80	0.46
10:F:91:LEU:HB3	10:F:96:MET:HB3	1.98	0.46
12:H:48:GLU:OE2	12:H:48:GLU:N	2.47	0.46
32:b:185:VAL:HG12	32:b:198:VAL:HG13	1.97	0.46
5:A:86:C:HO2'	5:A:348:A:H1'	1.81	0.46
14:J:17:ARG:HG3	14:J:17:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:534:A:H2'	31:a:535:G:C8	2.51	0.46
31:a:994:U:H2'	31:a:995:A:C8	2.49	0.46
31:a:1117:C:H2'	31:a:1118:U:H6	1.80	0.46
44:n:87:THR:HG23	44:n:92:ASP:HB2	1.98	0.46
51:u:17:ARG:HB3	51:u:20:LYS:HZ3	1.81	0.46
1:0:30:MET:HE1	5:A:2282:G:C6	2.51	0.46
5:A:1589:C:H2'	5:A:1590:A:H8	1.81	0.46
31:a:519:C:H41	42:l:50:ARG:NH2	2.14	0.46
32:b:45:LEU:O	32:b:49:VAL:HG13	2.16	0.46
5:A:498:U:H2'	5:A:499:G:O4'	2.16	0.46
5:A:2645:C:H2'	5:A:2646:U:C6	2.51	0.46
5:A:2727:G:H2'	5:A:2728:G:C8	2.51	0.46
9:E:3:LEU:HD12	9:E:13:LEU:HD12	1.97	0.46
12:H:52:ALA:HB1	12:H:56:LYS:NZ	2.30	0.46
31:a:1011:A:C2	31:a:1216:A:H1'	2.51	0.46
5:A:592:U:H2'	5:A:593:C:C6	2.51	0.45
5:A:596:U:H2'	5:A:597:A:H8	1.81	0.45
5:A:605:U:C5	5:A:618:G:C5	3.03	0.45
5:A:844:A:H4'	5:A:845:A:O5'	2.15	0.45
5:A:2683:U:H2'	5:A:2684:G:O4'	2.16	0.45
31:a:6:C:H42	31:a:610:C:H5''	1.81	0.45
32:b:79:SER:O	32:b:82:ILE:HG13	2.16	0.45
3:2:13:ARG:HD2	15:K:65:LYS:HG2	1.97	0.45
5:A:2784:C:H2'	5:A:2785:C:C6	2.51	0.45
13:I:2:LYS:HB2	20:P:93:ARG:HH12	1.81	0.45
31:a:37:G:H2'	31:a:38:C:C6	2.51	0.45
31:a:156:A:H2'	31:a:157:A:O4'	2.16	0.45
31:a:1093:C:O2	31:a:1167:A:O2'	2.34	0.45
31:a:1118:U:H2'	31:a:1119:U:C6	2.51	0.45
36:f:29:ILE:HD11	36:f:74:LEU:HD11	1.98	0.45
47:q:48:HIS:HB3	47:q:75:THR:HG22	1.99	0.45
7:C:107:PRO:HD2	7:C:110:LEU:HD22	1.97	0.45
23:S:6:ILE:HG21	23:S:48:LYS:HD3	1.98	0.45
31:a:421:G:H2'	31:a:422:U:C6	2.51	0.45
31:a:436:A:C4	31:a:437:A:C8	3.05	0.45
32:b:82:ILE:HD11	32:b:95:ASP:HA	1.98	0.45
34:d:67:TYR:OH	34:d:97:GLU:OE2	2.23	0.45
5:A:847:A:H2'	5:A:848:C:C6	2.51	0.45
13:I:98:GLU:H	13:I:98:GLU:CD	2.22	0.45
31:a:190:G:H4'	50:t:59:ASP:HB3	1.98	0.45
31:a:539:G:H5'	34:d:40:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:754:U:H2'	31:a:755:G:O4'	2.16	0.45
47:q:19:ASP:OD1	47:q:19:ASP:N	2.50	0.45
5:A:478:A:H4'	5:A:479:A:OP1	2.16	0.45
5:A:1108:A:C8	5:A:1109:G:H1'	2.48	0.45
5:A:1356:G:H2'	5:A:1357:C:C6	2.51	0.45
5:A:2736:A:H2'	5:A:2737:A:C8	2.51	0.45
5:A:2841:U:H5''	19:O:55:ASN:O	2.17	0.45
8:D:184:ASP:OD1	8:D:186:GLU:HG2	2.16	0.45
10:F:48:LYS:HD2	10:F:48:LYS:O	2.16	0.45
10:F:93:GLY:O	10:F:96:MET:HG3	2.16	0.45
15:K:95:GLU:CD	15:K:95:GLU:H	2.24	0.45
19:O:5:HIS:O	19:O:9:GLN:HG3	2.17	0.45
24:T:29:GLU:OE1	24:T:29:GLU:HA	2.17	0.45
25:U:53:LYS:HD2	25:U:53:LYS:HA	1.64	0.45
31:a:693:A:H2'	31:a:694:U:H6	1.82	0.45
44:n:56:SER:OG	44:n:58:VAL:HG22	2.17	0.45
52:v:29:C:H2'	52:v:30:G:C8	2.51	0.45
5:A:976:A:H2'	5:A:979:C:H42	1.81	0.45
5:A:2631:U:O2'	8:D:82:GLU:OE2	2.31	0.45
7:C:4:GLN:HE22	7:C:19:VAL:C	2.25	0.45
31:a:808:C:O2'	31:a:898:A:N1	2.49	0.45
31:a:887:G:H1'	31:a:903:A:N6	2.32	0.45
31:a:1260:A:H2'	31:a:1261:C:C6	2.52	0.45
35:e:40:ASP:OD2	35:e:44:ARG:HB2	2.17	0.45
43:m:12:ASN:OD1	43:m:46:ARG:NH1	2.50	0.45
5:A:687:A:H2'	5:A:688:U:C6	2.52	0.45
10:F:147:ASP:OD1	10:F:148:ARG:N	2.41	0.45
31:a:1335:G:H2'	31:a:1336:A:C8	2.51	0.45
32:b:8:MET:O	32:b:12:LEU:HD12	2.16	0.45
5:A:369:G:O2'	5:A:423:G:OP1	2.32	0.45
5:A:678:A:H2'	5:A:679:G:C8	2.51	0.45
5:A:1310:C:H2'	5:A:1311:A:H8	1.82	0.45
5:A:1458:A:H2'	5:A:1459:G:C8	2.52	0.45
5:A:2224:G:H2'	5:A:2225:U:H6	1.82	0.45
31:a:232:A:H2'	31:a:233:A:H8	1.80	0.45
31:a:489:C:H2'	31:a:490:A:C8	2.51	0.45
31:a:542:C:H5'	34:d:71:GLU:HB2	1.99	0.45
35:e:80:LEU:HB2	35:e:97:PRO:HG3	1.99	0.45
5:A:527:A:H5'	13:I:113:PRO:HG3	1.98	0.45
5:A:2021:C:H2'	5:A:2022:U:C6	2.52	0.45
6:B:17:A:H2'	6:B:18:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:63:THR:O	18:N:64:THR:HG22	2.17	0.45
31:a:1036:U:H2'	31:a:1037:A:C8	2.48	0.45
31:a:1248:A:H2'	31:a:1249:A:C8	2.52	0.45
14:J:63:VAL:HG12	14:J:106:LEU:HD11	1.99	0.45
31:a:319:U:H2'	31:a:320:G:O4'	2.16	0.45
31:a:577:C:H2'	31:a:578:G:O4'	2.16	0.45
5:A:1430:G:H2'	5:A:1431:G:C8	2.52	0.44
5:A:1805:A:H2'	5:A:1806:A:C8	2.52	0.44
15:K:112:ILE:HB	15:K:129:LEU:HD23	1.99	0.44
31:a:1034:C:H2'	31:a:1035:C:H6	1.83	0.44
35:e:68:ARG:HE	35:e:68:ARG:HB3	1.61	0.44
37:g:66:LEU:HD21	37:g:97:THR:HG23	1.99	0.44
5:A:794:C:H2'	5:A:795:U:C6	2.52	0.44
5:A:869:U:H2'	5:A:870:U:C6	2.53	0.44
5:A:1866:U:H2'	5:A:1867:A:O4'	2.18	0.44
5:A:2269:A:H2'	5:A:2270:A:C8	2.53	0.44
12:H:13:GLY:C	12:H:14:LYS:HD3	2.42	0.44
14:J:105:GLU:OE1	14:J:105:GLU:N	2.50	0.44
19:O:28:THR:CG2	19:O:91:ARG:HB3	2.47	0.44
26:V:20:MET:HE2	26:V:20:MET:HB2	1.91	0.44
31:a:491:G:O2'	31:a:493:A:H1'	2.17	0.44
31:a:915:A:H2'	31:a:916:A:C8	2.53	0.44
31:a:1097:C:H3'	32:b:97:ARG:NH2	2.32	0.44
31:a:1437:U:H2'	31:a:1438:A:N3	2.31	0.44
37:g:142:HIS:HB3	37:g:143:ARG:NH2	2.33	0.44
5:A:158:U:H2'	5:A:159:G:H8	1.82	0.44
32:b:68:LYS:HD3	32:b:69:VAL:N	2.32	0.44
5:A:178:U:H2'	5:A:179:U:C6	2.52	0.44
10:F:136:ILE:HG22	10:F:137:VAL:H	1.82	0.44
15:K:144:VAL:HG23	15:K:145:GLU:OE1	2.16	0.44
24:T:3:LYS:HE2	24:T:3:LYS:HA	1.99	0.44
31:a:521:G:H2'	31:a:522:C:C6	2.52	0.44
34:d:57:LEU:O	34:d:61:GLN:HG2	2.17	0.44
48:r:21:ILE:HG22	48:r:22:ASP:N	2.32	0.44
5:A:306:U:H2'	5:A:307:C:C6	2.52	0.44
5:A:1962:A:N3	5:A:2588:G:O2'	2.47	0.44
6:B:16:A:H2'	6:B:17:A:H8	1.82	0.44
31:a:35:A:H2'	31:a:36:C:C6	2.52	0.44
31:a:639:A:N7	38:h:108:SER:HA	2.32	0.44
34:d:22:LYS:HD2	34:d:31:LYS:HE3	1.99	0.44
5:A:79:A:H61	28:X:58:THR:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1151:C:H2'	5:A:1152:G:O4'	2.18	0.44
5:A:2302:C:H3'	5:A:2303:G:H5''	2.00	0.44
5:A:2456:U:C2	5:A:2457:A:C8	3.06	0.44
31:a:1483:G:H2'	31:a:1484:G:C8	2.53	0.44
33:c:210:GLY:O	33:c:214:VAL:HG23	2.18	0.44
41:k:106:ILE:HG13	51:u:6:LEU:HD13	2.00	0.44
5:A:2674:A:H2'	5:A:2675:A:H8	1.83	0.44
11:G:87:LEU:HD12	11:G:133:LEU:HD11	1.98	0.44
31:a:483:U:H2'	31:a:484:A:H8	1.83	0.44
32:b:10:ASP:O	32:b:13:GLN:HG3	2.18	0.44
34:d:158:LYS:O	34:d:161:ILE:HG12	2.18	0.44
5:A:34:G:H22	5:A:511:G:H1'	1.83	0.44
5:A:1665:G:O2'	5:A:1987:U:O4	2.33	0.44
5:A:2033:A:H2'	5:A:2034:G:C8	2.53	0.44
5:A:2793:U:O4	5:A:2797:G:N2	2.26	0.44
31:a:200:G:H2'	31:a:201:A:C8	2.52	0.44
31:a:518:G:OP2	42:l:51:LYS:NZ	2.51	0.44
31:a:919:G:H2'	31:a:920:A:H8	1.82	0.44
31:a:1031:G:C2	31:a:1032:A:C8	3.06	0.44
3:2:61:CYS:HB3	3:2:64:ILE:HG12	1.99	0.44
5:A:86:C:O2'	5:A:348:A:H1'	2.18	0.44
5:A:102:A:H2'	5:A:103:U:C6	2.53	0.44
5:A:2457:A:H2'	5:A:2458:C:C6	2.52	0.44
10:F:108:ILE:HG12	10:F:176:PRO:HG3	1.99	0.44
30:Z:31:GLN:OE1	30:Z:31:GLN:HA	2.17	0.44
31:a:993:A:H2'	31:a:994:U:C6	2.53	0.44
31:a:1118:U:H2'	31:a:1119:U:H6	1.83	0.44
31:a:1407:A:H2'	31:a:1408:C:C6	2.53	0.44
32:b:208:ALA:O	32:b:212:VAL:HG22	2.17	0.44
33:c:81:GLY:O	33:c:84:ILE:HG12	2.18	0.44
52:v:39:A:H2'	52:v:40:U:O4'	2.18	0.44
5:A:161:A:H2'	5:A:162:A:H8	1.81	0.43
10:F:4:LEU:O	10:F:6:ALA:N	2.51	0.43
18:N:52:ALA:HB3	18:N:77:ILE:HB	2.00	0.43
31:a:1144:C:O2'	39:i:5:TYR:OH	2.28	0.43
33:c:31:GLU:OE2	33:c:35:LYS:NZ	2.35	0.43
5:A:1194:U:H2'	5:A:1195:C:H6	1.83	0.43
5:A:1400:U:H2'	5:A:1401:U:C6	2.53	0.43
13:I:60:GLU:OE2	13:I:60:GLU:N	2.46	0.43
31:a:295:G:H2'	31:a:296:A:C8	2.53	0.43
31:a:1433:U:H2'	31:a:1434:A:C8	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:10:U:H2'	5:A:11:C:C6	2.54	0.43
18:N:67:ILE:O	18:N:71:THR:HG23	2.18	0.43
32:b:11:LEU:HD12	32:b:49:VAL:HG12	2.00	0.43
32:b:61:GLN:HB3	32:b:65:LYS:HZ1	1.83	0.43
40:j:42:MET:HB2	40:j:71:LYS:HB3	1.99	0.43
5:A:1276:G:H2'	5:A:1277:U:C6	2.54	0.43
5:A:2797:G:H2'	5:A:2798:U:C6	2.53	0.43
7:C:270:ASP:OD2	7:C:273:VAL:HG13	2.19	0.43
10:F:65:PRO:HB2	10:F:87:CYS:SG	2.58	0.43
31:a:536:A:H2'	31:a:537:G:H8	1.82	0.43
31:a:734:A:H2'	31:a:735:U:H6	1.83	0.43
31:a:1521:C:H2'	31:a:1522:G:C8	2.54	0.43
33:c:86:LYS:O	33:c:90:GLU:OE1	2.37	0.43
35:e:95:MET:HE3	35:e:95:MET:HB2	1.90	0.43
35:e:114:LEU:HD13	35:e:122:VAL:HG11	2.00	0.43
22:R:63:SER:O	22:R:63:SER:OG	2.24	0.43
31:a:457:A:H2'	31:a:458:G:H8	1.84	0.43
31:a:1001:A:H2'	31:a:1002:A:O4'	2.18	0.43
31:a:1008:C:H2'	31:a:1009:A:C8	2.54	0.43
33:c:77:ILE:HA	33:c:84:ILE:HG23	2.00	0.43
37:g:46:ALA:HA	37:g:121:ALA:HB2	2.00	0.43
5:A:521:G:H2'	5:A:522:C:C6	2.54	0.43
5:A:1316:A:C4	5:A:1317:A:C8	3.06	0.43
11:G:72:LEU:HA	11:G:75:LEU:HD12	2.00	0.43
19:O:94:ASP:OD1	19:O:116:LYS:NZ	2.39	0.43
31:a:380:C:H2'	31:a:381:C:H6	1.82	0.43
31:a:1068:C:H2'	31:a:1069:G:H8	1.83	0.43
33:c:84:ILE:O	33:c:88:GLN:HG3	2.18	0.43
45:o:75:HIS:O	45:o:79:THR:HG23	2.18	0.43
5:A:1924:A:H2'	5:A:1925:G:O4'	2.18	0.43
6:B:60:U:H2'	6:B:61:C:H6	1.84	0.43
19:O:27:ASP:OD1	19:O:92:ARG:HA	2.18	0.43
31:a:414:C:H2'	31:a:415:C:C6	2.53	0.43
31:a:1127:A:H2'	31:a:1128:G:H8	1.84	0.43
31:a:1493:C:H2'	31:a:1494:G:O4'	2.18	0.43
40:j:90:LEU:HD12	40:j:90:LEU:HA	1.81	0.43
41:k:92:ARG:H	41:k:92:ARG:HG2	1.59	0.43
47:q:76:LEU:HD12	47:q:77:VAL:N	2.34	0.43
5:A:292:U:H2'	5:A:293:U:C6	2.54	0.43
10:F:71:ARG:O	10:F:72:LYS:HB3	2.18	0.43
13:I:75:TYR:CE1	13:I:86:GLU:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:88:ASN:HB3	14:J:94:ILE:HG21	2.01	0.43
32:b:49:VAL:HG22	32:b:50:PRO:HD3	2.00	0.43
33:c:79:LYS:HD2	33:c:79:LYS:C	2.44	0.43
41:k:80:ASN:OD1	41:k:80:ASN:N	2.51	0.43
50:t:39:ILE:HD11	50:t:83:VAL:HG23	2.00	0.43
5:A:189:A:H2'	5:A:190:C:C6	2.54	0.43
5:A:715:C:H2'	5:A:716:A:O4'	2.18	0.43
5:A:2586:A:H2'	5:A:2587:C:C6	2.54	0.43
13:I:1:MET:SD	13:I:1:MET:N	2.89	0.43
26:V:46:HIS:CD2	26:V:77:ARG:HD2	2.54	0.43
31:a:917:U:H2'	31:a:918:U:C6	2.54	0.43
31:a:1093:C:H2'	31:a:1094:C:C6	2.54	0.43
32:b:198:VAL:HB	32:b:201:VAL:HG22	2.01	0.43
35:e:40:ASP:OD1	35:e:42:ASN:N	2.29	0.43
36:f:93:GLU:O	36:f:94:HIS:ND1	2.52	0.43
42:l:89:ASP:OD1	42:l:89:ASP:C	2.62	0.43
4:3:26:ILE:O	4:3:26:ILE:HG13	2.19	0.43
5:A:844:A:H5''	5:A:845:A:C8	2.54	0.43
5:A:1472:A:H2'	5:A:1473:G:O4'	2.18	0.43
5:A:2550:U:H2'	5:A:2551:U:C6	2.54	0.43
6:B:64:A:N6	6:B:104:U:H2'	2.34	0.43
7:C:160:ALA:HA	7:C:177:ARG:CZ	2.49	0.43
10:F:8:TYR:HA	10:F:12:LEU:HB2	2.01	0.43
18:N:68:GLU:OE1	18:N:68:GLU:N	2.52	0.43
31:a:588:U:H2'	31:a:589:A:H8	1.83	0.43
31:a:1034:C:H2'	31:a:1035:C:C6	2.54	0.43
32:b:9:ARG:HA	32:b:9:ARG:HD2	1.89	0.43
33:c:90:GLU:OE1	33:c:90:GLU:N	2.51	0.43
5:A:358:A:H2'	5:A:359:U:H6	1.84	0.42
5:A:1587:U:H2'	5:A:1588:A:H8	1.84	0.42
6:B:17:A:H2'	6:B:18:G:H8	1.84	0.42
31:a:144:G:O2'	31:a:1443:A:N3	2.46	0.42
31:a:204:U:H5''	31:a:205:U:OP1	2.19	0.42
31:a:650:A:C5	38:h:57:LYS:HG2	2.54	0.42
31:a:818:G:H2'	31:a:819:U:C6	2.54	0.42
31:a:1117:C:H2'	31:a:1118:U:C6	2.54	0.42
43:m:83:LEU:HD12	43:m:83:LEU:HA	1.86	0.42
9:E:163:LEU:HD23	9:E:163:LEU:HA	1.84	0.42
11:G:33:LEU:HB3	11:G:75:LEU:HD22	2.02	0.42
31:a:572:G:O2'	31:a:818:G:OP2	2.33	0.42
31:a:905:A:H2'	31:a:906:A:C8	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:211:MET:HE2	33:c:216:ASN:CG	2.44	0.42
34:d:4:TYR:CD1	34:d:4:TYR:C	2.96	0.42
1:0:34:LYS:HB2	1:0:45:PHE:CD1	2.54	0.42
5:A:198:A:H2'	5:A:199:G:N3	2.33	0.42
6:B:50:A:H8	6:B:50:A:OP2	2.03	0.42
10:F:32:THR:OG1	10:F:157:THR:O	2.31	0.42
10:F:49:LEU:HD12	10:F:148:ARG:NE	2.33	0.42
10:F:59:LEU:HD23	10:F:59:LEU:HA	1.86	0.42
31:a:358:G:N2	31:a:361:U:OP2	2.51	0.42
31:a:963:2MG:HM22	52:v:35:C:H5'	2.02	0.42
31:a:1115:U:H2'	31:a:1116:C:H6	1.84	0.42
33:c:79:LYS:HD2	33:c:80:LYS:HB2	2.00	0.42
36:f:19:VAL:O	36:f:23:GLU:HG2	2.19	0.42
44:n:73:TYR:CE2	44:n:75:ARG:HA	2.54	0.42
5:A:849:C:H2'	5:A:850:A:H8	1.84	0.42
5:A:1919:U:H2'	5:A:1920:C:C6	2.54	0.42
5:A:1942:U:H2'	5:A:1943:C:C6	2.55	0.42
18:N:54:THR:HB	18:N:64:THR:OG1	2.19	0.42
31:a:136:U:H2'	31:a:137:A:C8	2.54	0.42
31:a:1157:G:H1	31:a:1173:A:H61	1.67	0.42
38:h:67:PHE:CD2	38:h:68:GLU:HG3	2.54	0.42
1:0:6:ARG:HG3	1:0:50:ILE:HD12	2.02	0.42
5:A:12:A:H2'	5:A:13:A:H8	1.82	0.42
5:A:475:G:N1	5:A:478:A:OP2	2.49	0.42
5:A:1549:U:H2'	5:A:1550:G:O4'	2.19	0.42
5:A:1733:U:H3'	5:A:1734:G:C8	2.54	0.42
5:A:1993:C:OP2	8:D:132:THR:OG1	2.27	0.42
5:A:2428:A:H1'	52:v:76:C:O4'	2.18	0.42
14:J:71:ARG:HA	14:J:71:ARG:HD3	1.84	0.42
19:O:117:LEU:HA	19:O:118:PRO:HD2	1.88	0.42
20:P:78:ARG:HD3	20:P:78:ARG:HA	1.69	0.42
33:c:90:GLU:O	33:c:94:ILE:HG13	2.19	0.42
5:A:580:A:H2'	5:A:581:G:H8	1.84	0.42
5:A:1561:U:H2'	5:A:1562:C:C6	2.54	0.42
5:A:2247:OMG:HM23	5:A:2247:OMG:H1'	1.71	0.42
5:A:2448:C:H2'	5:A:2449:A:C8	2.55	0.42
7:C:144:VAL:HB	7:C:154:LEU:HB2	2.00	0.42
14:J:109:GLU:OE1	14:J:109:GLU:N	2.50	0.42
22:R:68:ASP:OD1	22:R:68:ASP:N	2.53	0.42
31:a:394:U:H2'	31:a:395:G:C8	2.55	0.42
34:d:63:VAL:HA	34:d:66:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:70:MET:HE3	35:e:70:MET:HB3	1.88	0.42
52:v:14:A:H3'	52:v:15:G:N2	2.34	0.42
53:w:2:U:H2'	53:w:3:G:C8	2.54	0.42
5:A:158:U:H2'	5:A:159:G:C8	2.55	0.42
5:A:997:A:H2'	5:A:998:A:C8	2.54	0.42
5:A:1533:U:H1'	5:A:1535:U:O2	2.19	0.42
13:I:7:LYS:HB2	13:I:10:GLU:HG3	2.02	0.42
31:a:979:U:H4'	31:a:980:A:O4'	2.20	0.42
31:a:1057:U:H2'	31:a:1058:G:H8	1.85	0.42
31:a:1352:G:H2'	31:a:1353:G:H8	1.85	0.42
34:d:107:MET:HE1	34:d:145:ILE:HD13	2.01	0.42
5:A:42:G:H8	5:A:42:G:OP2	2.03	0.42
5:A:125:A:H5'	5:A:126:A:H8	1.85	0.42
5:A:587:U:H2'	5:A:588:A:C8	2.55	0.42
7:C:123:PRO:O	7:C:128:ASN:ND2	2.35	0.42
7:C:256:LYS:HE2	7:C:273:VAL:O	2.20	0.42
31:a:23:G:H2'	31:a:24:G:C8	2.54	0.42
31:a:639:A:C5	38:h:108:SER:HA	2.54	0.42
31:a:684:A:C2	31:a:701:A:C5	3.07	0.42
31:a:878:G:P	42:l:9:ARG:HH22	2.43	0.42
31:a:1035:C:H2'	31:a:1036:U:C6	2.55	0.42
31:a:1115:U:H1'	31:a:1176:A:C5	2.54	0.42
33:c:132:ARG:HD2	33:c:136:ARG:HH21	1.85	0.42
46:p:66:GLU:OE1	46:p:69:ARG:NH1	2.53	0.42
5:A:637:U:H2'	5:A:638:C:H6	1.85	0.42
5:A:1428:A:H2'	5:A:1429:A:C8	2.55	0.42
5:A:1716:U:H2'	5:A:1717:G:O4'	2.19	0.42
5:A:2232:U:H2'	5:A:2233:G:O4'	2.20	0.42
24:T:2:ALA:HA	24:T:81:VAL:HB	2.01	0.42
31:a:79:U:H2'	31:a:80:A:C8	2.55	0.42
31:a:776:C:H2'	31:a:777:A:O4'	2.19	0.42
37:g:107:ALA:HB1	37:g:133:ALA:HB3	2.01	0.42
5:A:31:G:O2'	22:R:78:GLU:O	2.37	0.42
5:A:625:A:H5''	15:K:80:ARG:HH21	1.84	0.42
5:A:1422:A:H4'	5:A:1423:C:O4'	2.20	0.42
5:A:1666:A:O2'	5:A:1672:G:N7	2.48	0.42
9:E:1:MET:HE3	9:E:1:MET:HB3	1.73	0.42
11:G:52:LEU:HD13	11:G:52:LEU:HA	1.94	0.42
14:J:50:ALA:O	14:J:53:LYS:NZ	2.53	0.42
31:a:380:C:H2'	31:a:381:C:C6	2.55	0.42
31:a:601:G:H2'	31:a:602:U:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:674:U:H3	31:a:710:G:H22	1.68	0.42
31:a:1023:G:N3	31:a:1023:G:H2'	2.35	0.42
31:a:1163:G:N2	31:a:1167:A:OP2	2.49	0.42
32:b:66:LYS:HD3	32:b:66:LYS:HA	1.89	0.42
34:d:199:GLU:O	34:d:203:VAL:HG23	2.20	0.42
42:l:88:LYS:HB3	42:l:88:LYS:HE2	1.78	0.42
47:q:55:LYS:HB2	47:q:55:LYS:HE2	1.82	0.42
51:u:17:ARG:HA	51:u:20:LYS:CD	2.50	0.42
4:3:2:LYS:NZ	5:A:2474:A:OP2	2.44	0.41
5:A:142:A:H2'	5:A:143:C:H6	1.85	0.41
5:A:418:U:H2'	5:A:419:C:H6	1.85	0.41
7:C:256:LYS:HE2	7:C:273:VAL:HG23	2.01	0.41
10:F:140:GLU:HG2	10:F:141:ILE:O	2.20	0.41
31:a:632:A:H2'	31:a:633:U:C6	2.55	0.41
31:a:1050:G:H4'	31:a:1051:C:H3'	2.02	0.41
43:m:37:VAL:HG23	43:m:59:GLU:HG3	2.01	0.41
51:u:34:LYS:HA	51:u:34:LYS:HD3	1.64	0.41
5:A:596:U:H2'	5:A:597:A:C8	2.55	0.41
5:A:1314:C:O2'	5:A:1315:C:H5'	2.19	0.41
5:A:2805:A:H2'	5:A:2806:A:C8	2.55	0.41
14:J:4:THR:HG22	14:J:5:GLU:HG2	2.02	0.41
18:N:40:VAL:O	18:N:49:LEU:N	2.52	0.41
18:N:44:ASP:OD1	18:N:46:GLY:N	2.48	0.41
31:a:848:U:H2'	31:a:849:A:C8	2.55	0.41
31:a:897:A:H2'	31:a:898:A:C8	2.55	0.41
38:h:39:VAL:HG21	38:h:111:ILE:HG22	2.02	0.41
45:o:6:ALA:O	45:o:10:GLU:HG2	2.19	0.41
4:3:15:LYS:HE3	4:3:15:LYS:HB3	1.76	0.41
5:A:1412:C:O2'	5:A:1585:G:O2'	2.24	0.41
7:C:38:LYS:HE2	7:C:39:ARG:O	2.20	0.41
31:a:333:G:N7	55:a:1601:OIY:N52	2.68	0.41
31:a:610:C:H2'	31:a:611:C:H6	1.85	0.41
31:a:1312:U:H2'	31:a:1313:G:O4'	2.21	0.41
41:k:115:ILE:HD13	41:k:115:ILE:HA	1.88	0.41
44:n:11:LEU:HD23	44:n:11:LEU:HA	1.86	0.41
5:A:215:C:H2'	5:A:216:C:H6	1.85	0.41
5:A:1050:U:O4	5:A:1051:A:N6	2.53	0.41
5:A:2237:A:H2'	5:A:2238:G:C8	2.56	0.41
8:D:182:SER:HB3	8:D:191:VAL:HB	2.02	0.41
31:a:470:G:H2'	31:a:471:G:H8	1.86	0.41
31:a:590:U:H2'	31:a:591:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1141:G:N2	31:a:1143:A:H62	2.18	0.41
31:a:1527:G:H2'	31:a:1528:A:C8	2.55	0.41
33:c:86:LYS:O	33:c:89:ARG:N	2.53	0.41
37:g:108:ALA:O	37:g:119:ARG:HD2	2.20	0.41
38:h:112:MET:HE2	38:h:112:MET:HB3	1.92	0.41
41:k:79:LYS:H	41:k:79:LYS:HG2	1.76	0.41
51:u:49:LYS:HD2	51:u:49:LYS:HA	1.63	0.41
5:A:568:G:H2'	5:A:2026:6MZ:C8	2.51	0.41
5:A:1838:G:H2'	5:A:1839:C:H6	1.86	0.41
5:A:2295:G:N2	5:A:2314:G:C2	2.89	0.41
5:A:2379:G:HO2'	5:A:2380:U:P	2.42	0.41
5:A:2687:C:O2'	5:A:2867:U:O2'	2.36	0.41
15:K:84:LEU:HD23	15:K:84:LEU:HA	1.91	0.41
32:b:88:ARG:HH21	32:b:224:LEU:HD12	1.86	0.41
32:b:115:ARG:HA	32:b:118:ASP:OD2	2.20	0.41
52:v:14:A:H2'	52:v:15:G:H5'	2.02	0.41
52:v:21:U:OP2	52:v:49:C:N4	2.54	0.41
52:v:28:C:C2	52:v:29:C:C5	3.08	0.41
5:A:2641:U:H4'	5:A:2728:G:O2'	2.21	0.41
24:T:70:ILE:H	24:T:70:ILE:HG13	1.67	0.41
31:a:275:A:H5''	31:a:277:G:O4'	2.19	0.41
35:e:40:ASP:OD1	35:e:40:ASP:C	2.63	0.41
37:g:70:ARG:NH1	37:g:97:THR:OG1	2.53	0.41
41:k:111:ASP:OD1	41:k:113:THR:HG22	2.21	0.41
42:l:39:THR:CG2	42:l:49:MET:HG3	2.48	0.41
52:v:8:4SU:O2'	52:v:47:G:N2	2.54	0.41
52:v:47:G:H3'	52:v:48:U:C6	2.56	0.41
5:A:666:A:H2'	5:A:668:A:H62	1.86	0.41
5:A:2379:G:O2'	5:A:2380:U:OP1	2.32	0.41
28:X:42:GLU:H	28:X:42:GLU:CD	2.28	0.41
31:a:180:U:C2	31:a:181:C:C5	3.08	0.41
31:a:511:U:C2	31:a:512:G:C8	3.08	0.41
31:a:520:A:C2	42:l:88:LYS:HE3	2.55	0.41
31:a:673:A:H2'	31:a:674:U:H6	1.86	0.41
31:a:1005:U:H2'	31:a:1006:U:C6	2.56	0.41
31:a:1311:C:OP2	49:s:4:SER:OG	2.23	0.41
31:a:1519:U:H2'	31:a:1520:G:H8	1.86	0.41
32:b:33:ILE:HD11	32:b:191:THR:HG23	2.02	0.41
38:h:54:GLU:OE1	38:h:55:GLU:HB2	2.20	0.41
52:v:63:U:H2'	52:v:64:C:C6	2.56	0.41
5:A:189:A:H2'	5:A:190:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1344:C:C2	5:A:1345:C:C5	3.08	0.41
5:A:1501:C:H2'	5:A:1502:U:C6	2.55	0.41
5:A:2243:A:H2'	5:A:2244:C:H6	1.86	0.41
5:A:2573:A:H2'	5:A:2610:A:N6	2.35	0.41
5:A:2791:C:H2'	5:A:2792:U:C6	2.56	0.41
22:R:82:LEU:HB2	22:R:98:LYS:HB2	2.03	0.41
31:a:502:G:H2'	31:a:503:G:C8	2.55	0.41
31:a:1427:C:H2'	31:a:1428:A:C8	2.56	0.41
32:b:4:TYR:OH	32:b:60:ASN:ND2	2.53	0.41
34:d:190:ARG:HA	34:d:190:ARG:HD2	1.89	0.41
41:k:87:GLY:O	41:k:92:ARG:NH1	2.51	0.41
5:A:101:U:H2'	5:A:102:A:C8	2.55	0.41
5:A:324:A:OP2	9:E:162:ASN:HB2	2.21	0.41
5:A:1933:A:H1'	5:A:1935:5MU:H72	2.02	0.41
7:C:8:PRO:HB3	7:C:14:ARG:HG3	2.03	0.41
15:K:95:GLU:OE1	15:K:95:GLU:N	2.51	0.41
18:N:44:ASP:OD1	18:N:44:ASP:C	2.63	0.41
31:a:200:G:C8	31:a:461:A:N1	2.89	0.41
31:a:557:U:H5'	31:a:563:G:N2	2.35	0.41
32:b:21:GLN:HA	32:b:40:ILE:HA	2.02	0.41
34:d:90:GLU:N	34:d:90:GLU:OE1	2.54	0.41
47:q:58:ASP:OD1	47:q:58:ASP:N	2.53	0.41
52:v:55:5MU:H2'	52:v:56:PSU:C6	2.55	0.41
5:A:37:G:H2'	5:A:38:C:C6	2.56	0.41
5:A:1193:U:C2	5:A:1194:U:C5	3.09	0.41
5:A:1430:G:H2'	5:A:1431:G:H8	1.86	0.41
5:A:2883:C:H2'	5:A:2884:U:C6	2.55	0.41
7:C:167:ARG:HA	7:C:172:ALA:HA	2.02	0.41
10:F:152:MET:HE3	10:F:152:MET:HB2	1.95	0.41
28:X:42:GLU:OE1	28:X:42:GLU:N	2.53	0.41
31:a:185:C:H4'	31:a:186:G:O5'	2.21	0.41
31:a:1105:G:H2'	31:a:1105:G:N3	2.36	0.41
31:a:1504:A:H2'	31:a:1505:G:C8	2.56	0.41
33:c:130:PHE:O	33:c:134:MET:HG3	2.21	0.41
36:f:38:ARG:CB	36:f:63:ASN:HB2	2.50	0.41
5:A:932:U:H2'	5:A:933:C:H6	1.86	0.40
5:A:1587:U:C2	5:A:1588:A:C8	3.09	0.40
5:A:2302:C:C3'	5:A:2303:G:H5''	2.51	0.40
8:D:152:ASN:OD1	8:D:153:GLN:N	2.46	0.40
22:R:80:MET:HE3	22:R:80:MET:HB2	1.92	0.40
31:a:413:G:H2'	31:a:414:C:C6	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:670:A:H2'	31:a:671:G:H8	1.86	0.40
31:a:704:U:H2'	31:a:705:C:C6	2.56	0.40
31:a:1138:U:H2'	31:a:1139:G:H8	1.85	0.40
31:a:1163:G:O2'	31:a:1167:A:N6	2.54	0.40
5:A:46:G:H2'	5:A:47:U:C6	2.56	0.40
5:A:177:G:H2'	5:A:178:U:C6	2.56	0.40
5:A:1102:U:H2'	5:A:1103:A:C8	2.56	0.40
5:A:1442:C:H2'	5:A:1443:U:C6	2.55	0.40
5:A:1586:U:H2'	5:A:1587:U:C6	2.57	0.40
5:A:1682:A:H2'	5:A:1683:C:C6	2.56	0.40
5:A:1942:U:H2'	5:A:1943:C:H6	1.87	0.40
5:A:2068:C:H2'	5:A:2069:C:H6	1.85	0.40
5:A:2288:G:H2'	5:A:2289:C:C6	2.56	0.40
31:a:153:U:H2'	31:a:154:C:C6	2.55	0.40
31:a:218:U:H2'	31:a:219:A:H8	1.86	0.40
31:a:818:G:H2'	31:a:819:U:H6	1.87	0.40
31:a:1164:A:O2'	31:a:1166:A:OP2	2.23	0.40
31:a:1432:G:H2'	31:a:1433:U:C6	2.57	0.40
33:c:79:LYS:HE3	33:c:82:GLU:OE2	2.20	0.40
41:k:21:HIS:CD2	41:k:84:LEU:HD12	2.56	0.40
49:s:50:SER:HB3	49:s:57:HIS:HB3	2.03	0.40
52:v:23:G:H2'	52:v:24:A:H8	1.85	0.40
52:v:35:C:N4	53:w:3:G:H22	2.19	0.40
5:A:1193:U:H2'	5:A:1194:U:H6	1.84	0.40
5:A:1297:A:H5'	5:A:1606:A:OP2	2.22	0.40
5:A:1864:C:H2'	5:A:1865:G:O4'	2.21	0.40
28:X:4:LYS:HE2	28:X:4:LYS:HB2	1.74	0.40
28:X:41:HIS:ND1	28:X:42:GLU:OE1	2.54	0.40
31:a:1510:A:H2'	31:a:1511:G:H8	1.86	0.40
35:e:44:ARG:NH1	35:e:72:THR:OG1	2.55	0.40
5:A:141:U:H2'	5:A:142:A:H8	1.86	0.40
5:A:543:U:O2'	5:A:544:U:O2	2.30	0.40
5:A:691:A:H2'	5:A:692:U:C6	2.57	0.40
5:A:1681:U:H2'	5:A:1682:A:C8	2.56	0.40
11:G:7:ALA:O	11:G:69:ARG:HD2	2.20	0.40
12:H:44:THR:O	12:H:48:GLU:OE2	2.39	0.40
18:N:78:ALA:HB2	18:N:109:ALA:HA	2.03	0.40
25:U:8:ALA:HB2	25:U:46:LEU:HD23	2.04	0.40
28:X:2:LYS:O	28:X:6:LEU:HG	2.21	0.40
31:a:150:A:H2'	31:a:151:U:H6	1.86	0.40
31:a:754:U:OP1	31:a:819:U:O2'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1353:G:H2'	31:a:1354:A:H8	1.85	0.40
33:c:129:MET:HE2	33:c:129:MET:HA	2.03	0.40
34:d:111:SER:OG	34:d:115:GLU:OE2	2.36	0.40
34:d:172:TRP:NE1	34:d:188:PRO:HG3	2.36	0.40
48:r:65:LEU:HD23	48:r:65:LEU:HA	1.81	0.40
5:A:1047:A:C6	5:A:1048:G:C6	3.09	0.40
5:A:2306:A:H2	10:F:76:GLY:HA3	1.86	0.40
5:A:2601:PSU:H2'	5:A:2602:C:C6	2.56	0.40
31:a:218:U:H2'	31:a:219:A:C8	2.56	0.40
31:a:1037:A:H2'	31:a:1038:G:H8	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/51 (96%)	49 (100%)	0	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
7	C	270/274 (98%)	261 (97%)	8 (3%)	1 (0%)	30	33
8	D	209/212 (99%)	202 (97%)	7 (3%)	0	100	100
9	E	198/200 (99%)	197 (100%)	1 (0%)	0	100	100
10	F	172/178 (97%)	158 (92%)	11 (6%)	3 (2%)	7	5
11	G	172/177 (97%)	166 (96%)	5 (3%)	1 (1%)	21	22
12	H	58/148 (39%)	57 (98%)	1 (2%)	0	100	100
13	I	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
14	J	120/122 (98%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	K	142/146 (97%)	140 (99%)	2 (1%)	0	100	100
16	L	135/137 (98%)	134 (99%)	0	1 (1%)	18	18
17	M	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
18	N	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
19	O	115/122 (94%)	113 (98%)	2 (2%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
22	R	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
23	S	89/106 (84%)	89 (100%)	0	0	100	100
24	T	101/105 (96%)	98 (97%)	3 (3%)	0	100	100
25	U	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
26	V	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	W	75/78 (96%)	75 (100%)	0	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
30	Z	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	212 (95%)	9 (4%)	2 (1%)	14	13
33	c	213/250 (85%)	207 (97%)	6 (3%)	0	100	100
34	d	205/208 (99%)	202 (98%)	2 (1%)	1 (0%)	24	26
35	e	153/165 (93%)	152 (99%)	1 (1%)	0	100	100
36	f	102/127 (80%)	99 (97%)	3 (3%)	0	100	100
37	g	132/156 (85%)	128 (97%)	4 (3%)	0	100	100
38	h	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
39	i	124/128 (97%)	121 (98%)	3 (2%)	0	100	100
40	j	98/103 (95%)	95 (97%)	3 (3%)	0	100	100
41	k	115/128 (90%)	110 (96%)	5 (4%)	0	100	100
42	l	120/124 (97%)	117 (98%)	3 (2%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
45	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	p	80/101 (79%)	79 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	q	77/85 (91%)	76 (99%)	1 (1%)	0	100	100
48	r	50/75 (67%)	50 (100%)	0	0	100	100
49	s	80/91 (88%)	78 (98%)	2 (2%)	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	61/71 (86%)	61 (100%)	0	0	100	100
All	All	5414/5872 (92%)	5289 (98%)	116 (2%)	9 (0%)	44	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	5	LYS
10	F	137	VAL
16	L	79	LEU
32	b	8	MET
11	G	13	ASN
32	b	7	SER
34	d	128	ASN
10	F	72	LYS
7	C	3	ILE

