



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 07:26 AM EDT

PDB ID : 5WF0 / pdb_00005wf0
EMDB ID : EMD-8826
Title : 70S ribosome-EF-Tu H84A complex with GTP and near-cognate tRNA (Complex C2)
Authors : Fislage, M.; Frank, J.
Deposited on : 2017-07-11
Resolution : 3.60 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:

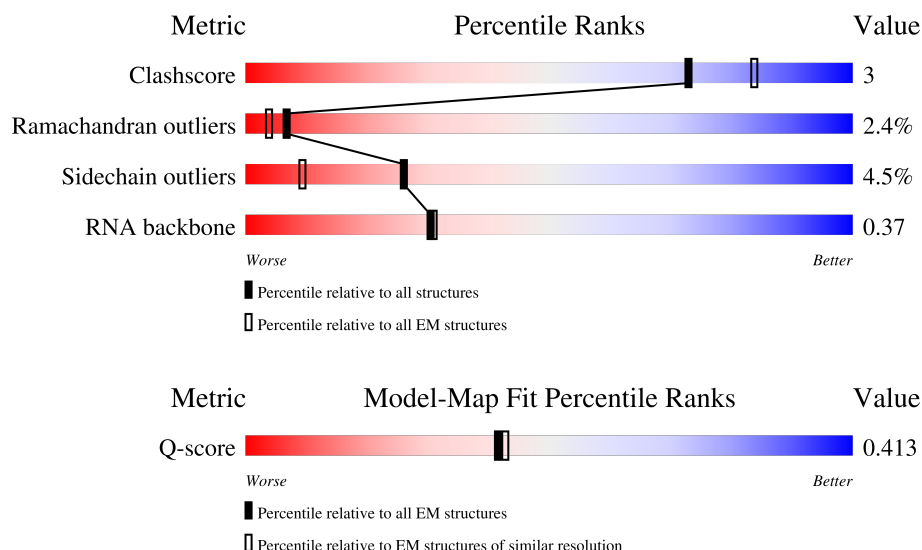
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.60 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.



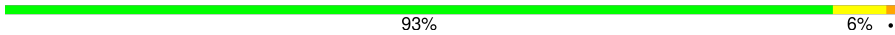
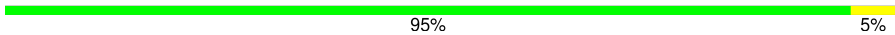
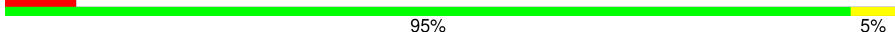
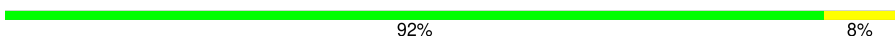
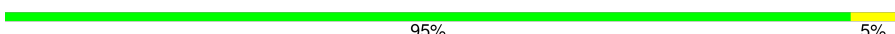
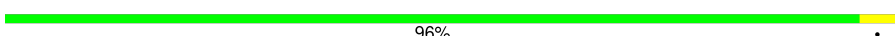
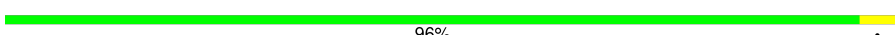
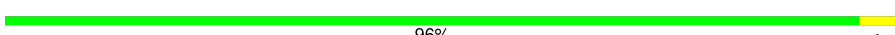
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	2903	 67% 28% 5%
2	B	120	 72% 27% 1%
3	C	271	 92% 8%

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Mol	Chain	Length	Quality of chain
4	D	208	 91% 7% .
5	E	200	 90% 9% .
6	F	177	 93% 6% .
7	G	174	 95% 5%
8	H	149	 8% 95% 5%
9	I	141	 16% 80% 17% .
10	J	141	 90% 9% .
11	K	122	 82% 16% ..
12	L	143	 90% 10% .
13	M	136	 93% 7%
14	N	119	 94% . .
15	O	116	 94% 5% .
16	P	114	 92% 8%
17	Q	115	 90% 10%
18	R	102	 88% 11% .
19	S	109	 88% 12%
20	T	92	 90% 10%
21	U	102	 88% 11% .
22	V	92	 95% 5%
23	W	75	 81% 16% .
24	X	77	 96% .
25	Y	60	 93% 7%
26	Z	56	 96% .
27	0	55	 84% 16%
28	1	51	 96% .

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Mol	Chain	Length	Quality of chain
29	2	45	
30	3	64	
31	4	38	
32	5	131	
33	6	66	
34	a	1540	
35	b	218	
36	c	206	
37	d	205	
38	e	157	
39	f	100	
40	g	151	
41	h	129	
42	i	127	
43	j	98	
44	k	116	
45	l	121	
46	m	115	
47	n	101	
48	o	88	
49	p	82	
50	q	80	
51	r	65	
52	s	79	
53	t	85	

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Mol	Chain	Length	Quality of chain
54	u	65	 72% 22% 6%
55	v	77	 73% 23%
55	w	77	 51% 36% 10%
56	x	12	 58% 42%
57	y	76	 96% 41% 8%
58	z	393	 96% 94% 6%

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 154600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2900	Total	C	N	O	P	0	0
			62277	27788	11459	20130	2900		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 216643
A	1723	G	A	conflict	GB 216643
A	1847	G	A	conflict	GB 216643

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1199817771

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1557	974	287	293	3		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	200	Total	C	N	O	S	0	0
			1544	969	282	289	4		

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1120	708	211	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	115	Total	C	N	O		0	0
			933	595	190	148			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	102	Total	C	N	O	S	0	0
			779	492	146	141			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	92	Total	C	N	O	S	0	0
			739	471	135	131	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	S	0	0
			572	355	116	100	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total	C	N	O	S	0	0
			494	305	96	91	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	56	Total	C	N	O	S	0	0
			434	273	85	74	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	51	Total	C	N	O	S	0	0
			417	269	76	72			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	0	0
			33050	14748	6057	10705	1540		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	121	Total	C	N	O	S	0	0
			940	581	193	162	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			810	502	165	140	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP B7MCS2

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 55 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0
55	w	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total	C	N	O	P	0	0
			252	113	43	84	12		

- Molecule 57 is a RNA chain called Phe-tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

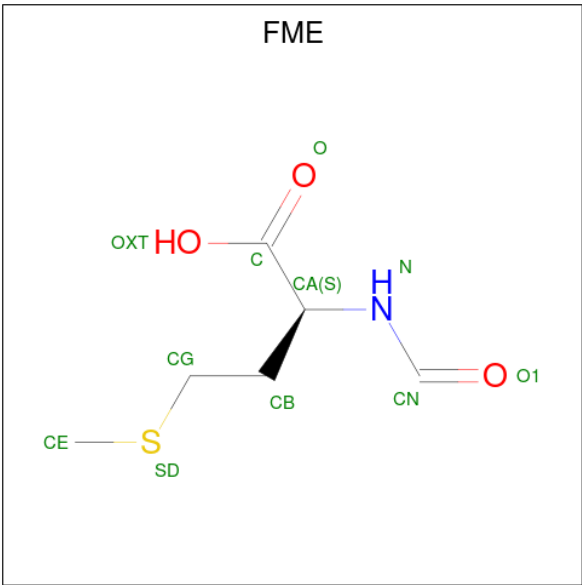
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3031	1915	522	581	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	84	ALA	HIS	engineered mutation	UNP A7ZUJ2

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
59	A	1	Total	C	N	O	S	0
			10	6	1	2	1	