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	47/47 (100%)	46 (98%)	1 (2%)	47	61
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	218/220 (99%)	211 (97%)	7 (3%)	34	45
8	D	166/167 (99%)	160 (96%)	6 (4%)	31	40
9	E	155/155 (100%)	152 (98%)	3 (2%)	50	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	F	144/147 (98%)	134 (93%)	10 (7%)	14	15
11	G	139/142 (98%)	134 (96%)	5 (4%)	31	40
12	H	45/112 (40%)	43 (96%)	2 (4%)	25	32
13	I	118/118 (100%)	117 (99%)	1 (1%)	73	84
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	104 (98%)	2 (2%)	50	64
16	L	113/113 (100%)	112 (99%)	1 (1%)	70	82
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	85/85 (100%)	84 (99%)	1 (1%)	63	76
19	O	99/102 (97%)	96 (97%)	3 (3%)	36	47
20	P	85/86 (99%)	84 (99%)	1 (1%)	63	76
21	Q	84/84 (100%)	83 (99%)	1 (1%)	63	76
22	R	88/88 (100%)	84 (96%)	4 (4%)	24	31
23	S	77/87 (88%)	76 (99%)	1 (1%)	61	75
24	T	83/85 (98%)	79 (95%)	4 (5%)	23	28
25	U	79/80 (99%)	78 (99%)	1 (1%)	61	75
26	V	59/64 (92%)	58 (98%)	1 (2%)	53	68
27	W	69/70 (99%)	68 (99%)	1 (1%)	59	73
28	X	53/56 (95%)	52 (98%)	1 (2%)	50	64
29	Y	53/54 (98%)	53 (100%)	0	100	100
30	Z	46/50 (92%)	46 (100%)	0	100	100
32	b	185/200 (92%)	180 (97%)	5 (3%)	39	52
33	c	175/198 (88%)	173 (99%)	2 (1%)	65	78
34	d	170/171 (99%)	167 (98%)	3 (2%)	51	66
35	e	113/120 (94%)	113 (100%)	0	100	100
36	f	94/111 (85%)	94 (100%)	0	100	100
37	g	113/128 (88%)	110 (97%)	3 (3%)	39	52
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	95 (96%)	4 (4%)	28	36
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	85 (97%)	3 (3%)	32	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	l	104/106 (98%)	97 (93%)	7 (7%)	15	16
43	m	95/98 (97%)	94 (99%)	1 (1%)	65	78
44	n	81/82 (99%)	80 (99%)	1 (1%)	63	76
45	o	71/72 (99%)	70 (99%)	1 (1%)	59	73
46	p	63/77 (82%)	63 (100%)	0	100	100
47	q	71/76 (93%)	69 (97%)	2 (3%)	38	50
48	r	46/66 (70%)	45 (98%)	1 (2%)	45	59
49	s	70/78 (90%)	70 (100%)	0	100	100
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	54/62 (87%)	53 (98%)	1 (2%)	50	64
All	All	4485/4756 (94%)	4394 (98%)	91 (2%)	48	63

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	33	LYS
7	C	19	VAL
7	C	118	SER
7	C	121	ASP
7	C	140	THR
7	C	198	GLN
7	C	228	ILE
7	C	272	ARG
8	D	95	VAL
8	D	98	THR
8	D	141	VAL
8	D	182	SER
8	D	186	GLU
8	D	192	VAL
9	E	1	MET
9	E	2	ASN
9	E	139	ASP
10	F	15	LYS
10	F	35	THR
10	F	51	ASP
10	F	59	LEU
10	F	88	LYS
10	F	91	LEU

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Mol	Chain	Res	Type
10	F	101	ASP
10	F	120	LYS
10	F	137	VAL
10	F	148	ARG
11	G	15	VAL
11	G	16	THR
11	G	17	VAL
11	G	18	THR
11	G	80	SER
12	H	19	VAL
12	H	30	LEU
13	I	2	LYS
15	K	29	VAL
15	K	144	VAL
16	L	110	ASN
18	N	36	ILE
19	O	28	THR
19	O	69	SER
19	O	73	VAL
20	P	15	LYS
21	Q	53	VAL
22	R	13	SER
22	R	66	VAL
22	R	72	SER
22	R	109	VAL
23	S	91	ASP
24	T	3	LYS
24	T	24	VAL
24	T	26	SER
24	T	66	SER
25	U	69	VAL
26	V	32	THR
27	W	2	SER
28	X	56	LEU
32	b	10	ASP
32	b	43	ILE
32	b	143	MET
32	b	154	LYS
32	b	188	ILE
33	c	186	THR
33	c	213	GLN
34	d	17	THR

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Mol	Chain	Res	Type
34	d	30	VAL
34	d	125	ILE
37	g	15	ASP
37	g	87	VAL
37	g	143	ARG
39	i	52	LEU
39	i	64	THR
39	i	102	VAL
39	i	128	ARG
41	k	31	VAL
41	k	83	VAL
41	k	110	THR
42	l	10	LYS
42	l	14	THR
42	l	16	VAL
42	l	49	MET
42	l	59	SER
42	l	78	SER
42	l	82	ILE
43	m	68	ASP
44	n	100	SER
45	o	47	LYS
47	q	6	VAL
47	q	56	ILE
48	r	47	THR
51	u	63	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	41	GLN
4	3	20	ASN
7	C	86	ASN
7	C	120	ASN
7	C	185	HIS
8	D	65	GLN
8	D	129	ASN
8	D	133	GLN
8	D	143	HIS
9	E	141	ASN
9	E	162	ASN
11	G	104	ASN

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Mol	Chain	Res	Type
13	I	47	HIS
13	I	63	GLN
15	K	101	ASN
19	O	59	ASN
21	Q	69	HIS
22	R	62	ASN
26	V	35	ASN
27	W	22	ASN
27	W	35	HIS
30	Z	25	ASN
33	c	3	GLN
33	c	19	ASN
33	c	54	ASN
34	d	61	GLN
34	d	91	ASN
34	d	159	ASN
35	e	85	ASN
35	e	137	ASN
36	f	58	HIS
38	h	4	GLN
44	n	90	GLN
48	r	52	GLN
49	s	57	HIS
50	t	3	ASN
50	t	20	HIS
50	t	80	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	201 (13%)	0
5	A	2726/2918 (93%)	358 (13%)	20 (0%)
52	v	76/77 (98%)	22 (28%)	0
53	w	2/3 (66%)	0	0
6	B	114/115 (99%)	11 (9%)	2 (1%)
All	All	4445/4657 (95%)	592 (13%)	22 (0%)

All (592) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	41	U

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Mol	Chain	Res	Type
5	A	42	G
5	A	50	G
5	A	53	G
5	A	58	G
5	A	65	G
5	A	67	G
5	A	78	A
5	A	81	A
5	A	82	G
5	A	92	G
5	A	104	C
5	A	107	U
5	A	109	G
5	A	110	A
5	A	117	G
5	A	125	A
5	A	126	A
5	A	127	U
5	A	138	A
5	A	147	A
5	A	149	G
5	A	170	A
5	A	203	A
5	A	206	A
5	A	222	G
5	A	223	A
5	A	229	A
5	A	235	U
5	A	236	U
5	A	240	A
5	A	246	U
5	A	252	G
5	A	255	G
5	A	257	G
5	A	262	A
5	A	278	U
5	A	279	U
5	A	285	A
5	A	297	G
5	A	313	A
5	A	331	G
5	A	332	A

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Mol	Chain	Res	Type
5	A	345	C
5	A	347	A
5	A	348	A
5	A	349	A
5	A	360	A
5	A	365	U
5	A	366	G
5	A	369	G
5	A	370	A
5	A	371	G
5	A	385	G
5	A	395	G
5	A	403	A
5	A	410	G
5	A	423	G
5	A	435	C
5	A	455	C
5	A	479	A
5	A	480	G
5	A	504	A
5	A	508	C
5	A	531	A
5	A	532	G
5	A	544	U
5	A	545	C
5	A	546	G
5	A	554	A
5	A	561	A
5	A	571	U
5	A	573	A
5	A	601	A
5	A	611	U
5	A	612	A
5	A	613	U
5	A	625	A
5	A	633	C
5	A	635	A
5	A	643	U
5	A	644	A
5	A	649	G
5	A	651	U
5	A	684	U

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Mol	Chain	Res	Type
5	A	714	A
5	A	728	A
5	A	745	U
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G
5	A	783	G
5	A	787	A
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	826	U
5	A	843	G
5	A	844	A
5	A	845	A
5	A	846	U
5	A	857	G
5	A	864	A
5	A	900	C
5	A	901	C
5	A	903	A
5	A	908	A
5	A	929	C
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C
5	A	971	G
5	A	980	A
5	A	993	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1019	G
5	A	1023	G
5	A	1030	U
5	A	1032	U
5	A	1033	G
5	A	1043	A
5	A	1044	G

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Mol	Chain	Res	Type
5	A	1103	A
5	A	1105	U
5	A	1106	C
5	A	1107	G
5	A	1108	A
5	A	1109	G
5	A	1125	G
5	A	1128	G
5	A	1129	U
5	A	1130	A
5	A	1131	A
5	A	1132	C
5	A	1140	A
5	A	1149	G
5	A	1168	A
5	A	1170	U
5	A	1173	G
5	A	1174	U
5	A	1175	A
5	A	1242	A
5	A	1248	A
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1296	A
5	A	1316	A
5	A	1324	U
5	A	1347	U
5	A	1360	A
5	A	1363	G
5	A	1374	U
5	A	1378	A
5	A	1390	A
5	A	1411	G
5	A	1413	G
5	A	1414	A
5	A	1422	A
5	A	1423	C
5	A	1428	A
5	A	1432	C
5	A	1433	U
5	A	1435	A

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Mol	Chain	Res	Type
5	A	1447	G
5	A	1448	U
5	A	1456	C
5	A	1462	G
5	A	1477	U
5	A	1485	A
5	A	1488	C
5	A	1489	A
5	A	1492	U
5	A	1504	U
5	A	1505	A
5	A	1511	A
5	A	1519	U
5	A	1523	A
5	A	1526	C
5	A	1528	G
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1535	U
5	A	1536	G
5	A	1538	A
5	A	1539	G
5	A	1540	C
5	A	1557	U
5	A	1564	A
5	A	1565	G
5	A	1567	A
5	A	1576	U
5	A	1580	C
5	A	1581	U
5	A	1582	U
5	A	1583	C
5	A	1586	U
5	A	1606	A
5	A	1607	A
5	A	1616	A
5	A	1644	C
5	A	1645	U

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Mol	Chain	Res	Type
5	A	1646	U
5	A	1647	G
5	A	1672	G
5	A	1723	A
5	A	1725	U
5	A	1726	C
5	A	1727	G
5	A	1728	C
5	A	1729	U
5	A	1760	G
5	A	1769	A
5	A	1776	A
5	A	1796	C
5	A	1797	A
5	A	1807	G
5	A	1812	C
5	A	1825	A
5	A	1844	A
5	A	1849	A
5	A	1872	A
5	A	1897	A
5	A	1902	G
5	A	1906	G
5	A	1908	A
5	A	1911	3TD
5	A	1923	A
5	A	1925	G
5	A	1926	G
5	A	1934	A
5	A	1936	U
5	A	1951	U
5	A	1959	U
5	A	1963	C
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1978	U
5	A	1987	U
5	A	1989	U
5	A	2018	U
5	A	2019	C
5	A	2026	6MZ

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Mol	Chain	Res	Type
5	A	2027	A
5	A	2029	A
5	A	2039	C
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2065	7MG
5	A	2089	G
5	A	2092	C
5	A	2093	U
5	A	2096	G
5	A	2194	A
5	A	2200	G
5	A	2207	G
5	A	2216	C
5	A	2221	A
5	A	2234	G
5	A	2235	G
5	A	2264	A
5	A	2275	G
5	A	2279	U
5	A	2283	A
5	A	2284	A
5	A	2299	G
5	A	2301	U
5	A	2303	G
5	A	2304	G
5	A	2305	A
5	A	2307	A
5	A	2314	G
5	A	2316	A
5	A	2317	G
5	A	2321	A
5	A	2323	A
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2378	G
5	A	2379	G
5	A	2380	U

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Mol	Chain	Res	Type
5	A	2381	C
5	A	2399	C
5	A	2402	U
5	A	2420	C
5	A	2421	A
5	A	2425	G
5	A	2426	A
5	A	2430	A
5	A	2431	A
5	A	2437	U
5	A	2444	A
5	A	2466	G
5	A	2469	U
5	A	2471	C
5	A	2472	A
5	A	2487	U
5	A	2498	G
5	A	2499	2MA
5	A	2503	C
5	A	2514	A
5	A	2516	C
5	A	2525	G
5	A	2543	A
5	A	2550	U
5	A	2562	A
5	A	2563	G
5	A	2598	A
5	A	2599	G
5	A	2605	U
5	A	2609	U
5	A	2625	U
5	A	2636	G
5	A	2661	A
5	A	2685	U
5	A	2686	A
5	A	2687	C
5	A	2710	G
5	A	2722	U
5	A	2729	A
5	A	2744	A
5	A	2754	A
5	A	2761	A

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Mol	Chain	Res	Type
5	A	2774	A
5	A	2776	A
5	A	2786	U
5	A	2787	A
5	A	2793	U
5	A	2796	U
5	A	2797	G
5	A	2800	C
5	A	2814	U
5	A	2816	G
5	A	2817	A
5	A	2830	G
5	A	2845	G
5	A	2851	U
5	A	2852	A
5	A	2854	U
5	A	2857	U
5	A	2863	A
5	A	2869	A
5	A	2876	C
5	A	2882	G
6	B	13	A
6	B	14	G
6	B	40	C
6	B	44	A
6	B	50	A
6	B	59	C
6	B	65	G
6	B	66	C
6	B	71	A
6	B	87	A
6	B	106	A
31	a	6	C
31	a	7	U
31	a	9	A
31	a	10	A
31	a	18	A
31	a	24	G
31	a	34	A
31	a	41	G
31	a	49	C
31	a	50	U

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Mol	Chain	Res	Type
31	a	53	A
31	a	62	A
31	a	66	G
31	a	80	A
31	a	81	G
31	a	82	C
31	a	83	U
31	a	84	U
31	a	85	G
31	a	91	G
31	a	97	A
31	a	117	U
31	a	123	G
31	a	126	A
31	a	127	U
31	a	159	G
31	a	160	G
31	a	163	U
31	a	170	A
31	a	184	A
31	a	185	C
31	a	186	G
31	a	193	A
31	a	205	U
31	a	208	G
31	a	216	G
31	a	241	U
31	a	243	G
31	a	247	G
31	a	262	G
31	a	263	C
31	a	276	C
31	a	285	G
31	a	324	C
31	a	325	A
31	a	340	A
31	a	341	C
31	a	343	G
31	a	348	C
31	a	350	G
31	a	363	U
31	a	368	C

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Mol	Chain	Res	Type
31	a	380	C
31	a	393	A
31	a	402	G
31	a	407	A
31	a	408	A
31	a	409	G
31	a	410	A
31	a	417	U
31	a	418	A
31	a	419	U
31	a	420	G
31	a	425	U
31	a	426	A
31	a	434	U
31	a	435	U
31	a	442	G
31	a	448	G
31	a	459	U
31	a	460	U
31	a	461	A
31	a	462	A
31	a	463	U
31	a	481	G
31	a	483	U
31	a	492	A
31	a	493	A
31	a	494	U
31	a	496	A
31	a	497	G
31	a	506	A
31	a	508	C
31	a	515	C
31	a	518	G
31	a	527	G
31	a	528	U
31	a	529	A
31	a	544	A
31	a	556	A
31	a	561	C
31	a	569	A
31	a	570	A
31	a	573	C

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Mol	Chain	Res	Type
31	a	593	A
31	a	615	C
31	a	630	G
31	a	639	A
31	a	650	A
31	a	662	A
31	a	684	A
31	a	685	G
31	a	700	G
31	a	720	U
31	a	721	G
31	a	752	G
31	a	774	A
31	a	790	U
31	a	791	A
31	a	812	A
31	a	814	C
31	a	840	U
31	a	841	G
31	a	842	A
31	a	846	U
31	a	887	G
31	a	888	U
31	a	911	A
31	a	923	G
31	a	924	G
31	a	931	C
31	a	932	A
31	a	957	U
31	a	963	2MG
31	a	966	A
31	a	972	A
31	a	973	G
31	a	974	A
31	a	989	U
31	a	990	G
31	a	1001	A
31	a	1007	U
31	a	1025	C
31	a	1026	U
31	a	1027	U
31	a	1028	C

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Mol	Chain	Res	Type
31	a	1029	G
31	a	1030	G
31	a	1051	C
31	a	1052	A
31	a	1062	U
31	a	1083	U
31	a	1091	G
31	a	1092	U
31	a	1095	C
31	a	1098	A
31	a	1101	G
31	a	1102	A
31	a	1134	C
31	a	1136	G
31	a	1140	G
31	a	1156	U
31	a	1157	G
31	a	1164	A
31	a	1165	C
31	a	1166	A
31	a	1168	A
31	a	1178	G
31	a	1179	G
31	a	1180	C
31	a	1188	A
31	a	1193	A
31	a	1194	A
31	a	1210	A
31	a	1224	A
31	a	1235	A
31	a	1255	G
31	a	1267	U
31	a	1276	A
31	a	1277	A
31	a	1284	A
31	a	1295	U
31	a	1297	G
31	a	1299	C
31	a	1302	G
31	a	1317	C
31	a	1337	A
31	a	1342	U

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Mol	Chain	Res	Type
31	a	1343	A
31	a	1350	G
31	a	1360	A
31	a	1361	U
31	a	1367	G
31	a	1378	U
31	a	1395	A
31	a	1416	G
31	a	1425	A
31	a	1438	A
31	a	1439	G
31	a	1443	A
31	a	1450	A
31	a	1451	A
31	a	1472	G
31	a	1490	A
31	a	1491	G
31	a	1494	G
31	a	1503	U
31	a	1514	G
31	a	1516	MA6
31	a	1526	G
31	a	1527	G
52	v	8	4SU
52	v	9	A
52	v	10	G
52	v	12	U
52	v	13	C
52	v	17	U
52	v	18	G
52	v	19	G
52	v	20	H2U
52	v	21	U
52	v	22	A
52	v	23	G
52	v	28	C
52	v	37	U
52	v	49	C
52	v	50	A
52	v	51	C
52	v	55	5MU
52	v	56	PSU

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Mol	Chain	Res	Type
52	v	58	A
52	v	61	U
52	v	65	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	91	A
5	A	109	G
5	A	256	C
5	A	365	U
5	A	368	C
5	A	424	G
5	A	478	A
5	A	507	U
5	A	782	G
5	A	844	A
5	A	1127	U
5	A	1179	G
5	A	1187	G
5	A	1437	U
5	A	1958	C
5	A	2379	G
5	A	2419	U
5	A	2443	G
5	A	2502	U
5	A	2786	U
6	B	13	A
6	B	86	U