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

Mol	Chain	Residues	Atoms		AltConf
60	A	1001	Total	Mg	0
			1001	1001	
60	B	34	Total	Mg	0
			34	34	
60	D	2	Total	Mg	0
			2	2	
60	E	2	Total	Mg	0
			2	2	
60	L	3	Total	Mg	0
			3	3	
60	M	1	Total	Mg	0
			1	1	
60	N	2	Total	Mg	0
			2	2	
60	Q	2	Total	Mg	0
			2	2	
60	T	1	Total	Mg	0
			1	1	
60	W	2	Total	Mg	0
			2	2	
60	X	2	Total	Mg	0
			2	2	

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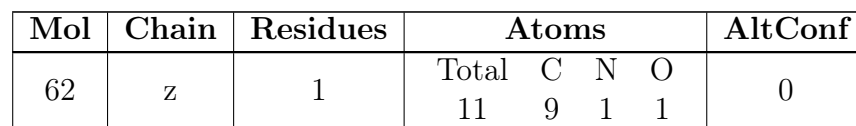
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Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total 1	Mg 1	0
60	4	1	Total 1	Mg 1	0
60	a	402	Total 402	Mg 402	0
60	d	3	Total 3	Mg 3	0
60	g	1	Total 1	Mg 1	0
60	i	2	Total 2	Mg 2	0
60	k	1	Total 1	Mg 1	0
60	m	1	Total 1	Mg 1	0
60	n	1	Total 1	Mg 1	0
60	o	2	Total 2	Mg 2	0
60	t	3	Total 3	Mg 3	0
60	v	8	Total 8	Mg 8	0
60	w	1	Total 1	Mg 1	0
60	x	1	Total 1	Mg 1	0

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

Mol	Chain	Residues	Atoms		AltConf
61	A	4	Total 4	K 4	0
61	a	1	Total 1	K 1	0

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



-
- The image displays the chemical structure of Guanosine Triphosphate (GTP). It consists of a guanine base (a purine ring system with an amino group at C2) linked to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is further linked to a chain of three phosphate groups (O3A, O3B, O3C) via phosphodiester bonds. The structure is color-coded: the guanine base is blue, the ribose sugar is green, and the phosphate groups are red. Stereochemistry is indicated with wedges and dashes, and atoms are labeled with their respective element symbols and numbers (e.g., N1, N2, N3, N4, N5, N6, N7, N8, N9, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799

Mol	Chain	Residues	Atoms					AltConf
63	z	1	Total	C	N	O	P	0
			32	10	5	14	3	

- 

Mol	Chain	Residues	Atoms	AltConf
64	A	463	Total O 463 463	0
64	B	11	Total O 11 11	0
64	C	5	Total O 5 5	0
64	D	1	Total O 1 1	0
64	E	1	Total O 1 1	0
64	G	3	Total O 3 3	0
64	J	2	Total O 2 2	0
64	L	3	Total O 3 3	0
64	M	2	Total O 2 2	0
64	N	4	Total O 4 4	0
64	O	1	Total O 1 1	0
64	Q	2	Total O 2 2	0
64	S	1	Total O 1 1	0
64	W	2	Total O 2 2	0
64	X	1	Total O 1 1	0
64	Z	2	Total O 2 2	0
64	0	1	Total O 1 1	0
64	3	2	Total O 2 2	0
64	a	160	Total O 160 160	0
64	d	1	Total O 1 1	0
64	i	1	Total O 1 1	0
64	s	3	Total O 3 3	0

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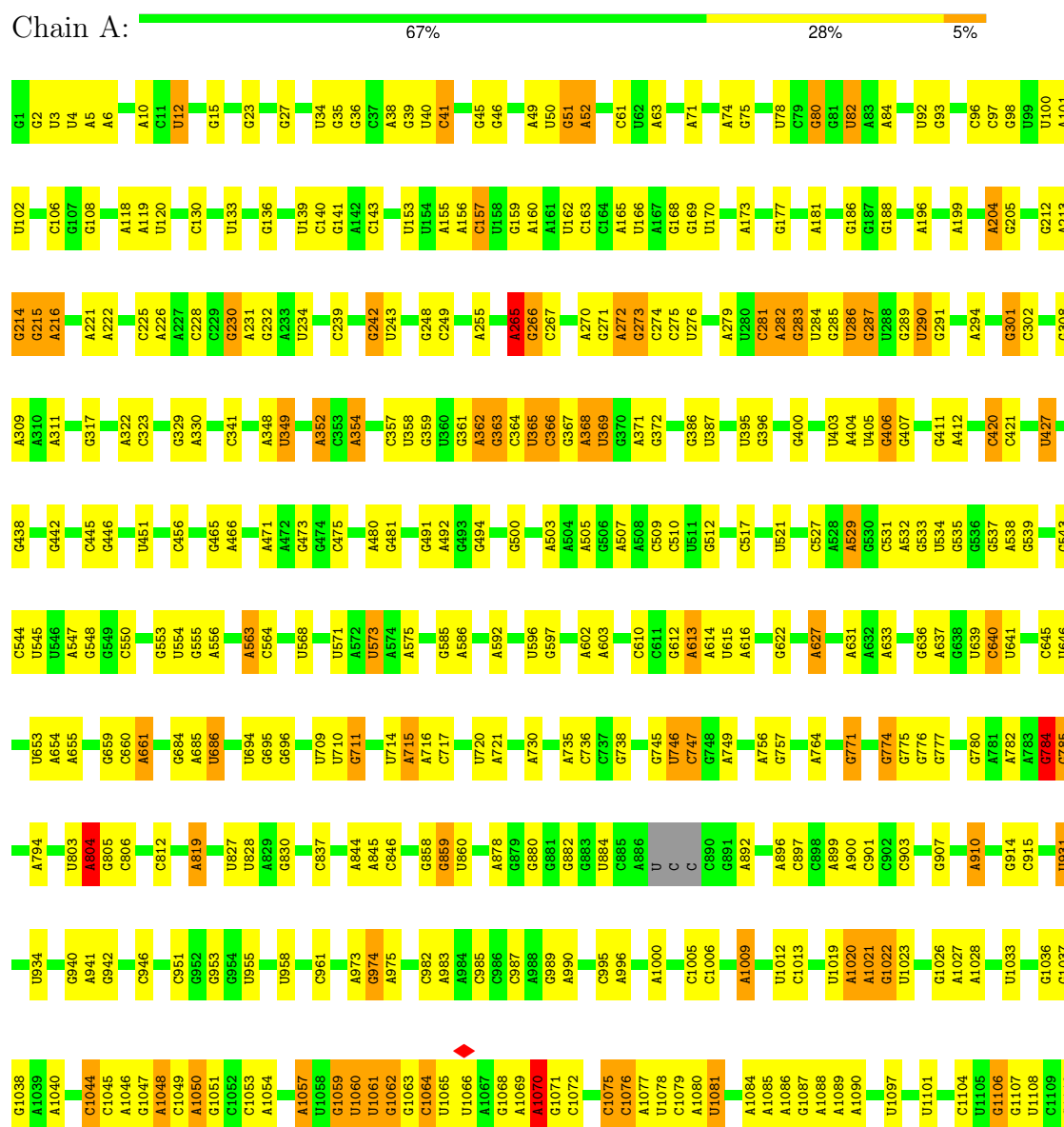
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
64	t	1	Total 1	O 1	0
64	u	1	Total 1	O 1	0
64	w	2	Total 2	O 2	0