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

28 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
5	PSU	A	1907	5	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
5	3TD	A	1911	5	19,22,23	4.42	6 (31%)	23,32,35	1.83	3 (13%)
31	7MG	a	524	31	23,26,27	1.08	1 (4%)	27,39,42	0.86	2 (7%)
31	2MG	a	1204	31	23,26,27	0.47	0	33,38,41	0.51	0
5	5MU	A	1935	5	19,22,23	0.45	0	27,32,35	0.48	0
5	7MG	A	2065	5	23,26,27	1.04	1 (4%)	27,39,42	0.91	2 (7%)
5	PSU	A	1913	5	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
31	5MC	a	964	31	19,22,23	0.56	0	26,32,35	0.60	0
5	PSU	A	2453	5	18,21,22	1.11	1 (5%)	21,30,33	1.97	6 (28%)
5	PSU	A	952	5	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
31	UR3	a	1495	31	19,22,23	2.88	7 (36%)	26,32,35	1.58	3 (11%)
31	2MG	a	963	31	23,26,27	0.48	0	33,38,41	0.49	0
5	PSU	A	2601	5	18,21,22	1.08	1 (5%)	21,30,33	1.95	5 (23%)
5	PSU	A	2500	5	18,21,22	1.10	1 (5%)	21,30,33	1.90	4 (19%)
31	4OC	a	1399	31	20,23,24	3.14	8 (40%)	25,32,35	0.91	1 (4%)
52	4SU	v	8	52	18,21,22	4.45	8 (44%)	25,30,33	2.23	4 (16%)
52	5MU	v	55	52	19,22,23	0.44	0	27,32,35	0.57	0
5	OMU	A	2548	5	19,22,23	3.01	8 (42%)	25,31,34	1.82	5 (20%)
5	PSU	A	2576	5	18,21,22	1.14	2 (11%)	21,30,33	2.07	6 (28%)
31	PSU	a	513	31	18,21,22	1.11	1 (5%)	21,30,33	1.94	5 (23%)
5	2MG	A	2441	5	23,26,27	0.51	0	33,38,41	0.49	0
31	MA6	a	1516	31	23,26,27	1.42	4 (17%)	33,38,41	3.26	12 (36%)
5	6MZ	A	2026	5	22,25,26	2.51	4 (18%)	29,36,39	3.31	10 (34%)
5	OMG	A	2247	5	23,26,27	0.50	0	32,38,41	0.46	0
52	H2U	v	20	52	18,21,22	0.47	0	19,30,33	1.30	3 (15%)
5	2MA	A	2499	5	22,25,26	3.92	9 (40%)	32,37,40	2.69	11 (34%)
31	MA6	a	1515	31	23,26,27	1.42	4 (17%)	33,38,41	3.22	12 (36%)
52	PSU	v	56	52	18,21,22	1.08	1 (5%)	21,30,33	1.84	4 (19%)

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
5	PSU	A	1907	5	-	1/7/25/26	0/2/2/2
5	3TD	A	1911	5	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	7MG	a	524	31	-	2/7/37/38	0/3/3/3
31	2MG	a	1204	31	-	0/9/27/28	0/3/3/3
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
5	7MG	A	2065	5	-	0/7/37/38	0/3/3/3
5	PSU	A	1913	5	-	0/7/25/26	0/2/2/2
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
31	2MG	a	963	31	-	0/9/27/28	0/3/3/3
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2500	5	-	2/7/25/26	0/2/2/2
31	4OC	a	1399	31	-	0/9/29/30	0/2/2/2
52	4SU	v	8	52	-	4/7/25/26	0/2/2/2
52	5MU	v	55	52	-	7/7/25/26	0/2/2/2
5	OMU	A	2548	5	-	0/9/27/28	0/2/2/2
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
31	PSU	a	513	31	-	0/7/25/26	0/2/2/2
5	2MG	A	2441	5	-	1/9/27/28	0/3/3/3
31	MA6	a	1516	31	-	1/11/29/30	0/3/3/3
5	6MZ	A	2026	5	-	2/9/27/28	0/3/3/3
5	OMG	A	2247	5	-	1/9/27/28	0/3/3/3
52	H2U	v	20	52	-	6/7/38/39	0/2/2/2
5	2MA	A	2499	5	-	2/7/25/26	0/3/3/3
31	MA6	a	1515	31	-	0/11/29/30	0/3/3/3
52	PSU	v	56	52	-	1/7/25/26	0/2/2/2

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C6-C5	13.19	1.49	1.35
5	A	2499	2MA	C4-N3	11.93	1.49	1.34
5	A	1911	3TD	C2-N1	10.79	1.50	1.37
5	A	2026	6MZ	C6-N6	10.02	1.45	1.34
52	v	8	4SU	C2-N1	9.71	1.53	1.38
52	v	8	4SU	C4-N3	8.70	1.46	1.37
52	v	8	4SU	C5-C4	7.49	1.51	1.42
5	A	2499	2MA	C2-N3	7.25	1.46	1.34
52	v	8	4SU	C2-N3	7.06	1.50	1.38
31	a	1495	UR3	C2-N1	7.05	1.48	1.38
5	A	2548	OMU	C2-N1	7.04	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1399	4OC	C4-N3	6.93	1.44	1.32
5	A	2499	2MA	C6-N1	6.83	1.44	1.35
31	a	1495	UR3	C6-C5	6.70	1.50	1.35
5	A	2548	OMU	C2-N3	6.62	1.49	1.38
52	v	8	4SU	C6-C5	6.51	1.50	1.35
31	a	1399	4OC	C6-C5	6.27	1.49	1.35
31	a	1399	4OC	C2-N3	6.19	1.48	1.36
5	A	2499	2MA	C2-N1	5.92	1.44	1.34
5	A	1911	3TD	C6-N1	5.77	1.45	1.36
5	A	2548	OMU	C6-C5	5.61	1.48	1.35
31	a	1495	UR3	C2-N3	5.52	1.49	1.39
5	A	1911	3TD	C2-N3	4.92	1.49	1.38
52	v	8	4SU	C4-S4	-4.88	1.60	1.68
31	a	1399	4OC	C4-N4	4.68	1.45	1.36
5	A	2499	2MA	C5-C6	4.52	1.53	1.41
31	a	524	7MG	C5-N7	4.49	1.41	1.35
5	A	2065	7MG	C5-N7	4.25	1.41	1.35
31	a	1399	4OC	C2-N1	4.21	1.48	1.40
5	A	2548	OMU	C4-N3	4.15	1.45	1.38
31	a	1516	MA6	C6-N6	3.87	1.47	1.36
31	a	1515	MA6	C6-N6	3.86	1.47	1.36
5	A	1907	PSU	C6-C5	3.69	1.39	1.35
5	A	1913	PSU	C6-C5	3.64	1.39	1.35
5	A	2499	2MA	C6-N6	-3.62	1.25	1.34
52	v	56	PSU	C6-C5	3.59	1.39	1.35
5	A	2500	PSU	C6-C5	3.56	1.39	1.35
31	a	513	PSU	C6-C5	3.55	1.39	1.35
31	a	1399	4OC	C5-C4	3.53	1.48	1.41
5	A	2453	PSU	C6-C5	3.53	1.39	1.35
5	A	2576	PSU	C6-C5	3.48	1.39	1.35
5	A	2601	PSU	C6-C5	3.41	1.39	1.35
5	A	952	PSU	C6-C5	3.41	1.39	1.35
31	a	1495	UR3	C6-N1	3.29	1.45	1.38
5	A	2026	6MZ	C5-N7	-3.22	1.33	1.39
31	a	1399	4OC	C6-N1	3.22	1.45	1.38
31	a	1515	MA6	C5-C4	-3.03	1.33	1.39
5	A	2548	OMU	O4-C4	-3.00	1.18	1.24
31	a	1516	MA6	C5-C4	-2.99	1.33	1.39
5	A	1911	3TD	C4-N3	2.98	1.46	1.40
5	A	2026	6MZ	C5-C4	-2.96	1.33	1.39
5	A	2548	OMU	C6-N1	2.78	1.44	1.38
31	a	1399	4OC	O2-C2	-2.75	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	8	4SU	C6-N1	2.69	1.44	1.38
5	A	2548	OMU	O2-C2	-2.63	1.18	1.23
5	A	2499	2MA	C5-N7	-2.61	1.34	1.39
5	A	2026	6MZ	C8-N9	-2.58	1.33	1.37
52	v	8	4SU	O2-C2	-2.58	1.18	1.23
31	a	1516	MA6	C5-N7	-2.55	1.34	1.39
31	a	1495	UR3	C4-N3	2.51	1.45	1.40
5	A	2499	2MA	C4-N9	-2.50	1.32	1.37
31	a	1515	MA6	C5-N7	-2.45	1.34	1.39
5	A	2548	OMU	C5-C4	2.32	1.48	1.43
31	a	1515	MA6	C8-N9	-2.29	1.33	1.37
31	a	1516	MA6	C8-N9	-2.26	1.33	1.37
31	a	1495	UR3	C5-C4	2.25	1.49	1.43
5	A	1911	3TD	O2-C2	-2.23	1.19	1.23
5	A	2499	2MA	C8-N7	2.09	1.35	1.31
5	A	2576	PSU	O4'-C1'	-2.06	1.41	1.43
31	a	1495	UR3	O2-C2	-2.02	1.18	1.22

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1516	MA6	N1-C6-N6	-11.88	102.38	116.86
31	a	1515	MA6	N1-C6-N6	-11.58	102.75	116.86
5	A	2026	6MZ	C4-N9-C1'	-8.96	105.67	126.63
5	A	2026	6MZ	C1'-N9-C8	8.79	146.60	127.09
31	a	1516	MA6	C5-C6-N6	7.96	137.93	125.33
31	a	1515	MA6	C5-C6-N6	7.68	137.48	125.33
52	v	8	4SU	C4-N3-C2	-7.62	120.01	127.31
5	A	2499	2MA	C1'-N9-C8	-7.10	111.33	127.09
5	A	2499	2MA	N9-C8-N7	-6.04	105.36	113.94
5	A	2026	6MZ	C5-C4-N3	-5.92	118.57	126.72
5	A	2548	OMU	C4-N3-C2	-5.72	119.51	126.61
5	A	1911	3TD	N1-C2-N3	5.70	120.27	116.13
31	a	1515	MA6	N1-C2-N3	-5.68	119.98	128.58
31	a	1516	MA6	N1-C2-N3	-5.63	120.07	128.58
31	a	1495	UR3	C4-N3-C2	-5.49	120.16	124.58
52	v	8	4SU	C5-C4-N3	5.40	119.77	114.75
5	A	2499	2MA	C4-N9-C8	5.33	111.33	105.74
5	A	2499	2MA	C5-C4-N3	-5.30	121.60	127.18
5	A	2026	6MZ	N1-C2-N3	-5.25	120.63	128.58
5	A	2576	PSU	N1-C2-N3	5.16	120.61	115.17
5	A	2026	6MZ	C4-C5-C6	5.10	121.02	116.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	952	PSU	N1-C2-N3	5.03	120.47	115.17
5	A	2453	PSU	N1-C2-N3	5.00	120.44	115.17
5	A	2601	PSU	N1-C2-N3	4.92	120.36	115.17
5	A	952	PSU	C4-N3-C2	-4.90	119.62	126.37
5	A	2453	PSU	C4-N3-C2	-4.89	119.63	126.37
5	A	2601	PSU	C4-N3-C2	-4.88	119.65	126.37
5	A	1907	PSU	C4-N3-C2	-4.86	119.67	126.37
5	A	2500	PSU	N1-C2-N3	4.83	120.26	115.17
5	A	2576	PSU	C4-N3-C2	-4.82	119.74	126.37
31	a	513	PSU	N1-C2-N3	4.78	120.21	115.17
52	v	56	PSU	C4-N3-C2	-4.78	119.79	126.37
31	a	1516	MA6	C5-C4-N3	-4.77	120.15	126.72
52	v	56	PSU	N1-C2-N3	4.76	120.19	115.17
5	A	1907	PSU	N1-C2-N3	4.76	120.19	115.17
5	A	2500	PSU	C4-N3-C2	-4.75	119.83	126.37
31	a	513	PSU	C4-N3-C2	-4.74	119.85	126.37
31	a	1515	MA6	C5-C4-N3	-4.73	120.20	126.72
5	A	1913	PSU	N1-C2-N3	4.67	120.10	115.17
5	A	1913	PSU	C4-N3-C2	-4.67	119.94	126.37
5	A	2499	2MA	C4-N9-C1'	4.58	137.33	126.63
31	a	1515	MA6	N9-C8-N7	-4.41	107.68	113.94
5	A	1911	3TD	C4-N3-C2	-4.33	120.03	124.61
31	a	1516	MA6	N9-C8-N7	-4.31	107.83	113.94
5	A	2026	6MZ	N3-C4-N9	4.09	134.12	127.17
5	A	2499	2MA	N3-C4-N9	4.05	132.13	126.99
31	a	1516	MA6	C4-C5-C6	3.97	120.01	115.91
31	a	1515	MA6	C4-C5-C6	3.91	119.95	115.91
5	A	2548	OMU	N3-C2-N1	3.86	119.92	114.89
5	A	2026	6MZ	N9-C8-N7	-3.78	108.57	113.94
5	A	2548	OMU	C5-C4-N3	3.76	120.06	114.80
52	v	8	4SU	N3-C2-N1	3.74	119.77	114.89
31	a	1495	UR3	C5-C4-N3	3.71	119.92	115.04
52	v	20	H2U	C5-C4-N3	-3.53	112.94	116.69
5	A	2026	6MZ	C2-N3-C4	3.51	120.39	111.83
31	a	1516	MA6	C2-N1-C6	3.44	120.24	111.83
31	a	1515	MA6	C2-N1-C6	3.43	120.21	111.83
5	A	2499	2MA	C5-N7-C8	3.41	108.81	103.45
5	A	2499	2MA	N3-C2-N1	-3.35	119.87	125.77
52	v	8	4SU	C5-C4-S4	-3.31	120.52	124.31
31	a	1515	MA6	C2-N3-C4	3.30	119.90	111.83
31	a	1516	MA6	C2-N3-C4	3.28	119.84	111.83
31	a	1515	MA6	N3-C4-N9	2.99	132.25	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2500	PSU	O2-C2-N1	-2.94	119.75	122.79
31	a	1516	MA6	C5-N7-C8	2.92	108.04	103.45
31	a	513	PSU	O2-C2-N1	-2.92	119.78	122.79
31	a	1515	MA6	C5-N7-C8	2.89	107.99	103.45
31	a	1516	MA6	N3-C4-N9	2.89	132.07	127.17
5	A	2576	PSU	O2-C2-N1	-2.88	119.82	122.79
5	A	2026	6MZ	C5-N7-C8	2.87	107.96	103.45
5	A	2548	OMU	O4-C4-C5	-2.87	120.22	125.16
52	v	20	H2U	O2-C2-N1	2.83	126.50	123.10
5	A	2576	PSU	C6-N1-C2	-2.82	120.08	122.69
5	A	1913	PSU	O2-C2-N1	-2.79	119.91	122.79
5	A	952	PSU	O2-C2-N1	-2.77	119.93	122.79
31	a	1515	MA6	C4-N9-C8	2.70	108.58	105.74
5	A	1907	PSU	O2-C2-N1	-2.68	120.03	122.79
5	A	2576	PSU	O4'-C1'-C2'	2.65	108.82	105.15
5	A	2453	PSU	O2-C2-N1	-2.63	120.08	122.79
31	a	513	PSU	C6-N1-C2	-2.61	120.27	122.69
5	A	2500	PSU	C6-N1-C2	-2.61	120.27	122.69
52	v	56	PSU	O2-C2-N1	-2.61	120.10	122.79
5	A	1911	3TD	C6-C5-C4	2.55	119.90	118.19
5	A	1913	PSU	C6-N1-C2	-2.50	120.37	122.69
5	A	952	PSU	C6-N1-C2	-2.48	120.39	122.69
31	a	524	7MG	C4-C5-N7	2.46	108.28	105.38
5	A	2453	PSU	C6-N1-C2	-2.45	120.41	122.69
52	v	56	PSU	C6-N1-C2	-2.44	120.43	122.69
31	a	1516	MA6	C4-N9-C8	2.41	108.27	105.74
5	A	2601	PSU	O2-C2-N1	-2.36	120.36	122.79
5	A	2065	7MG	C5-C4-N9	2.35	109.34	106.33
5	A	2576	PSU	C6-C5-C4	2.34	119.75	118.17
5	A	2601	PSU	C6-N1-C2	-2.33	120.53	122.69
31	a	513	PSU	O4'-C1'-C2'	2.32	108.37	105.15
5	A	2065	7MG	C4-C5-N7	2.31	108.10	105.38
31	a	1399	4OC	C6-C5-C4	2.30	119.78	117.00
5	A	1907	PSU	C6-N1-C2	-2.28	120.57	122.69
5	A	2601	PSU	C6-C5-C4	2.25	119.69	118.17
5	A	2499	2MA	N6-C6-N1	2.23	120.03	117.03
5	A	2499	2MA	CM2-C2-N1	2.22	120.45	117.13
31	a	1516	MA6	C4-C5-N7	-2.18	108.09	110.58
31	a	524	7MG	C5-C4-N9	2.16	109.11	106.33
5	A	2453	PSU	C6-C5-C4	2.15	119.63	118.17
5	A	2548	OMU	O2-C2-N1	-2.15	120.00	122.80
5	A	1907	PSU	C6-C5-C4	2.14	119.62	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2453	PSU	O4'-C1'-C2'	2.13	108.09	105.15
5	A	2026	6MZ	C5-C6-N1	2.12	120.42	118.15
31	a	1495	UR3	C6-N1-C2	-2.10	120.08	121.80
31	a	1515	MA6	C4-C5-N7	-2.08	108.20	110.58
5	A	2499	2MA	C4-C5-N7	-2.06	108.22	110.58
52	v	20	H2U	O2-C2-N3	-2.05	117.72	121.49

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	v	8	4SU	O4'-C1'-N1-C2
52	v	20	H2U	O4'-C1'-N1-C6
52	v	55	5MU	C2'-C1'-N1-C6
52	v	55	5MU	O4'-C4'-C5'-O5'
5	A	1911	3TD	O4'-C4'-C5'-O5'
5	A	2247	OMG	C1'-C2'-O2'-CM2
52	v	55	5MU	C2'-C1'-N1-C2
52	v	55	5MU	C3'-C4'-C5'-O5'
5	A	2499	2MA	O4'-C4'-C5'-O5'
31	a	524	7MG	C3'-C4'-C5'-O5'
52	v	20	H2U	C3'-C4'-C5'-O5'
5	A	1911	3TD	C3'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
5	A	2026	6MZ	O4'-C4'-C5'-O5'
5	A	2026	6MZ	C3'-C4'-C5'-O5'
52	v	8	4SU	O4'-C1'-N1-C6
52	v	20	H2U	C2'-C1'-N1-C2
5	A	2500	PSU	O4'-C4'-C5'-O5'
31	a	524	7MG	O4'-C4'-C5'-O5'
52	v	20	H2U	C2'-C1'-N1-C6
5	A	2441	2MG	C3'-C4'-C5'-O5'
52	v	8	4SU	O4'-C4'-C5'-O5'
52	v	20	H2U	O4'-C4'-C5'-O5'
52	v	20	H2U	O4'-C1'-N1-C2
52	v	8	4SU	C4'-C5'-O5'-P
52	v	55	5MU	C4'-C5'-O5'-P
52	v	55	5MU	O4'-C1'-N1-C6
52	v	55	5MU	O4'-C1'-N1-C2
52	v	56	PSU	C4'-C5'-O5'-P
5	A	1907	PSU	O4'-C4'-C5'-O5'
31	a	1516	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
5	A	2500	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1911	3TD	1	0
5	A	1935	5MU	1	0
31	a	963	2MG	1	0
5	A	2601	PSU	1	0
52	v	8	4SU	1	0
52	v	55	5MU	1	0
5	A	2026	6MZ	2	0
5	A	2247	OMG	1	0
52	v	20	H2U	1	0
52	v	56	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z > 2$
55	OIY	A	3003	-	41,42,55	1.69	9 (21%)	43,58,74	1.70	6 (13%)
55	OIY	A	3006	-	36,37,55	1.33	6 (16%)	37,52,74	1.90	6 (16%)
55	OIY	A	3005	-	54,55,55	1.80	11 (20%)	55,74,74	1.54	6 (10%)
55	OIY	A	3002	-	54,55,55	1.78	11 (20%)	55,74,74	1.58	7 (12%)
55	OIY	a	1603	-	54,55,55	1.78	11 (20%)	55,74,74	1.54	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	OIY	a	1602	-	54,55,55	1.79	10 (18%)	55,74,74	1.51	7 (12%)
55	OIY	A	3004	-	48,49,55	1.84	11 (22%)	50,67,74	1.92	10 (20%)
55	OIY	A	3001	-	32,33,55	1.43	6 (18%)	34,47,74	1.77	5 (14%)
55	OIY	a	1601	-	36,37,55	1.33	6 (16%)	37,52,74	1.77	6 (16%)
55	OIY	N	201	-	36,37,55	1.37	6 (16%)	37,52,74	1.71	5 (13%)
55	OIY	a	1604	-	36,37,55	1.36	6 (16%)	37,52,74	1.66	4 (10%)