3 Residue-property plots

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

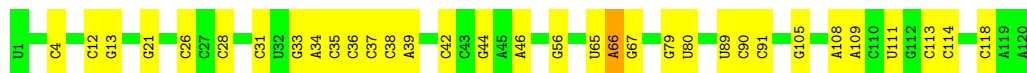
• Molecule 1: 23S rRNA



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G2799	U2689	U2552	G2424	A2311	A2163	G2056	A1919	A1809	U1716	A1569	U1485		A1226	G1112
A2800	U2689	U2552	A2425	C2313	C2164	A2060	G1929	A1810	A1717	U1578			G1227	G1115
A2802	U2689	U2554	G2428	G2318	A2170	G2061	G1930	G1816	U1720	A1579			G1236	G1116
U2804	U2689	U2554	G2429	A2171	A2171	G2062	G1930	G1817	G1721	A1580			A1237	G1117
C2805	U2707	A2566	A2430	G2319	U2172	A2063	A1936	U1818	A1722	G1581			G1238	G1118
C2806	U2713	A2567	A2435	G2323	A2173	G2069	A1937	G1826	G1723	C1582			G1245	U1119
C2807	U2713	U2568	G2435	U2324	U2180	A2070	A1938	G1826	G1724	A1583			G1245	
U2808	G2715	G2569	U2441	U2325	U2180	A2071	G1939	C1833	G1726	U1584			A1246	G1124
A2809	C2716	G2570	U2441	C2326	G2186	C2072	U1940	C1833	G1726	C1585			A1247	G1125
A2810	U2720	U2571	G2445	A2327	U2192	A2077	C1941	U1834	A1727	A1586			G1248	
G2811	U2720	A2572	G2446	A2328	U2192	C2078	C1942	G1835	G1728	G1587				U1130
	U2724	C2573	G2447	U2329	A2198	C2078	U1955	G1841	U1729	G1588			A1253	G1131
U2818	U2724	G2578	A2448	G2330	A2198	A2080	U1955	G1842	U1730	U1589			G1256	U1132
A2819	A2726	C2579	U2449	G2331	G2204	U2092	C1962	G1847	G1731	A1505			C1257	C1135
A2820	A2726	U2580	U2449	A2332	A2205	G2093	U1963	G1847	G1737	A1506			U1258	
	A2727	G2581	U2457	A2333	C2206	C2093	G1964	U1851	G1738	C1592			A1262	G1139
U2833	U2728	G2581	U2457	U2334	C2206	C2096	C1965	U1852	A1739	G1595				A1140
	U2733	U2585	A2469	U2335	C2208	A2097	A1966	U1852	G1740	A1596			G1271	U1141
G2838	A2734	U2586	G2470	A2336	C2208	U2098	C1967	A1854	U1742	C1597			A1272	A1143
G2839	G2735		G2475	C2342	A2211	U2099	A1970	G1857	G1743	C1605			U1273	
	G2742	A2602	A2476	C2350	U2212	G2100	U1971	A1858	A1744	A1608			G1429	G1149
U2849	U2743	U2604		G2350	U2213	A2101	G1972	A1858	A1745	A1609			G1300	G1150
A2850	G2744	U2605	C2480	G2357	C2214	G2102	U1976	G1862	A1746	A1610			A1301	A1151
U2861	G2745	G2608	G2481	G2357	G2221	C2103	U1976	G1862	U1747	C1615			C1305	C1152
G2862	C2746	U2609	U2491	G2361	G2221	U2105	G1980	A1866	C1748	A1616				C1153
C2863	U2746	U2609	U2491	G2361	G2221	C2105	A1981	A1866	A1749	G1617			G1320	G1154
	G2747	U2613	G2494	G2373	A2225	U2106	U1982	G1869	G1750	A1618				A1155
G2867	A2748	A2614		G2373	C2226	G2107	U1982	C1870	C1752	G1619				
A2868		U2615	C2498	A2378	G2238	A2108	U1991	A1871	U1758	G1642			A1327	G1171
A2872	C2752	U2615	U2499	G2379	G2239	U2109	G1992	A1871	U1758	G1642			A1328	C1172
A2873	U2754	G2623	U2500	G2379	G2239	G2110	U1993	G1873	G1643	U1534			U1329	U1174
C2874		G2624	U2500	G2383	G2251	U2112	U1993	G1873	G1643	G1534			C1330	A1175
	A2757	U2629	G2501	U2384	G2251	U2113	C1997	G1875	G1764	A1647			G1331	U1176
C2880	A2758	U2629	G2502	U2384	G2251	U2113	C1997	G1875	A1773	U1648			G1332	U1177
A2883	C2762	U2636	A2503	C2385	U2262	U2118	G2004	A1876	A1773	G1649			C1345	G1178
U2884	G2763	U2637	G2504	C2386	C2264	G2120	G2004	A1876	A1773	G1649				C1179
G2885	A2764	U2638	U2504	C2386	C2264	G2120	G2004	A1876	A1773	G1649			U1352	U1180
A2886	A2765	A2639	U2506	A2392	A2274	U2122	A2013	U1882	G1776	A1650			C1357	U1181
	C2773	G2645	A2513	A2392	A2274	U2122	A2013	U1882	G1776	A1650			G1358	U1182
A2900	U2778	U2654	U2514	G2399	A2278	G2127	A2020	G1884	U1779	A1651			A1359	U1184
C2901	U2779	U2655	C2515	G2400	G2279	G2127	A2021	A1885	U1781	G1674			C1363	A1189
C2902	G2780	U2656	A2516	U2401	G2279	G2127	A2021	A1885	U1782	C1675			A1366	G1190
U2903	C2788	A2657	A2517	G2402	G2283	U2131	U2028	G1903	A1784	U1688			G1367	
	C2789	U2658	A2518	U2404	C2283	U2132	U2028	G1903	A1791	U1688			A1368	G1193
	C2790	U2659	A2519	G2405	G2286	U2133	A2030	G1906	A1794	U1693			G1368	U1203
	U2791	U2660	A2520	A2406	A2287	A2134	A2031	G1907	C1795	C1694				G1210
	G2791	A2661	A2521	U2408	A2288	G2141	A2032	U1911	U1796	G1695			U1476	
	A2792	G2662	A2531	U2408	U2296	C2145	A2033	A1912	A1700	A1700			A1378	A1210
	C2793	A2663	A2531	A2411	A2297	C2146	G2038	A1913	G1710	G1710			U1379	
	U2794	G2664	A2535	A2412	A2297	A2147	U2039	C1914	A1801	A1801				G1216
	C2795	U2664	A2542	G2415	U2305	A2147	U2039	A1916	A1802	A1802			A1383	U1217
		A2682		A2415	A2309	G2157	C2043	A1916	A1803	A1803			A1387	G1218
				A2309	A2309	G2157	C2043	A1916	A1803	A1803				