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
55	OIY	A	3003	-	-	7/28/73/89	0/3/3/3
55	OIY	A	3006	-	-	8/22/67/89	0/3/3/3
55	OIY	A	3005	-	-	17/44/89/89	0/3/3/3
55	OIY	A	3002	-	-	8/44/89/89	0/3/3/3
55	OIY	a	1603	-	-	14/44/89/89	0/3/3/3
55	OIY	a	1602	-	-	11/44/89/89	0/3/3/3
55	OIY	A	3004	-	-	16/36/81/89	0/3/3/3
55	OIY	A	3001	-	-	9/17/62/89	0/3/3/3
55	OIY	a	1601	-	-	3/22/67/89	0/3/3/3
55	OIY	N	201	-	-	3/22/67/89	0/3/3/3
55	OIY	a	1604	-	-	3/22/67/89	0/3/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3004	OIY	C34-N33	6.79	1.49	1.33
55	a	1602	OIY	C34-N33	6.75	1.49	1.33
55	A	3003	OIY	C34-N33	6.71	1.49	1.33
55	A	3005	OIY	C34-N33	6.70	1.49	1.33
55	A	3002	OIY	C34-N33	6.69	1.49	1.33
55	a	1603	OIY	C34-N33	6.67	1.49	1.33
55	A	3005	OIY	C42-N41	6.16	1.48	1.33
55	A	3002	OIY	C42-N41	6.12	1.47	1.33
55	a	1603	OIY	C42-N41	6.11	1.47	1.33
55	a	1602	OIY	C42-N41	6.07	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3004	OIY	C42-N41	5.11	1.47	1.34
55	a	1602	OIY	C05-N07	3.89	1.40	1.33
55	A	3001	OIY	C05-N07	3.88	1.40	1.33
55	N	201	OIY	C05-N07	3.87	1.40	1.33
55	a	1603	OIY	C05-N07	3.87	1.40	1.33
55	a	1604	OIY	C05-N07	3.86	1.40	1.33
55	A	3005	OIY	C05-N07	3.86	1.40	1.33
55	A	3002	OIY	C05-N07	3.77	1.40	1.33
55	A	3004	OIY	C05-N07	3.75	1.40	1.33
55	A	3006	OIY	C05-N07	3.72	1.40	1.33
55	a	1601	OIY	C05-N07	3.70	1.40	1.33
55	A	3003	OIY	C05-N07	3.64	1.39	1.33
55	A	3006	OIY	C01-C02	3.25	1.55	1.52
55	a	1601	OIY	C01-C02	3.22	1.55	1.52
55	A	3001	OIY	C01-C02	3.21	1.55	1.52
55	a	1604	OIY	C01-C02	3.19	1.55	1.52
55	N	201	OIY	C01-C02	3.16	1.55	1.52
55	A	3003	OIY	C01-C02	3.16	1.55	1.52
55	a	1603	OIY	C01-C02	3.14	1.55	1.52
55	A	3004	OIY	C01-C02	3.13	1.55	1.52
55	A	3002	OIY	C01-C02	3.09	1.55	1.52
55	a	1602	OIY	C01-C02	3.08	1.55	1.52
55	A	3005	OIY	C01-C02	3.07	1.55	1.52
55	a	1604	OIY	C02-C03	-2.99	1.50	1.53
55	A	3005	OIY	C02-C03	-2.89	1.50	1.53
55	A	3001	OIY	C02-C03	-2.89	1.50	1.53
55	A	3004	OIY	C02-C03	-2.87	1.50	1.53
55	a	1602	OIY	C02-C03	-2.87	1.50	1.53
55	N	201	OIY	C02-C03	-2.84	1.50	1.53
55	a	1603	OIY	C02-C03	-2.84	1.50	1.53
55	A	3003	OIY	C02-C03	-2.75	1.50	1.53
55	A	3002	OIY	C02-C03	-2.73	1.50	1.53
55	a	1601	OIY	C02-C03	-2.73	1.50	1.53
55	A	3001	OIY	C01-N07	2.71	1.49	1.46
55	a	1603	OIY	C01-N07	2.70	1.49	1.46
55	a	1604	OIY	C01-N07	2.70	1.49	1.46
55	A	3006	OIY	C02-C03	-2.69	1.50	1.53
55	A	3002	OIY	C01-N07	2.69	1.49	1.46
55	A	3004	OIY	C01-N07	2.64	1.49	1.46
55	A	3005	OIY	C01-N07	2.64	1.49	1.46
55	N	201	OIY	C01-N07	2.59	1.49	1.46
55	A	3006	OIY	C01-N07	2.56	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1602	OIY	C01-N07	2.56	1.49	1.46
55	a	1601	OIY	C01-N07	2.52	1.48	1.46
55	A	3001	OIY	C26-N25	2.44	1.39	1.34
55	A	3006	OIY	C26-N25	2.42	1.39	1.34
55	A	3002	OIY	C26-N25	2.41	1.39	1.34
55	A	3004	OIY	C44-C42	2.40	1.55	1.50
55	N	201	OIY	C26-N25	2.39	1.39	1.34
55	A	3005	OIY	C26-N25	2.38	1.39	1.34
55	A	3004	OIY	C26-N25	2.38	1.39	1.34
55	a	1602	OIY	C26-N25	2.36	1.39	1.34
55	a	1603	OIY	C26-N25	2.36	1.39	1.34
55	a	1601	OIY	C26-N25	2.35	1.39	1.34
55	a	1604	OIY	C26-N25	2.35	1.39	1.34
55	A	3003	OIY	C26-N25	2.33	1.39	1.34
55	A	3003	OIY	C01-N07	2.33	1.48	1.46
55	A	3003	OIY	C36-C34	2.32	1.56	1.51
55	a	1602	OIY	C21-N23	2.31	1.37	1.33
55	a	1601	OIY	C21-N23	2.30	1.37	1.33
55	A	3005	OIY	C21-N23	2.30	1.37	1.33
55	N	201	OIY	C21-N23	2.29	1.37	1.33
55	A	3002	OIY	C21-N23	2.28	1.37	1.33
55	a	1603	OIY	C21-N23	2.28	1.37	1.33
55	a	1604	OIY	C21-N23	2.27	1.37	1.33
55	A	3003	OIY	C21-N23	2.27	1.37	1.33
55	A	3006	OIY	C21-N23	2.25	1.37	1.33
55	A	3004	OIY	C21-N23	2.24	1.37	1.33
55	A	3001	OIY	C21-N23	2.24	1.37	1.33
55	a	1603	OIY	O43-C42	-2.15	1.19	1.23
55	A	3004	OIY	C36-C34	2.15	1.56	1.51
55	A	3002	OIY	O43-C42	-2.15	1.19	1.23
55	A	3005	OIY	O43-C42	-2.14	1.19	1.23
55	A	3002	OIY	O35-C34	-2.13	1.19	1.23
55	a	1602	OIY	O43-C42	-2.12	1.19	1.23
55	A	3003	OIY	O35-C34	-2.11	1.19	1.23
55	a	1602	OIY	O35-C34	-2.10	1.19	1.23
55	A	3005	OIY	O35-C34	-2.09	1.19	1.23
55	A	3004	OIY	O35-C34	-2.07	1.19	1.23
55	A	3002	OIY	C36-C34	2.07	1.56	1.51
55	a	1603	OIY	O35-C34	-2.06	1.19	1.23
55	a	1603	OIY	C36-C34	2.04	1.56	1.51
55	A	3005	OIY	C36-C34	2.03	1.56	1.51

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A	3003	OIY	C02-C01-N07	7.85	117.82	109.83
55	A	3004	OIY	C02-C01-N07	7.71	117.68	109.83
55	a	1601	OIY	C02-C01-N07	7.62	117.59	109.83
55	A	3006	OIY	C02-C01-N07	7.42	117.39	109.83
55	A	3002	OIY	C02-C01-N07	7.33	117.30	109.83
55	A	3005	OIY	C02-C01-N07	7.24	117.21	109.83
55	A	3001	OIY	C02-C01-N07	7.20	117.17	109.83
55	N	201	OIY	C02-C01-N07	7.20	117.16	109.83
55	a	1602	OIY	C02-C01-N07	7.18	117.15	109.83
55	a	1604	OIY	C02-C01-N07	7.15	117.11	109.83
55	a	1603	OIY	C02-C01-N07	7.11	117.07	109.83
55	A	3004	OIY	O17-C12-C13	5.12	112.47	108.97
55	A	3006	OIY	C12-C13-N25	4.35	116.43	111.12
55	A	3004	OIY	C36-C34-N33	4.02	122.18	115.97
55	A	3004	OIY	C16-O17-C12	3.89	117.88	112.47
55	A	3006	OIY	O06-C05-N07	3.53	127.19	122.41
55	a	1601	OIY	C28-C26-N25	-3.51	111.47	116.25
55	A	3002	OIY	C28-C26-N25	-3.50	111.48	116.25
55	A	3002	OIY	O06-C05-N07	3.49	127.14	122.41
55	a	1601	OIY	O17-C12-C13	3.48	111.34	108.97
55	A	3006	OIY	C28-C26-N25	-3.47	111.52	116.25
55	N	201	OIY	C28-C26-N25	-3.40	111.61	116.25
55	a	1604	OIY	O06-C05-N07	3.37	126.98	122.41
55	a	1602	OIY	C28-C26-N25	-3.36	111.66	116.25
55	N	201	OIY	O17-C12-C13	3.35	111.25	108.97
55	a	1603	OIY	C28-C26-N25	-3.31	111.73	116.25
55	A	3005	OIY	C28-C26-N25	-3.28	111.78	116.25
55	A	3001	OIY	O06-C05-N07	3.26	126.83	122.41
55	A	3004	OIY	C28-C26-N25	-3.24	111.83	116.25
55	A	3003	OIY	C28-C26-N25	-3.22	111.86	116.25
55	A	3005	OIY	O06-C05-N07	3.22	126.77	122.41
55	N	201	OIY	O06-C05-N07	3.19	126.74	122.41
55	a	1603	OIY	O06-C05-N07	3.16	126.69	122.41
55	a	1604	OIY	C28-C26-N25	-3.14	111.97	116.25
55	a	1601	OIY	O06-C05-N07	3.13	126.65	122.41
55	a	1603	OIY	C36-C34-N33	3.12	120.79	115.97
55	A	3004	OIY	O06-C05-N07	3.10	126.61	122.41
55	a	1602	OIY	C03-N10-C09	-3.06	107.06	112.17
55	A	3002	OIY	C36-C34-N33	3.06	120.69	115.97
55	a	1602	OIY	O06-C05-N07	2.84	126.26	122.41
55	a	1604	OIY	C03-N10-C09	-2.84	107.42	112.17
55	A	3001	OIY	C12-C13-N25	2.83	114.58	111.12
55	A	3006	OIY	C03-N10-C09	-2.83	107.44	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	1603	OIY	C03-N10-C09	-2.83	107.44	112.17
55	A	3005	OIY	C03-N10-C09	-2.82	107.45	112.17
55	N	201	OIY	C03-N10-C09	-2.80	107.48	112.17
55	A	3002	OIY	C03-N10-C09	-2.79	107.51	112.17
55	A	3001	OIY	C03-N10-C09	-2.78	107.52	112.17
55	A	3003	OIY	O06-C05-N07	2.70	126.07	122.41
55	a	1603	OIY	C44-C42-N41	2.61	120.00	115.97
55	A	3005	OIY	C44-C42-N41	2.57	119.95	115.97
55	A	3004	OIY	C03-N10-C09	-2.57	107.87	112.17
55	a	1601	OIY	C03-N10-C09	-2.57	107.88	112.17
55	A	3005	OIY	C36-C34-N33	2.55	119.91	115.97
55	A	3002	OIY	C44-C42-N41	2.52	119.86	115.97
55	A	3001	OIY	C28-C26-N25	-2.49	111.48	115.86
55	a	1602	OIY	C40-N41-C42	-2.38	118.39	122.82
55	A	3006	OIY	C13-N25-C26	2.30	126.29	122.90
55	A	3004	OIY	C44-C42-N41	2.27	119.99	116.12
55	a	1602	OIY	O17-C12-N11	2.22	112.19	108.12
55	a	1602	OIY	C36-C34-N33	2.21	119.39	115.97
55	A	3003	OIY	C03-N10-C09	-2.20	108.49	112.17
55	A	3003	OIY	O17-C12-N11	2.18	112.12	108.12
55	A	3002	OIY	O17-C12-C13	2.12	110.42	108.97
55	A	3003	OIY	C36-C34-N33	2.08	120.13	116.34
55	A	3004	OIY	O35-C34-N33	-2.05	119.01	123.03
55	A	3004	OIY	N11-C09-N10	-2.03	115.43	122.00
55	a	1601	OIY	N11-C09-N10	-2.02	115.48	122.00

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	3001	OIY	N23-C21-O20-C15
55	A	3001	OIY	O22-C21-O20-C15
55	A	3002	OIY	C26-C28-C29-N52
55	A	3004	OIY	C26-C28-C29-C30
55	A	3004	OIY	C26-C28-C29-N52
55	A	3004	OIY	C28-C29-C30-C31
55	A	3004	OIY	N52-C29-C30-C31
55	A	3004	OIY	C36-C37-C38-C39
55	A	3004	OIY	N51-C37-C38-C39
55	A	3005	OIY	N23-C21-O20-C15
55	A	3005	OIY	O22-C21-O20-C15
55	A	3005	OIY	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
55	A	3005	OIY	N52-C29-C30-C31
55	A	3005	OIY	C34-C36-C37-N51
55	A	3006	OIY	C14-C15-O20-C21
55	A	3006	OIY	C16-C15-O20-C21
55	A	3006	OIY	C26-C28-C29-C30
55	A	3006	OIY	C26-C28-C29-N52
55	a	1602	OIY	C26-C28-C29-N52
55	a	1602	OIY	C34-C36-C37-C38
55	a	1602	OIY	C34-C36-C37-N51
55	a	1603	OIY	C34-C36-C37-N51
55	a	1603	OIY	C36-C37-C38-C39
55	a	1603	OIY	C44-C45-C46-C47
55	a	1603	OIY	O17-C16-C18-O19
55	A	3004	OIY	C36-C34-N33-C32
55	a	1602	OIY	C44-C42-N41-C40
55	a	1603	OIY	C36-C34-N33-C32
55	A	3002	OIY	O17-C16-C18-O19
55	A	3001	OIY	C15-C16-C18-O19
55	A	3003	OIY	O17-C16-C18-O19
55	A	3003	OIY	C15-C16-C18-O19
55	a	1604	OIY	O17-C16-C18-O19
55	A	3003	OIY	C30-C31-C32-N33
55	A	3002	OIY	C15-C16-C18-O19
55	a	1603	OIY	C15-C16-C18-O19
55	A	3004	OIY	O35-C34-N33-C32
55	a	1602	OIY	O43-C42-N41-C40
55	a	1603	OIY	O35-C34-N33-C32
55	A	3001	OIY	O17-C16-C18-O19
55	A	3004	OIY	C38-C39-C40-N41
55	a	1603	OIY	C38-C39-C40-N41
55	A	3002	OIY	C30-C31-C32-N33
55	a	1602	OIY	C38-C39-C40-N41
55	a	1604	OIY	C15-C16-C18-O19
55	A	3005	OIY	C15-C16-C18-O19
55	A	3004	OIY	O17-C16-C18-O19
55	A	3005	OIY	O17-C16-C18-O19
55	A	3004	OIY	C29-C30-C31-C32
55	A	3002	OIY	C26-C28-C29-C30
55	A	3004	OIY	C31-C32-N33-C34
55	a	1602	OIY	O17-C16-C18-O19
55	a	1603	OIY	C30-C31-C32-N33
55	A	3002	OIY	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
55	A	3001	OIY	C12-C13-N25-C26
55	A	3005	OIY	C12-C13-N25-C26
55	A	3006	OIY	C12-C13-N25-C26
55	A	3005	OIY	C37-C38-C39-C40
55	a	1601	OIY	C26-C28-C29-C30
55	A	3003	OIY	C34-C36-C37-N51
55	A	3005	OIY	C29-C30-C31-C32
55	A	3005	OIY	C38-C39-C40-N41
55	A	3001	OIY	C14-C15-O20-C21
55	A	3003	OIY	C14-C15-O20-C21
55	a	1602	OIY	C14-C15-O20-C21
55	a	1602	OIY	C44-C45-C46-C47
55	a	1602	OIY	N50-C45-C46-C47
55	a	1603	OIY	N50-C45-C46-C47
55	A	3005	OIY	C42-C44-C45-C46
55	a	1603	OIY	C37-C38-C39-C40
55	A	3004	OIY	C30-C31-C32-N33
55	A	3001	OIY	C14-C13-N25-C26
55	A	3005	OIY	C14-C13-N25-C26
55	a	1602	OIY	C29-C30-C31-C32
55	A	3004	OIY	N33-C34-C36-C37
55	A	3004	OIY	O35-C34-C36-C37
55	A	3006	OIY	C14-C13-N25-C26
55	A	3006	OIY	O22-C21-O20-C15
55	A	3003	OIY	C26-C28-C29-N52
55	N	201	OIY	C26-C28-C29-N52
55	A	3005	OIY	N33-C34-C36-C37
55	a	1601	OIY	C14-C15-O20-C21
55	a	1603	OIY	C29-C30-C31-C32
55	A	3002	OIY	C38-C39-C40-N41
55	A	3001	OIY	O17-C12-N11-C09
55	A	3005	OIY	O17-C12-N11-C09
55	A	3005	OIY	O35-C34-C36-C37
55	A	3001	OIY	N08-C09-N11-C12
55	A	3002	OIY	N08-C09-N11-C12
55	A	3003	OIY	N08-C09-N11-C12
55	A	3004	OIY	N08-C09-N11-C12
55	A	3005	OIY	N08-C09-N11-C12
55	A	3006	OIY	N08-C09-N11-C12
55	N	201	OIY	N52-C29-C30-C31
55	N	201	OIY	N08-C09-N11-C12
55	a	1601	OIY	N08-C09-N11-C12

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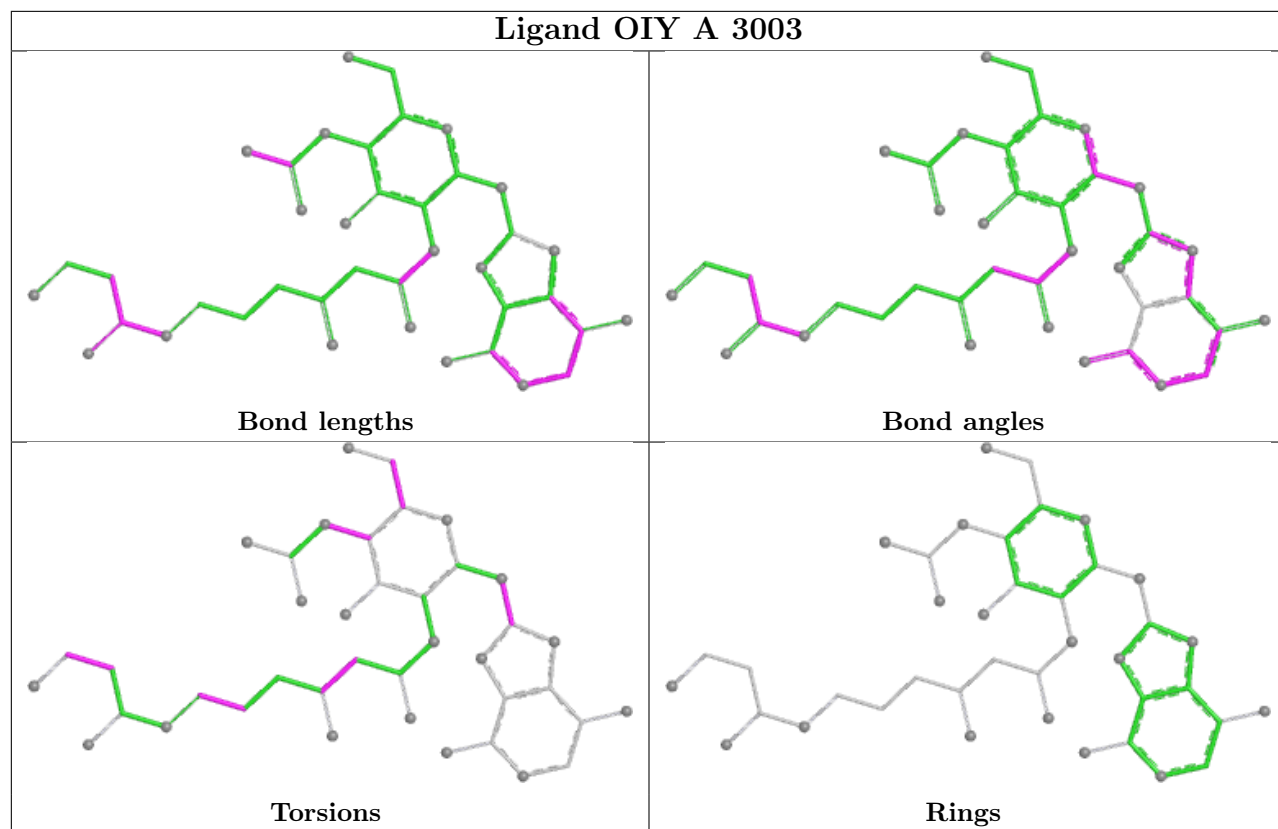
Mol	Chain	Res	Type	Atoms
55	a	1603	OIY	N51-C37-C38-C39
55	a	1604	OIY	N08-C09-N11-C12
55	a	1603	OIY	C34-C36-C37-C38

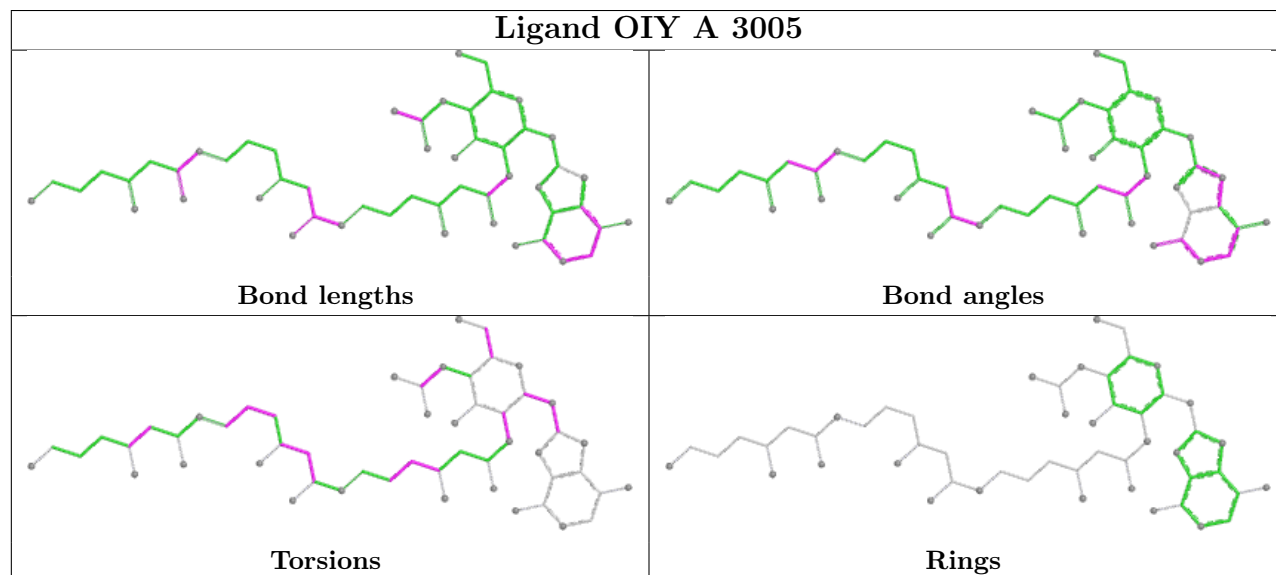
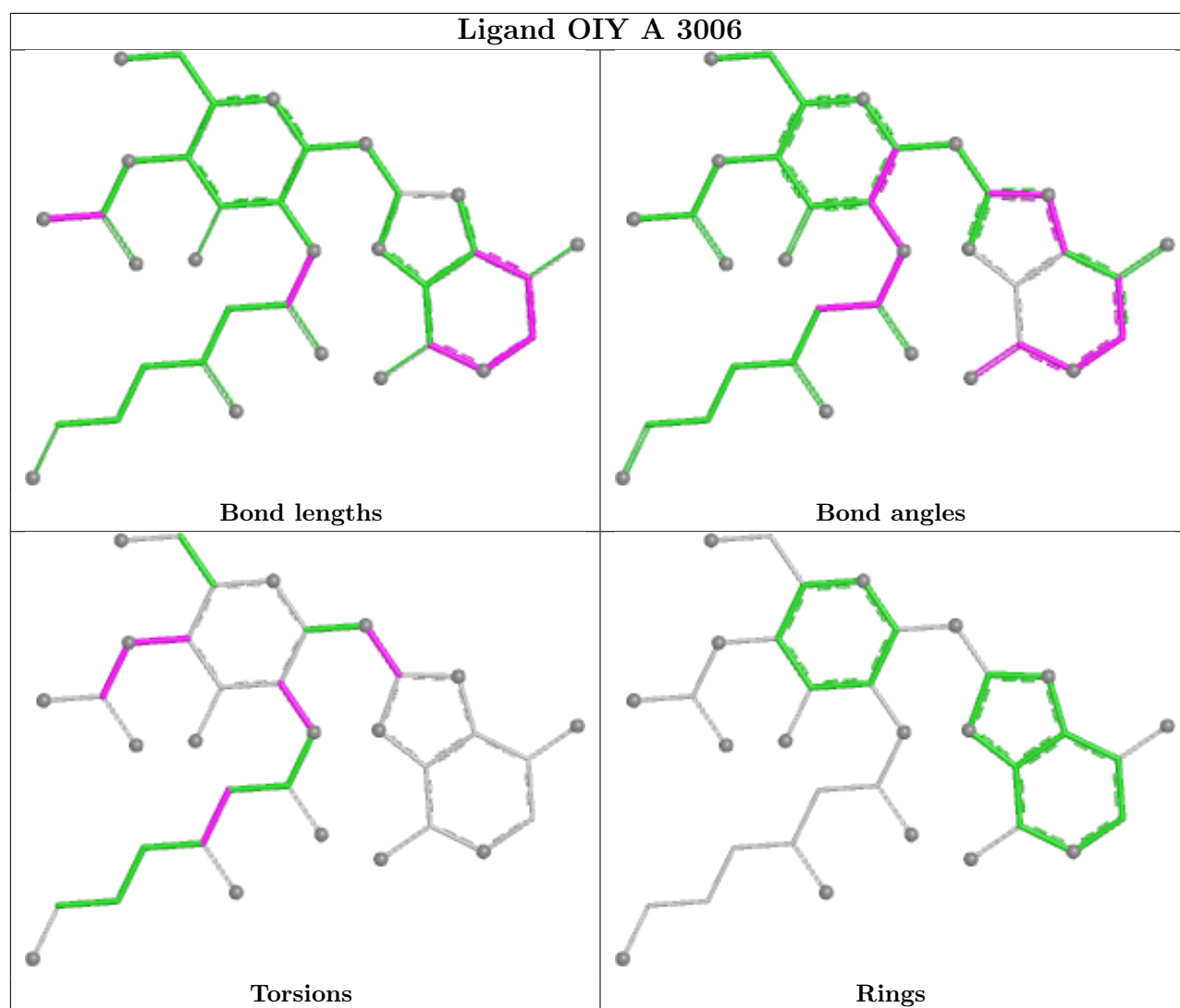
There are no ring outliers.

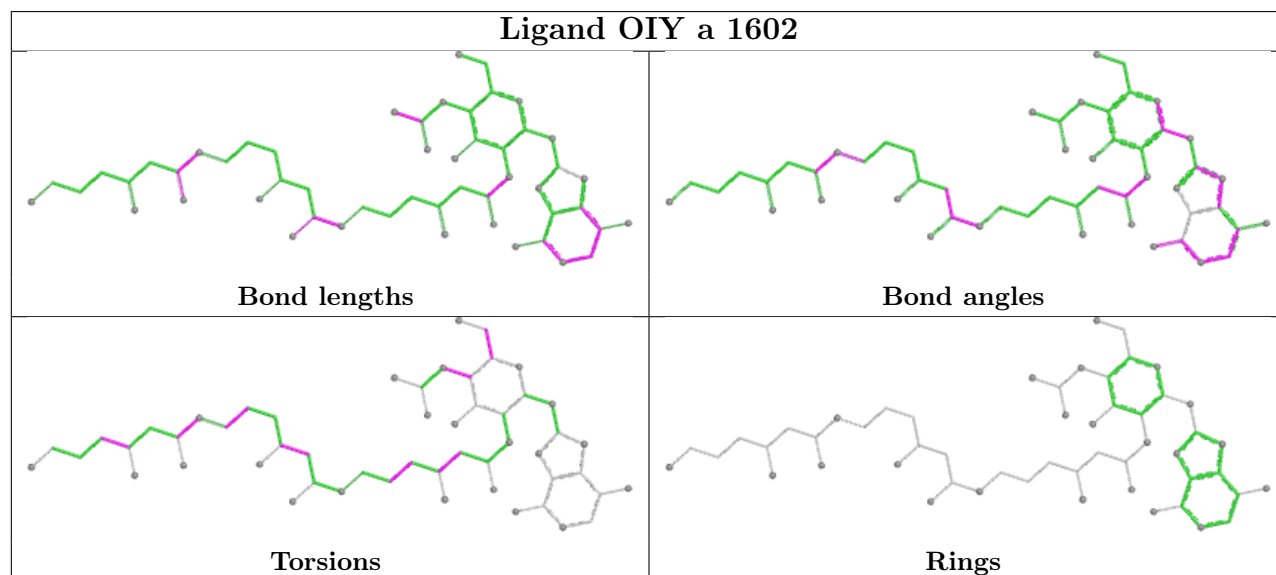
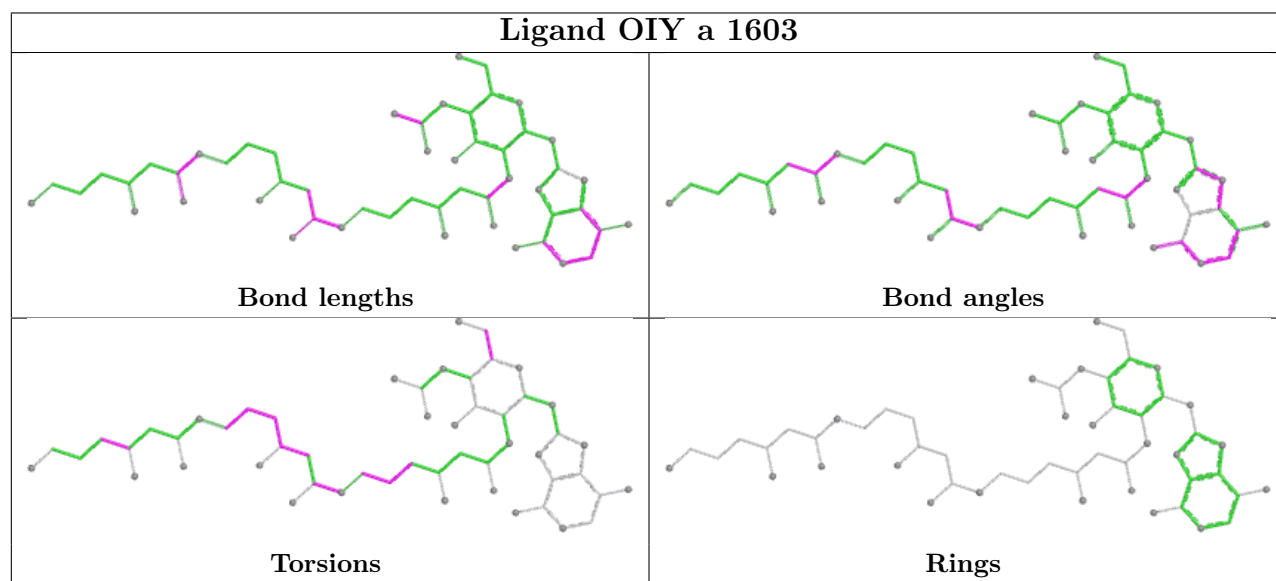
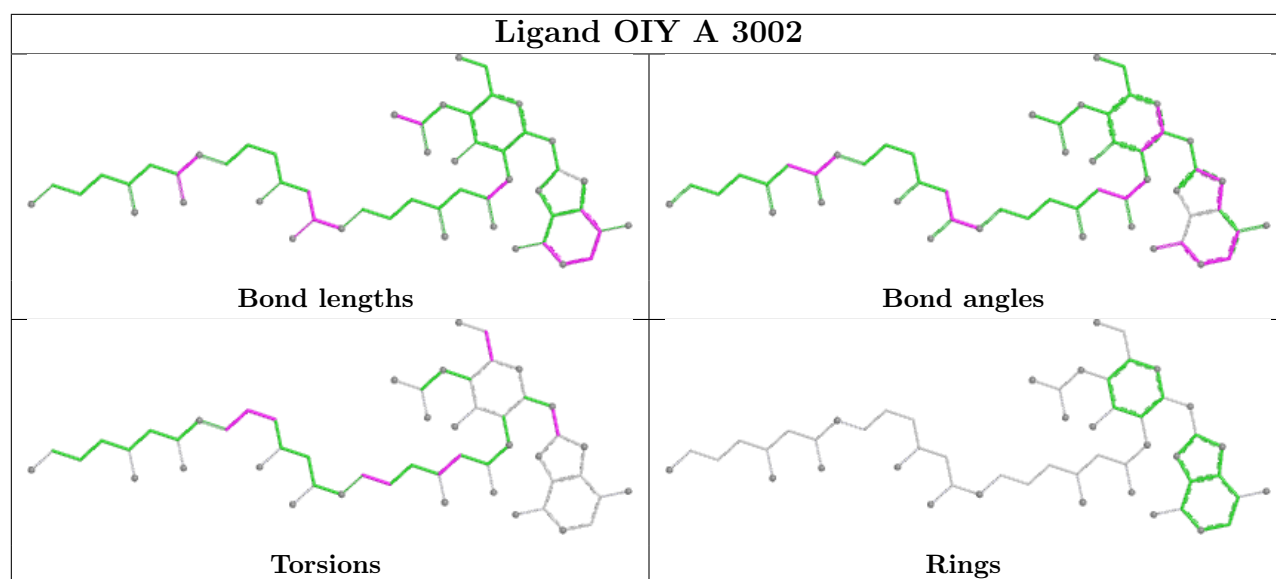
7 monomers are involved in 7 short contacts:

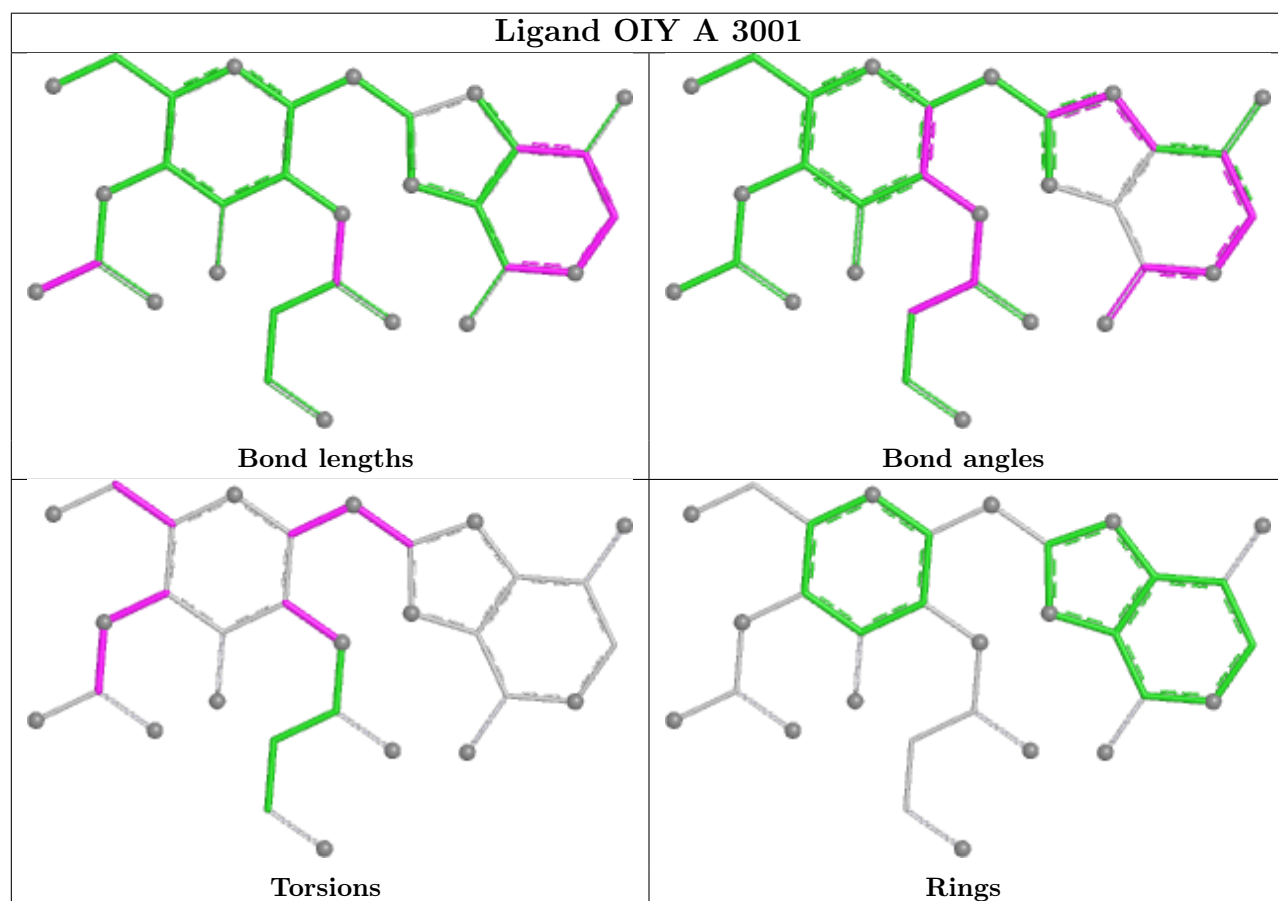
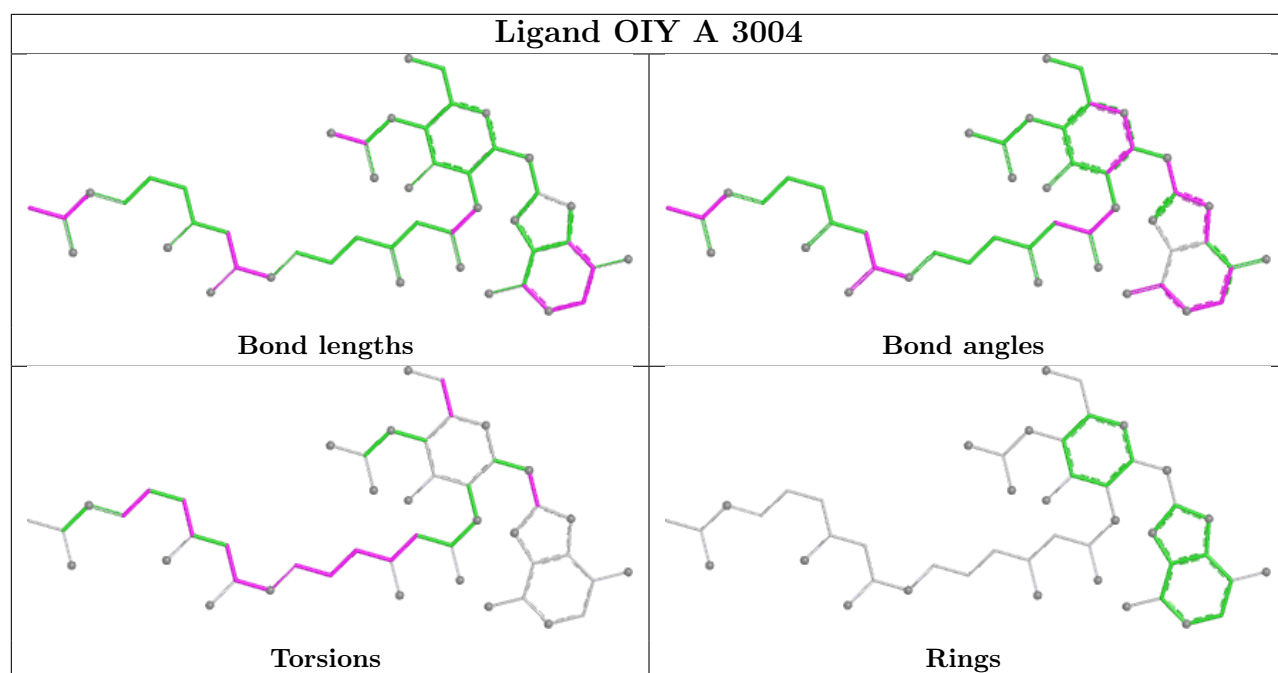
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	A	3006	OIY	1	0
55	A	3005	OIY	1	0
55	a	1602	OIY	1	0
55	A	3001	OIY	1	0
55	a	1601	OIY	1	0
55	N	201	OIY	1	0
55	a	1604	OIY	1	0