- Molecule 2: 5S rRNA

Chain B:  72% 27%



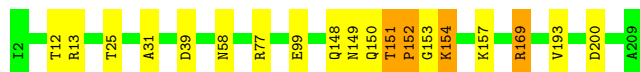
- Molecule 3: 50S ribosomal protein L2

Chain C:  92% 8%



- Molecule 4: 50S ribosomal protein L3

Chain D:  91% 7%



- Molecule 5: 50S ribosomal protein L4

Chain E:  90% 9%

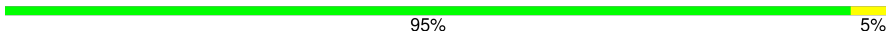


- Molecule 6: 50S ribosomal protein L5

Chain F:  93% 6%

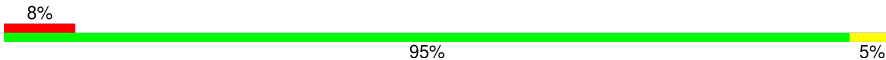


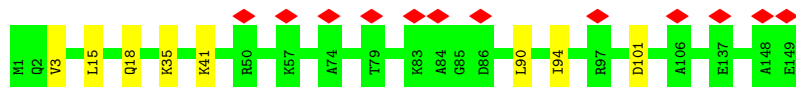
- Molecule 7: 50S ribosomal protein L6

Chain G:  95% 5%

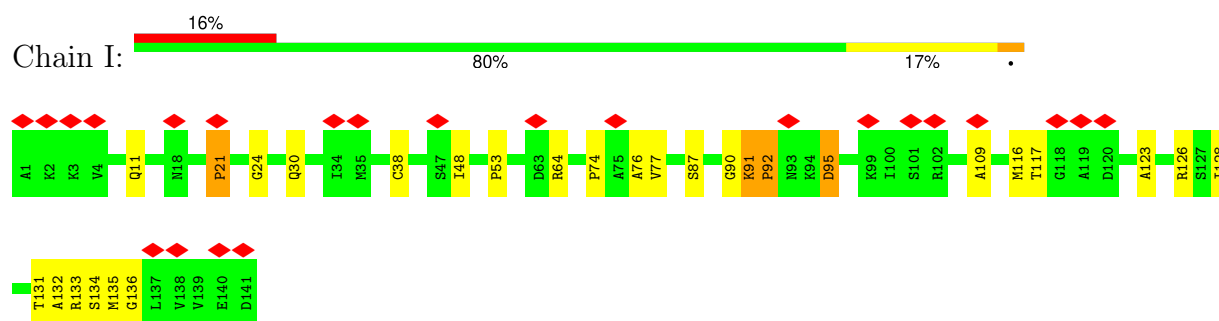


- Molecule 8: 50S ribosomal protein L9

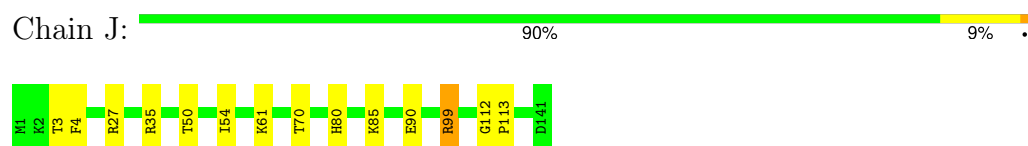
Chain H:  8% 95% 5%



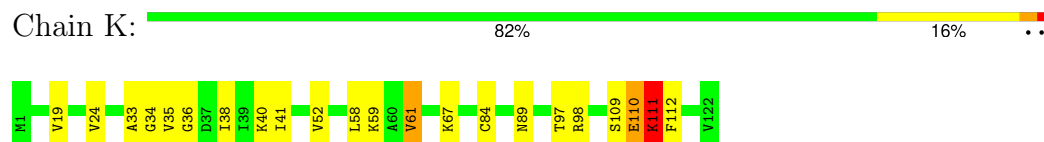
- Molecule 9: 50S ribosomal protein L11



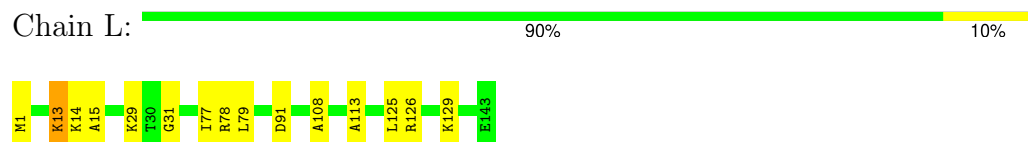
- Molecule 10: 50S ribosomal protein L13



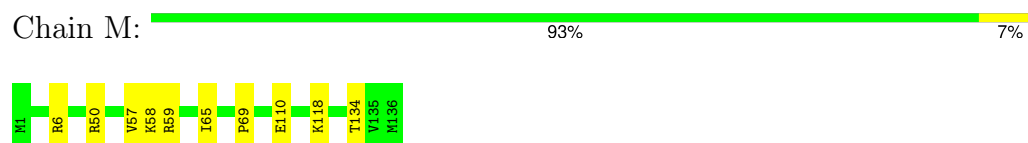
- Molecule 11: 50S ribosomal protein L14



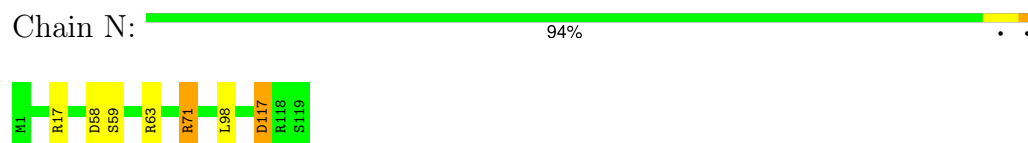
- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L18





- Molecule 16: 50S ribosomal protein L19

Chain P: 92% 8%



- Molecule 17: 50S ribosomal protein L20

Chain Q: 90% 10%



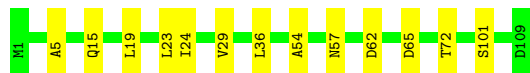
- Molecule 18: 50S ribosomal protein L21

Chain R: 88% 11%



- Molecule 19: 50S ribosomal protein L22

Chain S: 88% 12%



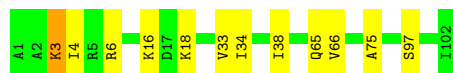
- Molecule 20: 50S ribosomal protein L23

Chain T: 90% 10%



- Molecule 21: 50S ribosomal protein L24

Chain U: 88% 11%



- Molecule 22: 50S ribosomal protein L25

Chain V: 95% 5%



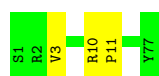
- Molecule 23: 50S ribosomal protein L27

Chain W: 81% 16%



- Molecule 24: 50S ribosomal protein L28

Chain X: 96%



- Molecule 25: 50S ribosomal protein L29

Chain Y: 93% 7%



- Molecule 26: 50S ribosomal protein L30

Chain Z: 96%



- Molecule 27: 50S ribosomal protein L32

Chain 0: 84% 16%



- Molecule 28: 50S ribosomal protein L33

Chain 1: 96%



- Molecule 29: 50S ribosomal protein L34

Chain 2: 80% 20%



- Molecule 30: 50S ribosomal protein L35

Chain 3: 97% .



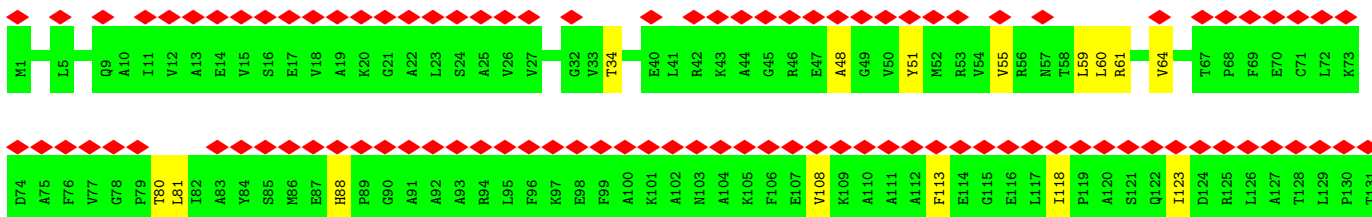
- Molecule 31: 50S ribosomal protein L36 1

Chain 4: 100%

There are no outlier residues recorded for this chain.