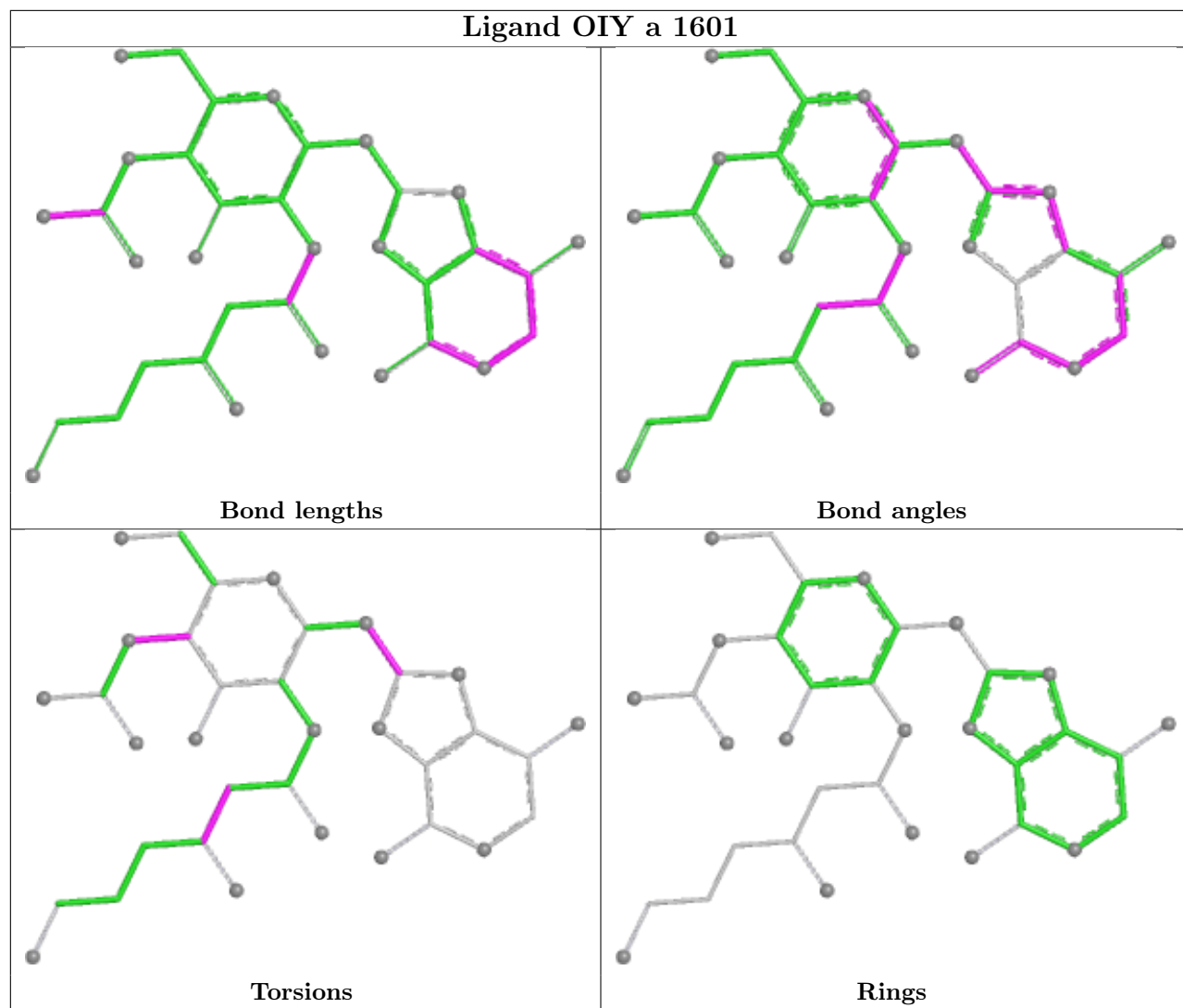
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

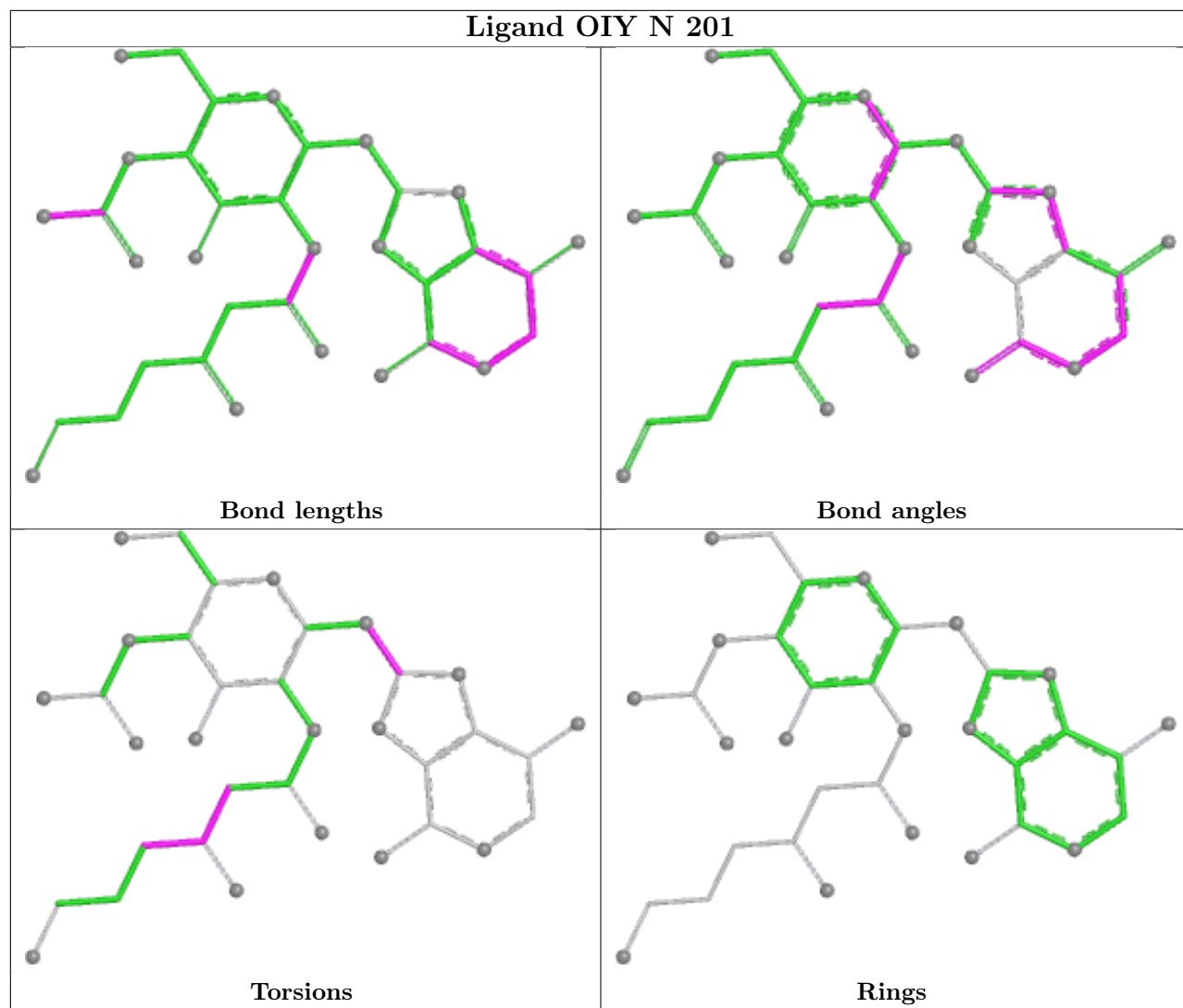


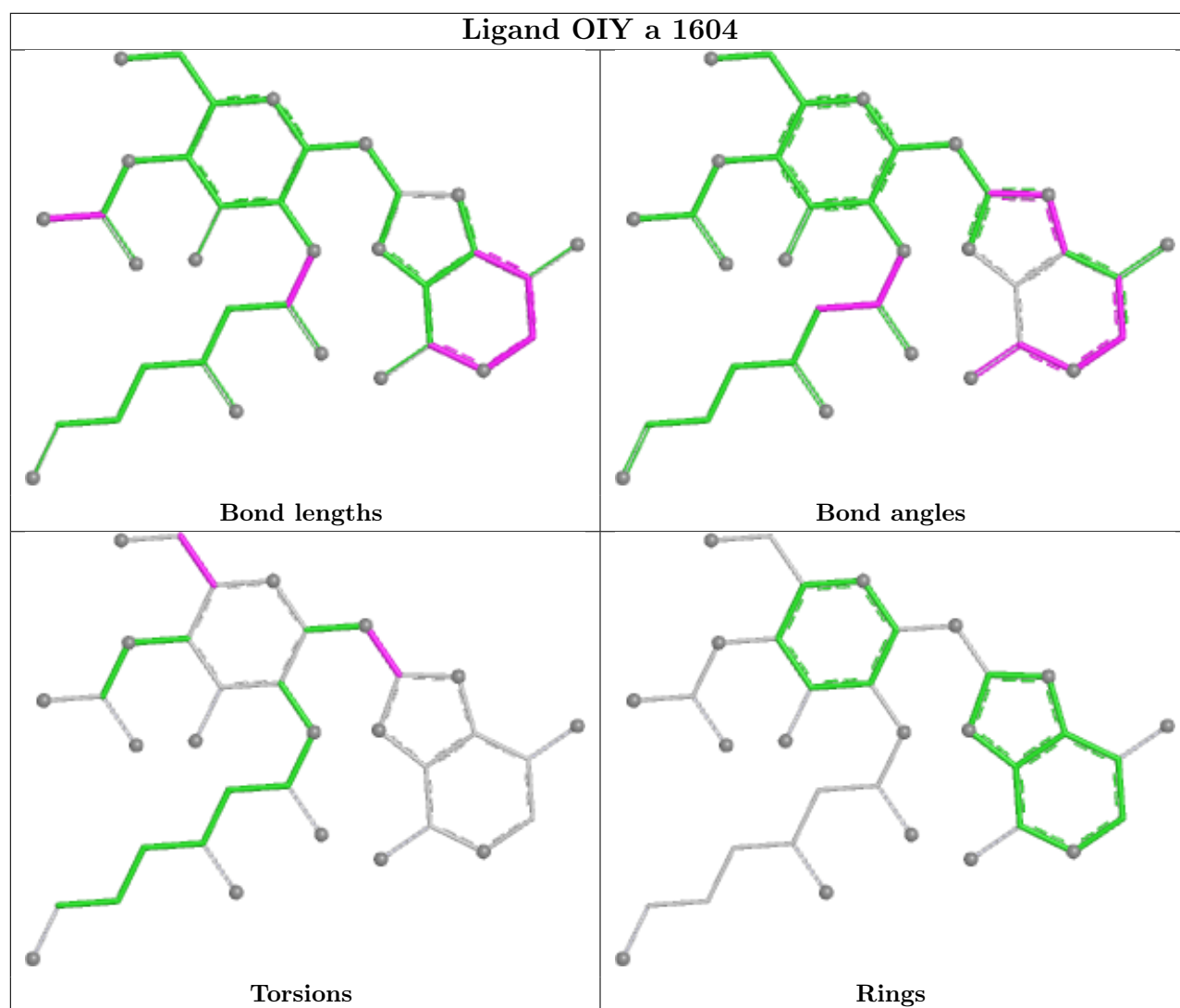












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

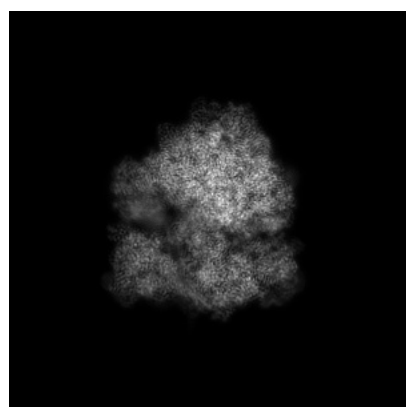
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26821. These allow visual inspection of the internal detail of the map and identification of artifacts.

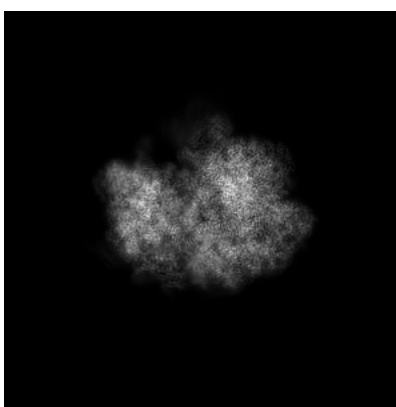
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

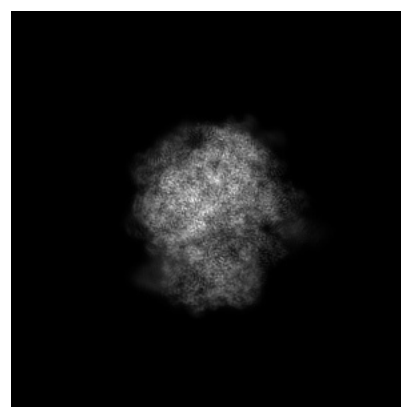
6.1.1 Primary map



X



Y



Z

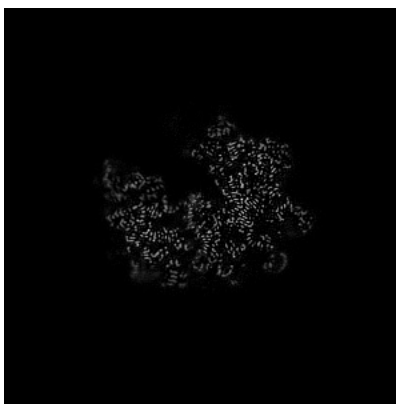
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 320



Y Index: 320

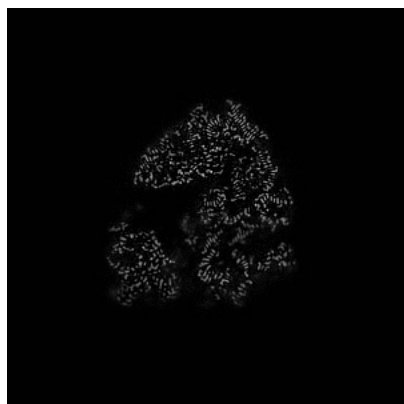


Z Index: 320

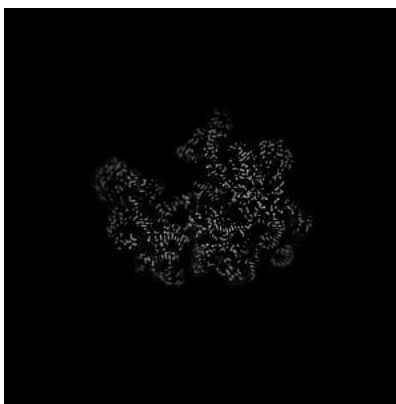
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

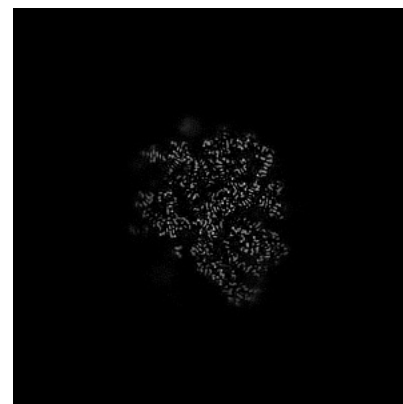
6.3.1 Primary map



X Index: 320



Y Index: 335

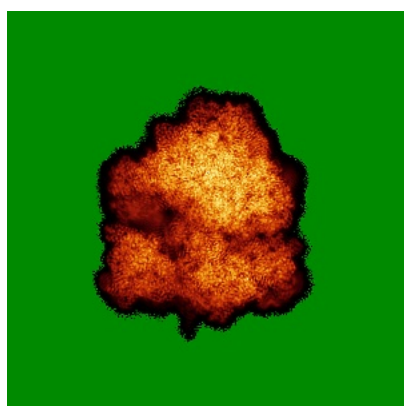


Z Index: 375

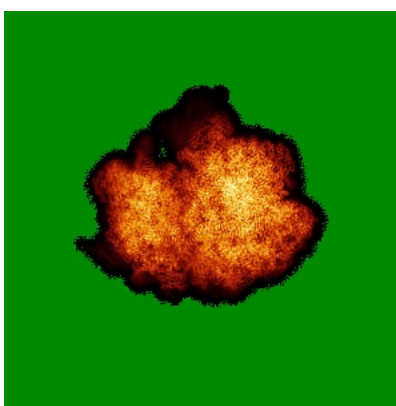
The images above show the largest variance slices of the map in three orthogonal directions.

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

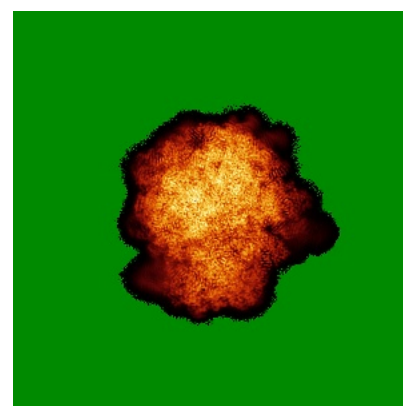
6.4.1 Primary map



X



Y

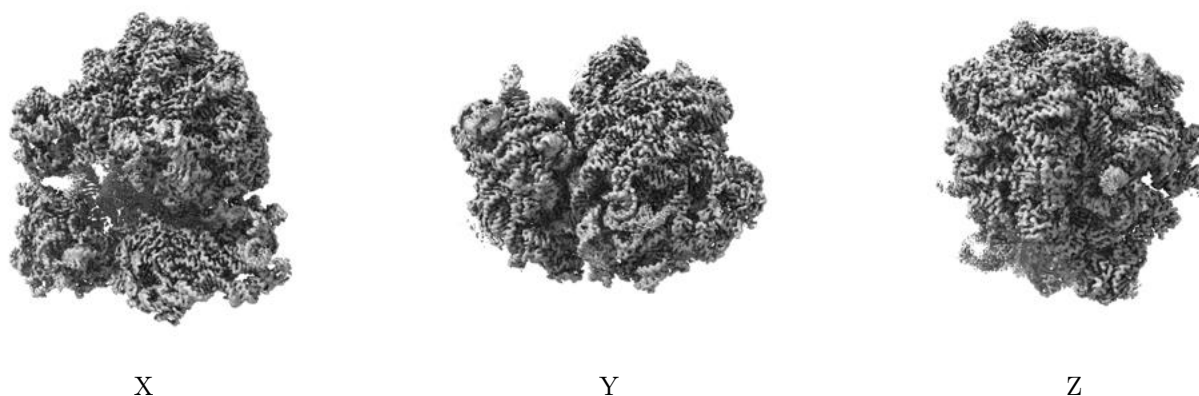


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

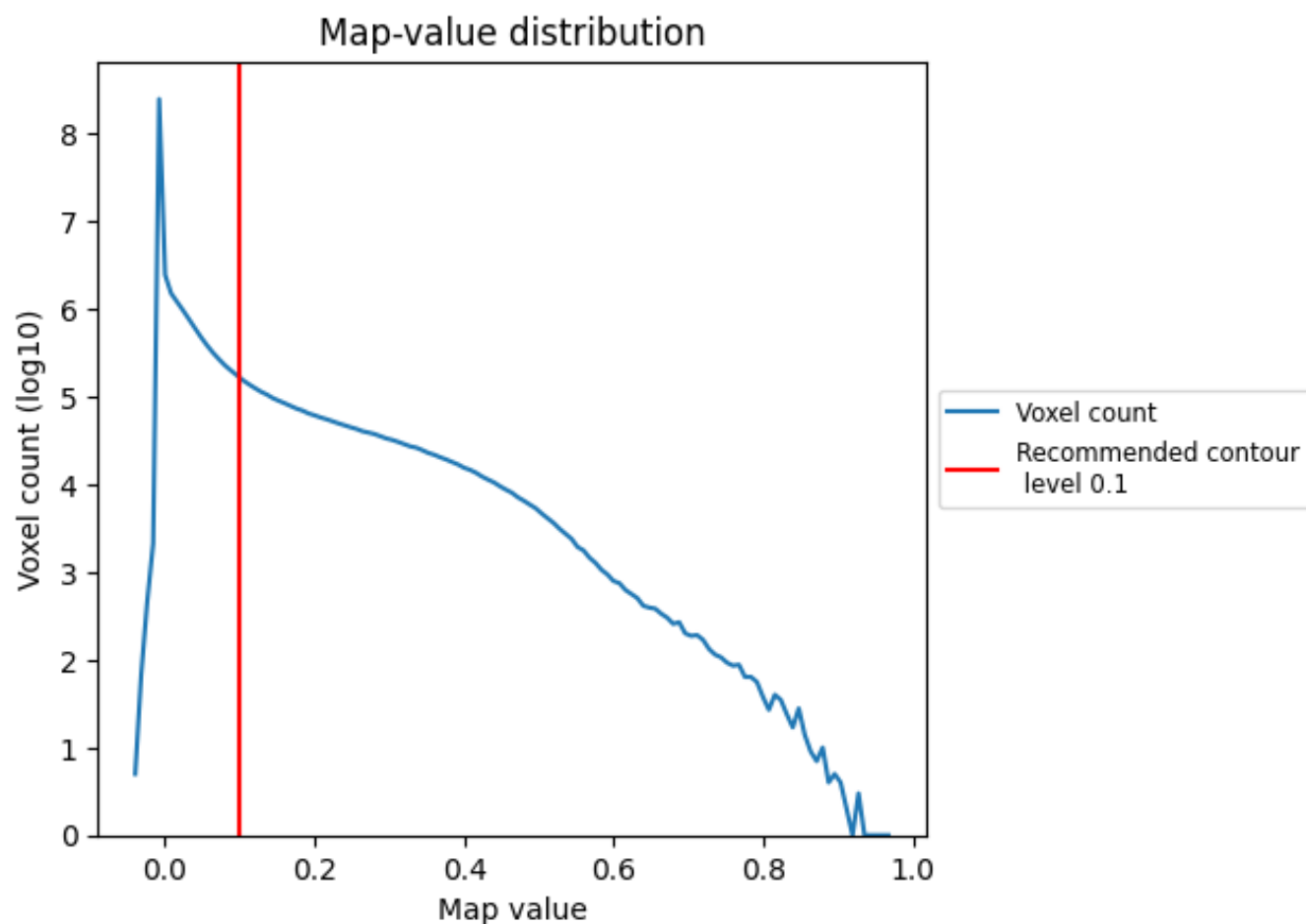
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

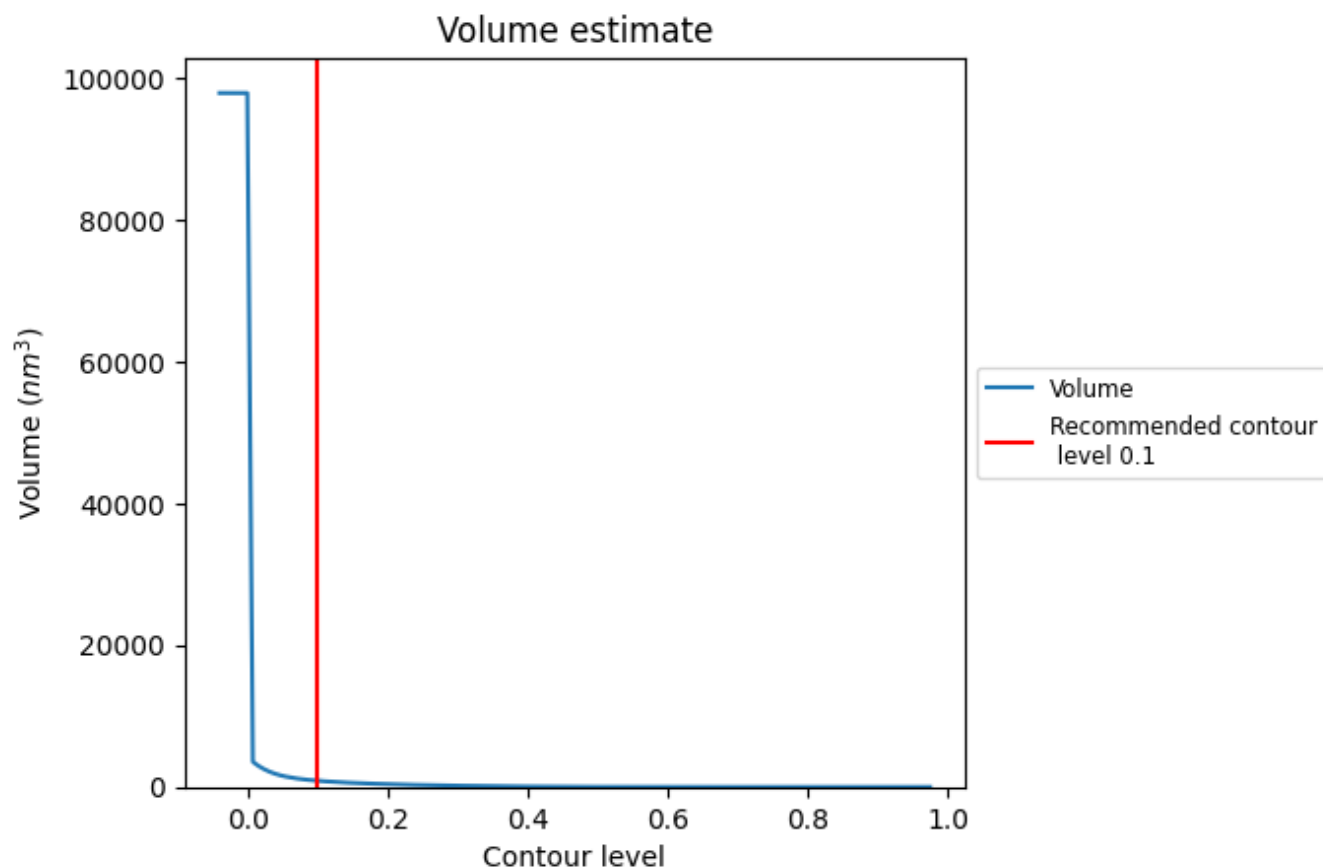
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

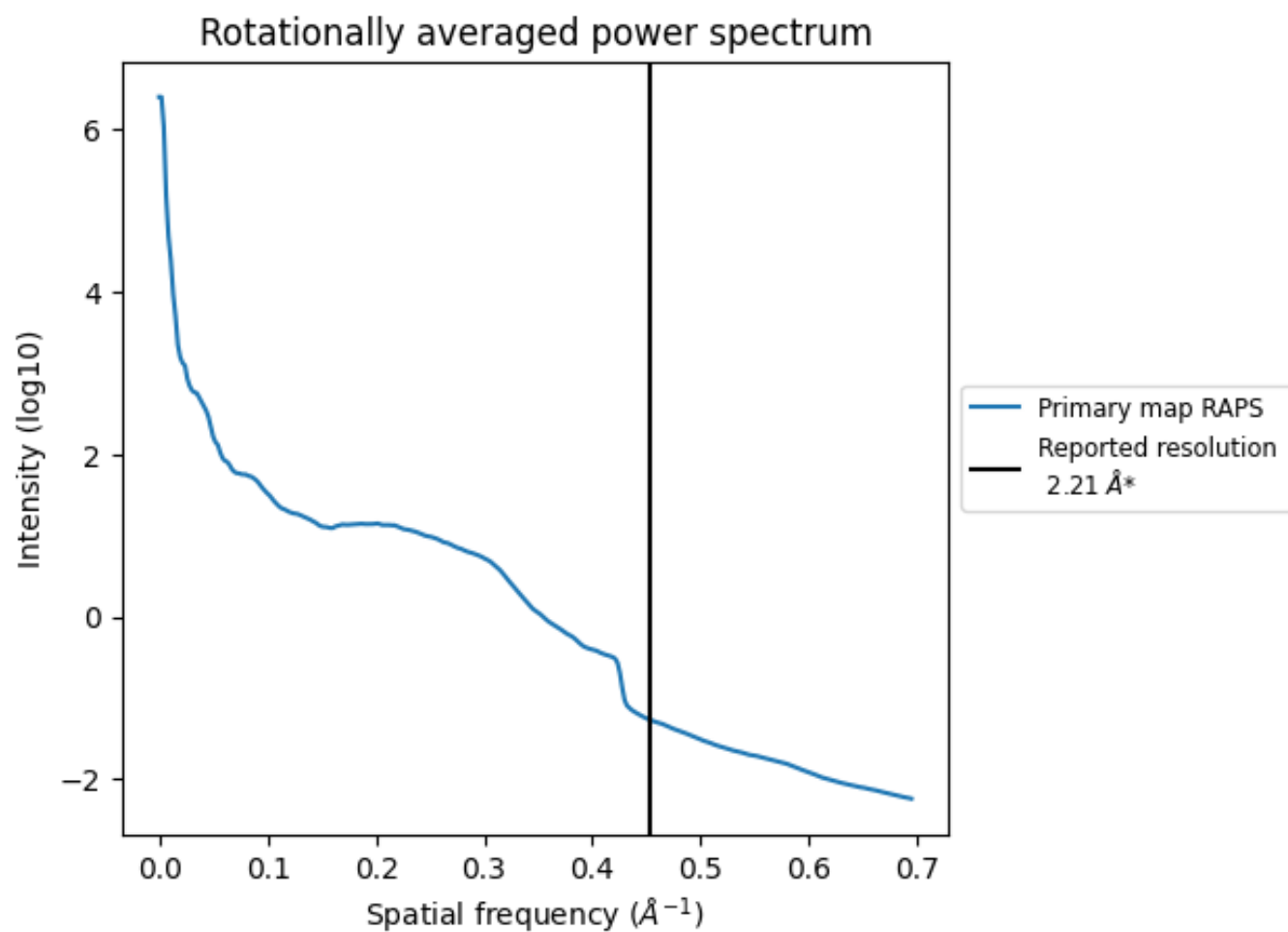
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 876 nm^3 ; this corresponds to an approximate mass of 792 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 0.452 Å⁻¹

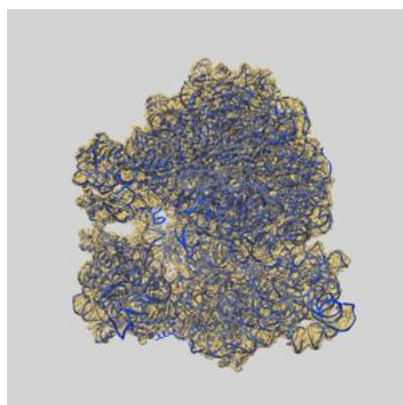
8 Fourier-Shell correlation

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

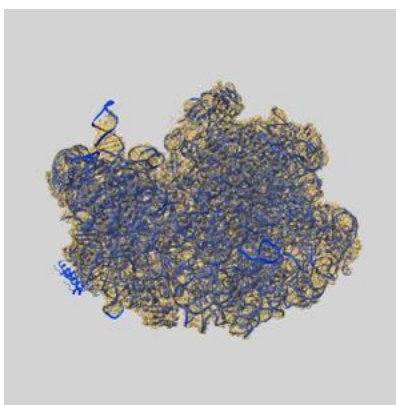
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26821 and PDB model 7UVZ. Per-residue inclusion information can be found in section 3 on page 15.

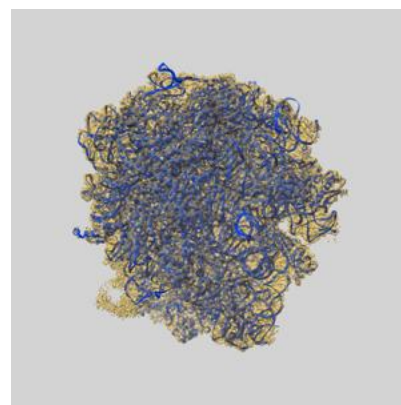
9.1 Map-model overlay [i](#)



X



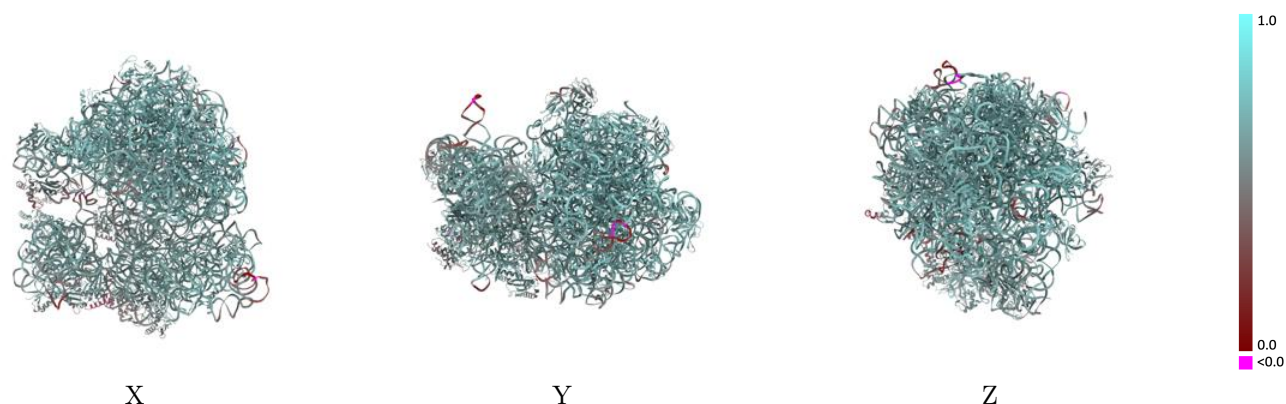
Y



Z

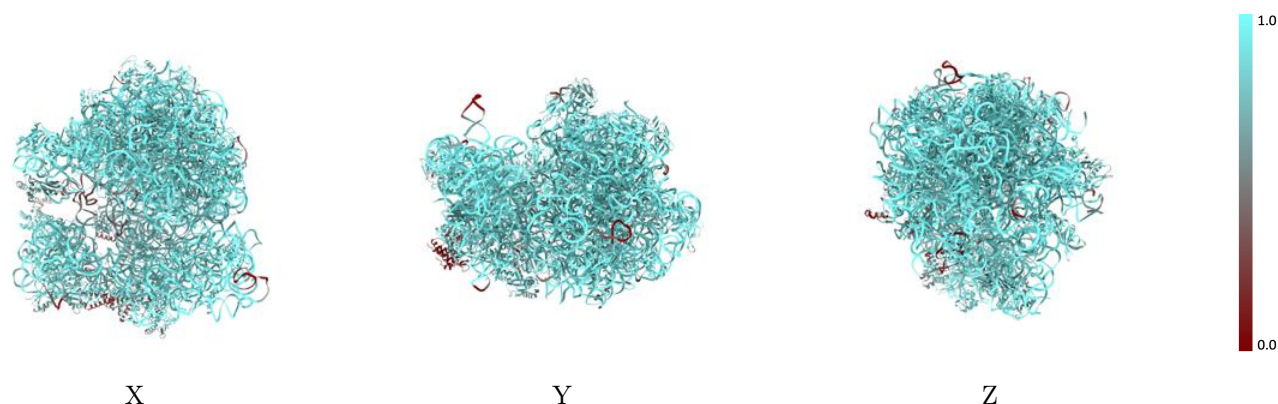
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



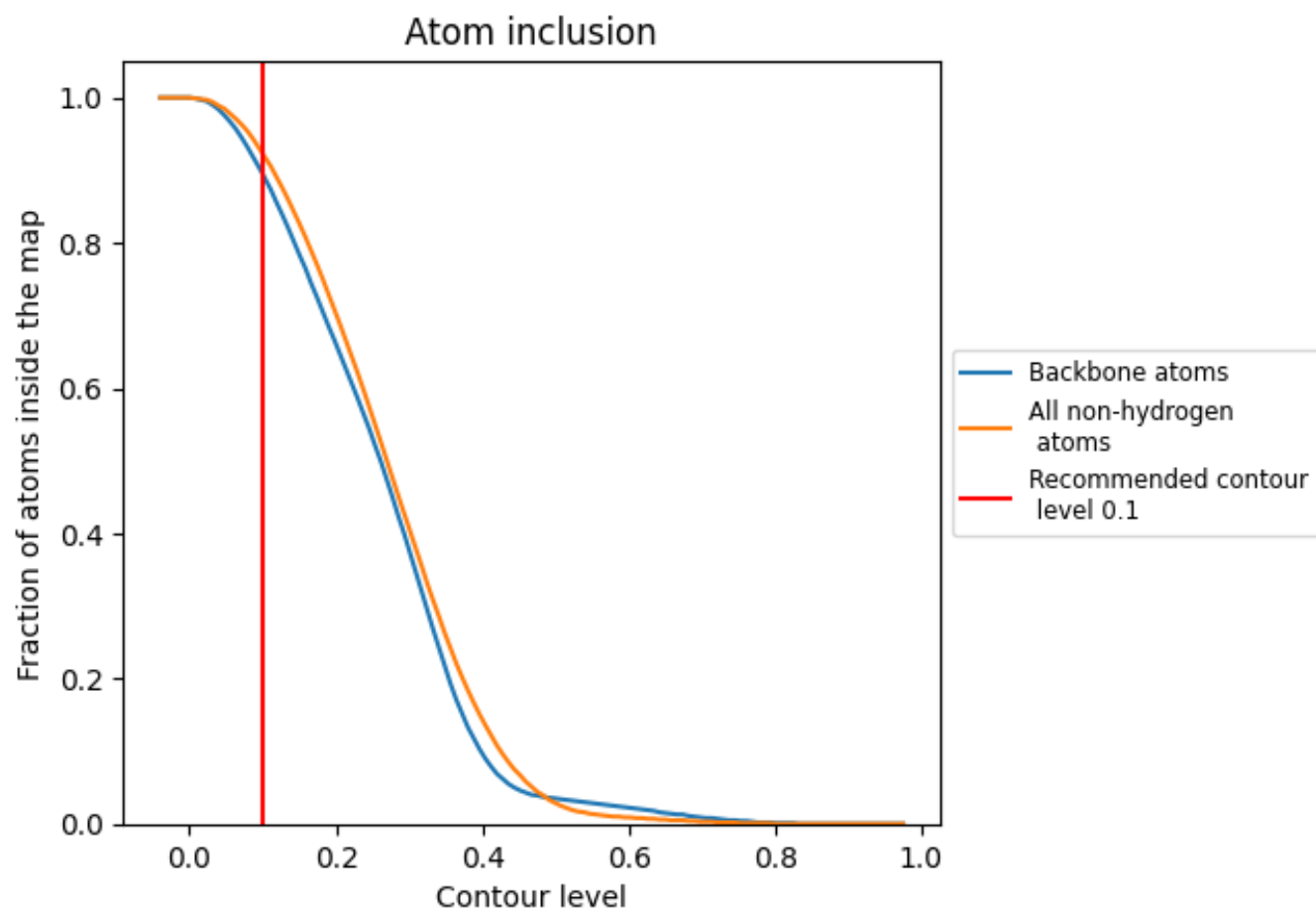
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 92% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9230	 0.6370
0	 0.9090	 0.6820
1	 0.9830	 0.7290
2	 0.9960	 0.7230
3	 0.9580	 0.6840
A	 0.9700	 0.6630
B	 0.9770	 0.6090
C	 0.9600	 0.6980
D	 0.9680	 0.7120
E	 0.9460	 0.6910
F	 0.5880	 0.4580
G	 0.8230	 0.5870
H	 0.5010	 0.4620
I	 0.9660	 0.7050
J	 0.9510	 0.6910
K	 0.9660	 0.7030
L	 0.9390	 0.6860
M	 0.9850	 0.7180
N	 0.8950	 0.6210
O	 0.9330	 0.6830
P	 0.9920	 0.7200
Q	 0.9580	 0.6930
R	 0.9600	 0.7110
S	 0.9040	 0.6650
T	 0.8650	 0.6260
U	 0.9030	 0.6560
V	 0.9700	 0.7120
W	 0.9410	 0.6940
X	 0.8550	 0.6110
Y	 0.9690	 0.6970
Z	 0.9370	 0.7020
a	 0.9510	 0.6100
b	 0.1330	 0.4040
c	 0.8880	 0.6150
d	 0.7710	 0.5350



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Chain	Atom inclusion	Q-score
e	 0.9470	 0.6470
f	 0.8080	 0.5770
g	 0.6450	 0.5290
h	 0.9490	 0.6530
i	 0.9240	 0.6380
j	 0.8430	 0.6140
k	 0.7850	 0.5590
l	 0.8170	 0.6260
m	 0.9110	 0.6310
n	 0.9160	 0.6360
o	 0.9430	 0.6480
p	 0.9580	 0.6550
q	 0.9210	 0.6260
r	 0.9080	 0.6140
s	 0.9510	 0.6420
t	 0.9560	 0.6430
u	 0.2890	 0.4950
v	 0.4850	 0.4010
w	 0.6770	 0.3910