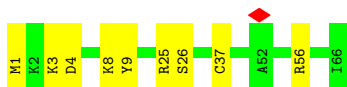
- Molecule 32: 50S ribosomal protein L10

Chain 5: 76%
89% 11%



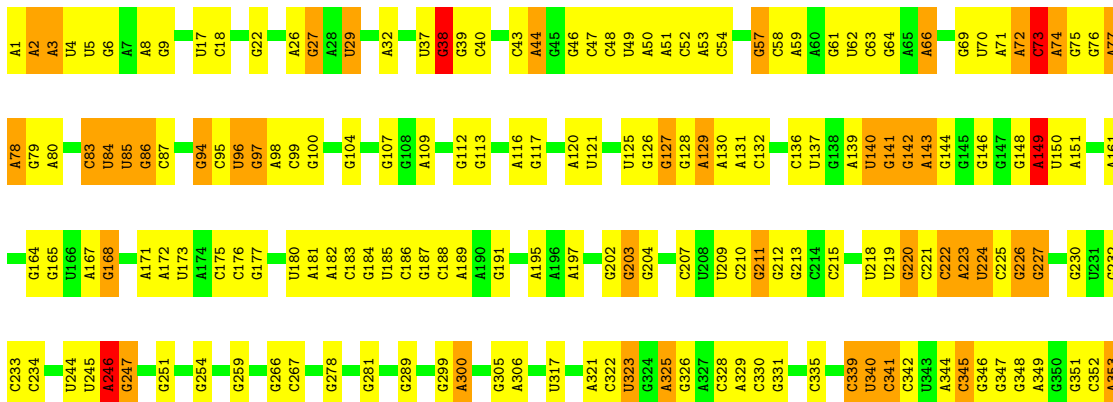
- Molecule 33: 50S ribosomal protein L31

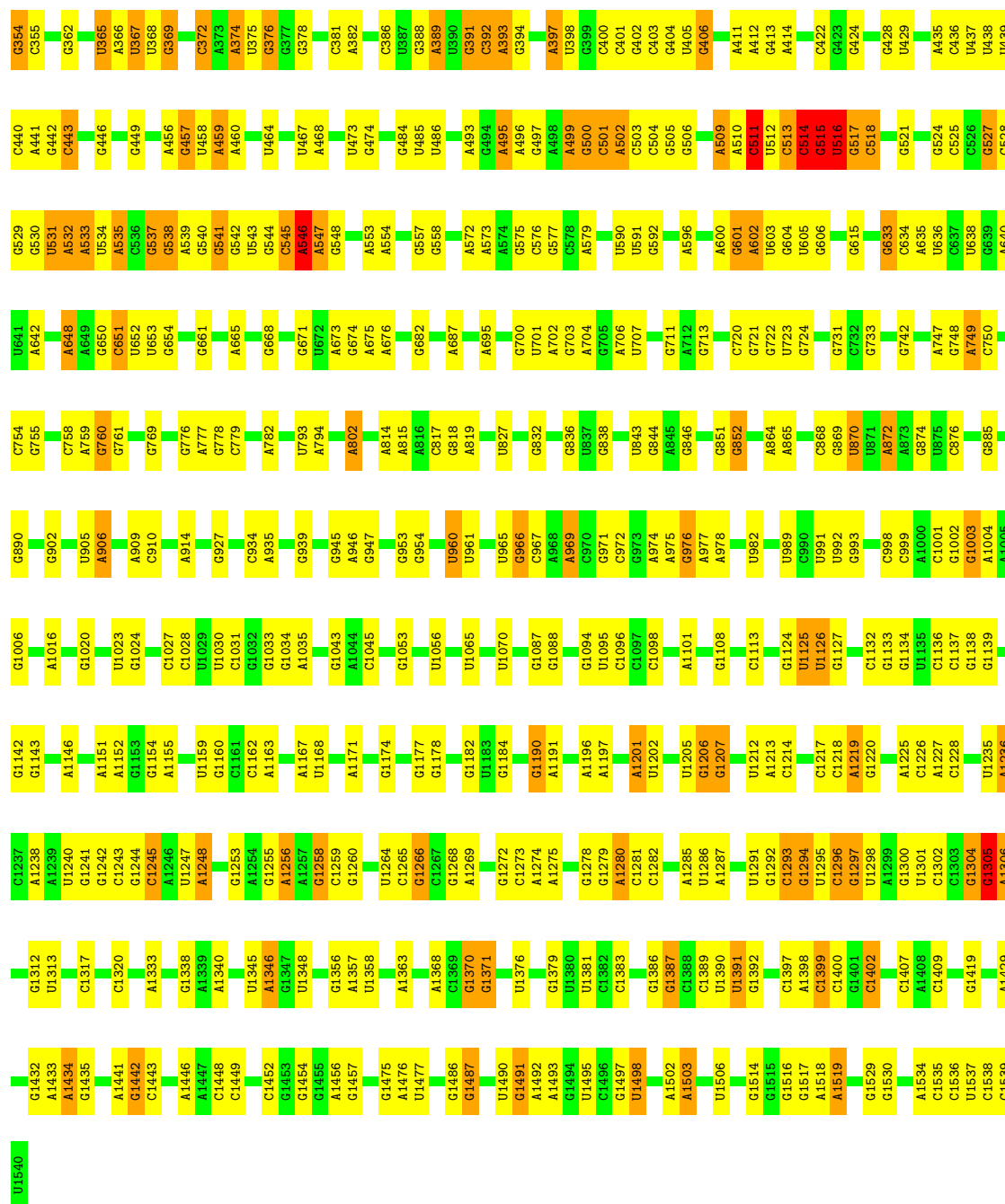
Chain 6: 86% 14%



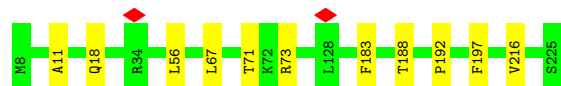
- Molecule 34: 16S rRNA

Chain a: 59% 32% 8%





- Molecule 35: 30S ribosomal protein S2



- Molecule 36: 30S ribosomal protein S3





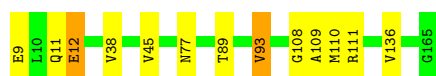
- Molecule 37: 30S ribosomal protein S4

Chain d: 96% .



- Molecule 38: 30S ribosomal protein S5

Chain e: 92% 7% .



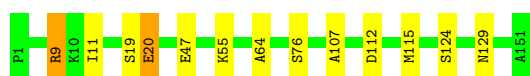
- Molecule 39: 30S ribosomal protein S6

Chain f: 91% 7% .



- Molecule 40: 30S ribosomal protein S7

Chain g: 91% 7% .



- Molecule 41: 30S ribosomal protein S8

Chain h: 93% 7% .



- Molecule 42: 30S ribosomal protein S9

Chain i: 83% 16% .

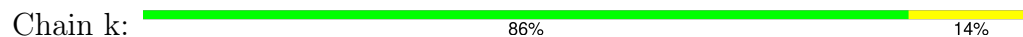


- Molecule 43: 30S ribosomal protein S10

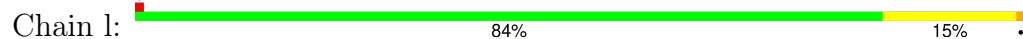
Chain j: 86% 10% .



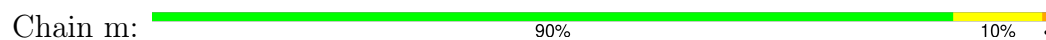
- Molecule 44: 30S ribosomal protein S11



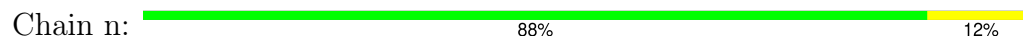
- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13



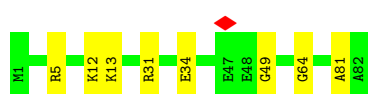
- Molecule 47: 30S ribosomal protein S14



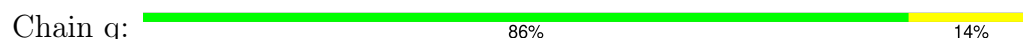
- Molecule 48: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S16

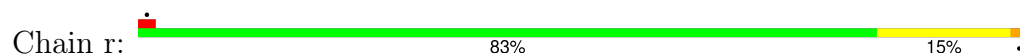


- Molecule 50: 30S ribosomal protein S17

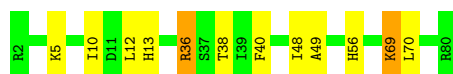
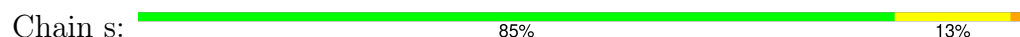




- Molecule 51: 30S ribosomal protein S18



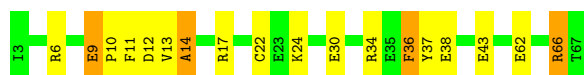
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



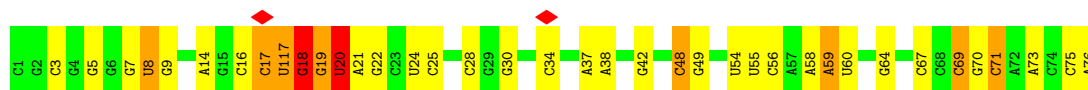
- Molecule 54: 30S ribosomal protein S21



- Molecule 55: tRNA-fMet



- Molecule 55: tRNA-fMet

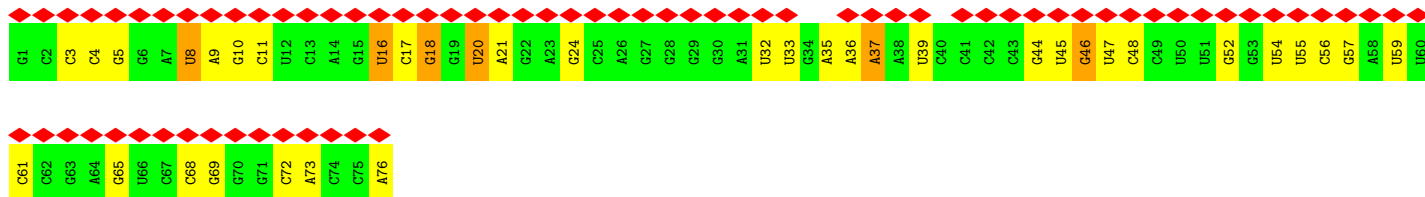


- Molecule 56: mRNA

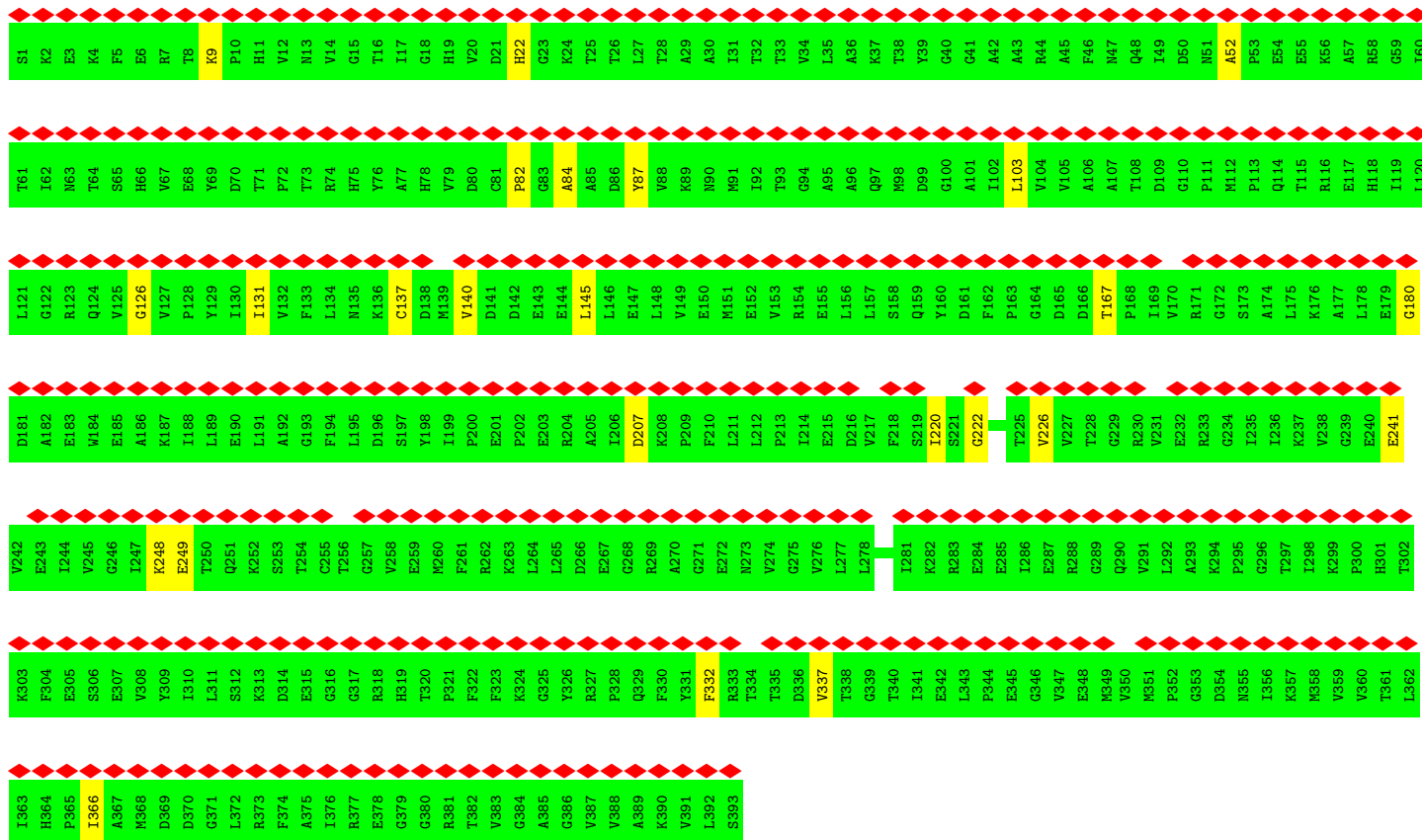




• Molecule 57: Phe-tRNA-Phe



• Molecule 58: Elongation factor Tu 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30623	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.00371	Depositor
Map size (Å)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, MG, MIA, 4OC, 5MU, OMG, PSU, K, 6MZ, MA6, 7MG, OMC, 5MC, 2MG, UR3, 3TD, H2U, 2MA, 1MG, OMU, FME, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/69174	0.71	32/107907 (0.0%)
2	B	0.37	0/2876	0.68	2/4483 (0.0%)
3	C	0.51	0/2121	0.75	0/2852
4	D	0.52	0/1578	0.78	1/2124 (0.0%)
5	E	0.50	0/1563	0.81	0/2103
6	F	0.54	0/1434	0.82	0/1926
7	G	0.54	0/1324	0.75	0/1794
8	H	0.57	0/1122	0.76	0/1515
9	I	0.70	0/1046	0.97	3/1410 (0.2%)
10	J	0.52	0/1143	0.81	2/1540 (0.1%)
11	K	0.52	0/947	0.74	0/1268
12	L	0.52	0/1052	0.86	0/1401
13	M	0.49	0/1093	0.80	0/1460
14	N	0.55	0/964	0.87	0/1289
15	O	0.55	0/902	0.88	0/1209
16	P	0.50	0/929	0.74	0/1242
17	Q	0.52	0/946	0.93	0/1260
18	R	0.50	0/823	0.78	2/1100 (0.2%)
19	S	0.50	0/852	0.82	0/1142
20	T	0.54	0/736	0.79	0/984
21	U	0.51	0/787	0.77	0/1051
22	V	0.51	0/752	0.75	0/1008
23	W	0.45	0/579	0.69	0/767
24	X	0.48	0/635	0.71	0/848
25	Y	0.53	0/495	0.86	0/658
26	Z	0.54	0/438	0.86	0/586
27	0	0.48	0/440	0.80	0/588
28	1	0.48	0/424	0.69	0/565
29	2	0.55	0/370	0.94	0/487
30	3	0.47	0/513	0.83	0/676
31	4	0.46	0/303	0.73	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.66	0/1001	0.85	0/1350
33	6	0.57	0/531	0.83	0/709
34	a	0.37	0/36725	0.73	26/57285 (0.0%)
35	b	0.57	0/1735	0.81	0/2338
36	c	0.54	0/1651	0.79	0/2225
37	d	0.55	0/1665	0.83	0/2227
38	e	0.54	0/1169	0.83	0/1573
39	f	0.57	0/835	0.82	0/1128
40	g	0.54	0/1195	0.83	0/1602
41	h	0.52	0/989	0.84	1/1326 (0.1%)
42	i	0.56	0/1034	0.77	0/1375
43	j	0.58	0/796	0.75	0/1077
44	k	0.54	0/885	0.80	0/1195
45	l	0.58	0/954	0.80	1/1282 (0.1%)
46	m	0.58	0/900	0.86	0/1204
47	n	0.56	0/822	0.81	0/1095
48	o	0.52	0/722	0.88	0/964
49	p	0.55	0/659	0.82	0/884
50	q	0.56	0/657	0.72	0/881
51	r	0.57	0/544	0.79	0/731
52	s	0.56	0/652	0.76	0/877
53	t	0.55	0/671	0.90	0/888
54	u	0.66	0/550	0.94	0/728
55	v	0.40	1/1747 (0.1%)	0.70	0/2721
55	w	0.42	1/1747 (0.1%)	0.87	7/2721 (0.3%)
56	x	0.40	0/280	0.78	0/433
57	y	0.39	0/1607	0.71	0/2501
58	z	0.57	0/3086	0.76	0/4175
All	All	0.43	2/164170 (0.0%)	0.74	77/245135 (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
34	a	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-6.40	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	7	4SU	O3'-P	5.15	1.61	1.56

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	17	C	O3'-P-O5'	16.31	128.46	104.00
55	w	117	U	P-O3'-C3'	11.04	136.76	120.20
1	A	242	G	C2'-C3'-O3'	10.92	125.88	109.50
34	a	1305	G	C2'-C3'-O3'	9.76	124.15	109.50
1	A	1022	G	C2'-C3'-O3'	9.27	123.40	109.50
1	A	204	A	C4'-C3'-O3'	9.09	123.03	109.40
34	a	515	G	C2'-C3'-O3'	8.31	126.16	113.70
1	A	1730	U	C2'-C3'-O3'	8.14	121.71	109.50
1	A	2407	A	C2'-C3'-O3'	7.97	125.65	113.70
1	A	1378	A	C4'-C3'-O3'	7.85	121.17	109.40
1	A	265	A	C4'-C3'-O3'	7.72	120.98	109.40
1	A	2296	U	C4'-C3'-O3'	7.62	120.83	109.40
55	w	18	G	C1'-C2'-O2'	-7.52	100.53	111.80
1	A	1130	U	C4'-C3'-O3'	-7.33	102.00	113.00
34	a	514	C	C4'-C3'-O3'	7.04	123.57	113.00
34	a	1190	G	C2'-C3'-O3'	7.04	120.07	109.50
34	a	500	G	O4'-C1'-C2'	-7.04	100.56	107.60
2	B	66	A	C4'-C3'-O3'	7.03	123.55	113.00
55	w	117	U	O3'-P-O5'	6.97	114.45	104.00
34	a	63	C	C2'-C3'-O3'	6.92	124.08	113.70
34	a	1201	A	C2'-C3'-O3'	6.86	119.79	109.50
34	a	246	A	C4'-C3'-O3'	6.84	119.66	109.40
1	A	859	G	C2'-C3'-O3'	6.80	119.69	109.50
1	A	1857	G	C4'-C3'-O3'	6.78	119.57	109.40
1	A	613	A	C4'-C3'-O3'	6.47	119.11	109.40
1	A	1020	A	C4'-C3'-O3'	6.44	119.06	109.40
34	a	374	A	C2'-C3'-O3'	-6.33	104.21	113.70
34	a	94	G	C2'-C3'-O3'	6.15	118.73	109.50
2	B	66	A	C2'-C3'-O3'	-6.15	104.48	113.70
4	D	152	PRO	N-CA-C	-6.10	105.58	113.57
18	R	51	VAL	CA-C-N	-6.10	112.22	119.84
18	R	51	VAL	C-N-CA	-6.10	112.22	119.84
1	A	1940	U	C4'-C3'-O3'	6.09	118.54	109.40
1	A	1475	G	C2'-C3'-O3'	6.08	118.61	109.50
1	A	1070	A	C2'-C3'-O3'	6.07	118.60	109.50
34	a	428	G	C4'-C3'-O3'	6.05	118.47	109.40
1	A	2391	G	C4'-C3'-O3'	6.05	122.07	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	804	A	C4'-C3'-O3'	-6.02	103.97	113.00
34	a	515	G	N9-C1'-C2'	6.02	121.03	112.00
1	A	1475	G	C4'-C3'-O3'	6.00	118.39	109.40
34	a	960	U	C2'-C3'-O3'	5.93	118.40	109.50
34	a	1297	G	C2'-C3'-O3'	5.88	118.32	109.50
55	w	117	U	OP2-P-O3'	-5.85	90.45	108.00
9	I	21	PRO	N-CA-C	5.79	117.76	110.70
45	l	20	VAL	N-CA-C	5.72	113.72	107.60
34	a	1399	C	C4'-C3'-O3'	5.71	117.96	109.40
1	A	301	G	C2'-C3'-O3'	5.69	118.03	109.50
1	A	2566	A	C4'-C3'-O3'	5.66	117.89	109.40
1	A	301	G	C4'-C3'-O3'	5.62	117.83	109.40
34	a	73	C	N1-C1'-C2'	5.56	120.34	112.00
34	a	960	U	C4'-C3'-O3'	5.55	117.73	109.40
1	A	1140	C	C2'-C3'-O3'	5.54	122.01	113.70
1	A	774	G	C2'-C3'-O3'	5.49	117.73	109.50
1	A	1078	U	C2'-C3'-O3'	-5.48	105.47	113.70
34	a	1432	G	C3'-C2'-O2'	5.47	118.90	110.70
34	a	1399	C	C2'-C3'-O3'	5.44	117.66	109.50
34	a	1272	G	C4'-C3'-O3'	-5.41	104.88	113.00
9	I	91	LYS	CA-C-N	5.39	126.58	119.84
9	I	91	LYS	C-N-CA	5.39	126.58	119.84
34	a	546	A	N9-C1'-C2'	5.38	120.07	112.00
55	w	69	C	C2'-C3'-O3'	5.37	121.75	113.70
34	a	511	C	C4'-C3'-O3'	-5.36	101.36	109.40
1	A	1081	U	C3'-C2'-O2'	5.35	118.72	110.70
34	a	38	G	C4'-C3'-O3'	-5.30	105.04	113.00
34	a	1201	A	C4'-C3'-O3'	5.28	117.32	109.40
1	A	982	C	C2'-C3'-O3'	-5.27	105.79	113.70
1	A	1970	A	C2'-C3'-O3'	5.25	117.38	109.50
41	h	26	MET	N-CA-C	5.16	112.86	108.22
1	A	96	C	C4'-C3'-O3'	-5.15	105.28	113.00
1	A	1496	A	C3'-C2'-O2'	5.13	118.40	110.70
34	a	63	C	C3'-C2'-O2'	5.12	118.37	110.70
34	a	149	A	C1'-C2'-O2'	5.11	116.06	108.40
10	J	112	GLY	CA-C-N	5.09	125.12	119.32
10	J	112	GLY	C-N-CA	5.09	125.12	119.32
1	A	784	G	C2'-C3'-O3'	-5.05	106.12	113.70
1	A	2326	C	C4'-C3'-O3'	5.05	120.58	113.00
55	w	17	C	OP2-P-O3'	-5.04	92.89	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	a	502	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62277	0	31338	328	0
2	B	2572	0	1302	3	0
3	C	2082	0	2157	7	0
4	D	1557	0	1604	6	0
5	E	1544	0	1607	6	0
6	F	1410	0	1447	6	0
7	G	1304	0	1348	3	0
8	H	1111	0	1148	1	0
9	I	1032	0	1088	21	0
10	J	1120	0	1151	5	0
11	K	938	0	1012	11	0
12	L	1043	0	1123	7	0
13	M	1074	0	1157	1	0
14	N	951	0	994	3	0
15	O	892	0	923	2	0
16	P	917	0	965	3	0
17	Q	933	0	1006	8	0
18	R	810	0	834	5	0
19	S	845	0	909	4	0
20	T	730	0	795	1	0
21	U	779	0	834	2	0
22	V	739	0	763	1	0
23	W	572	0	593	9	0
24	X	625	0	655	3	0
25	Y	494	0	530	1	0
26	Z	434	0	477	1	0
27	0	434	0	448	8	0
28	1	417	0	451	0	0
29	2	367	0	405	4	0
30	3	504	0	574	0	0
31	4	302	0	343	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	5	988	0	1025	4	0
33	6	522	0	524	2	0
34	a	33050	0	16655	296	0
35	b	1704	0	1732	2	0
36	c	1624	0	1699	3	0
37	d	1643	0	1710	4	0
38	e	1156	0	1199	3	0
39	f	817	0	808	6	0
40	g	1181	0	1240	4	0
41	h	979	0	1034	2	0
42	i	1022	0	1070	19	0
43	j	786	0	828	7	0
44	k	869	0	878	2	0
45	l	940	0	1001	5	0
46	m	891	0	955	2	0
47	n	810	0	852	0	0
48	o	714	0	736	13	0
49	p	649	0	666	2	0
50	q	648	0	691	1	0
51	r	535	0	552	2	0
52	s	637	0	665	6	0
53	t	665	0	714	14	0
54	u	544	0	579	6	0
55	v	1644	0	840	1	0
55	w	1644	0	840	13	0
56	x	252	0	130	2	0
57	y	1632	0	843	3	0
58	z	3031	0	3052	5	0
59	A	10	0	10	0	0
60	0	1	0	0	0	0
60	4	1	0	0	0	0
60	A	1001	0	0	0	0
60	B	34	0	0	0	0
60	D	2	0	0	0	0
60	E	2	0	0	0	0
60	L	3	0	0	0	0
60	M	1	0	0	0	0
60	N	2	0	0	0	0
60	Q	2	0	0	0	0
60	T	1	0	0	0	0
60	W	2	0	0	0	0
60	X	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	a	402	0	0	0	0
60	d	3	0	0	0	0
60	g	1	0	0	0	0
60	i	2	0	0	0	0
60	k	1	0	0	0	0
60	m	1	0	0	0	0
60	n	1	0	0	0	0
60	o	2	0	0	0	0
60	t	3	0	0	0	0
60	v	8	0	0	0	0
60	w	1	0	0	0	0
60	x	1	0	0	0	0
61	A	4	0	0	0	0
61	a	1	0	0	0	0
62	z	11	0	8	0	0
63	z	32	0	12	0	0
64	0	1	0	0	0	0
64	3	2	0	0	0	0
64	A	463	0	0	0	0
64	B	11	0	0	0	0
64	C	5	0	0	0	0
64	D	1	0	0	0	0
64	E	1	0	0	0	0
64	G	3	0	0	0	0
64	J	2	0	0	0	0
64	L	3	0	0	0	0
64	M	2	0	0	0	0
64	N	4	0	0	0	0
64	O	1	0	0	0	0
64	Q	2	0	0	0	0
64	S	1	0	0	0	0
64	W	2	0	0	0	0
64	X	1	0	0	0	0
64	Z	2	0	0	0	0
64	a	160	0	0	1	0
64	d	1	0	0	0	0
64	i	1	0	0	0	0
64	s	3	0	0	0	0
64	t	1	0	0	0	0
64	u	1	0	0	0	0
64	w	2	0	0	0	0
All	All	154600	0	103529	799	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 3.

All (799) 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)
34:a:514:C:O2	34:a:538:G:N2	1.62	1.30
1:A:627:A:OP1	12:L:78:ARG:NH1	1.71	1.22
1:A:2013:A:N1	1:A:2613:U:O4	1.71	1.21
1:A:714:U:OP2	48:o:88:ARG:NH1	1.76	1.19
34:a:502:A:H61	34:a:544:G:N2	1.43	1.17
34:a:219:U:C2'	34:a:220:G:H5'	1.74	1.16
34:a:143:A:H2	34:a:220:G:O6	1.29	1.15
34:a:143:A:C2	34:a:220:G:O6	1.99	1.14
43:j:88:MET:O	43:j:90:LEU:N	1.79	1.14
34:a:219:U:H2'	34:a:220:G:H5'	1.17	1.12
1:A:1915:3TD:C1'	1:A:1915:3TD:O4'	1.66	1.12
1:A:51:G:O2'	1:A:52:A:OP2	1.66	1.10
34:a:142:G:O6	34:a:221:C:N4	1.85	1.09
34:a:502:A:N6	34:a:544:G:N2	2.00	1.08
48:o:44:GLU:HG2	48:o:45:HIS:HD2	1.16	1.06
1:A:931:U:O4	1:A:1183:U:O2'	1.76	1.02
1:A:2029:G:H2'	1:A:2031:A:OP1	1.59	1.02
34:a:1376:U:O4	40:g:9:ARG:NH2	1.91	1.02
1:A:1713:A:N1	1:A:1745:A:N6	2.08	1.02
34:a:600:A:H2'	34:a:601:G:C5'	1.90	1.01
1:A:2773:C:OP1	4:D:169:ARG:NH1	1.96	0.98
34:a:539:A:N6	34:a:540:G:C2	2.31	0.98
34:a:969:A:H61	42:i:129:ARG:NH1	1.62	0.96
34:a:600:A:C2'	34:a:601:G:H5''	1.96	0.96
34:a:143:A:H2	34:a:220:G:C6	1.83	0.95
1:A:78:U:O2	1:A:108:G:O6	1.85	0.94
1:A:1469:A:N7	1:A:1522:A:N6	2.15	0.94
1:A:2638:G:O2'	1:A:2639:A:H8	1.49	0.93
1:A:596:U:H3	1:A:661:A:H61	1.12	0.93
34:a:827:U:N3	34:a:872:A:N6	2.15	0.93
42:i:126:PHE:HE1	42:i:128:LYS:HG3	1.34	0.92
1:A:230:G:N1	1:A:231:A:C2	2.38	0.92
55:w:59:A:P	55:w:60:U:H5	1.94	0.91
1:A:596:U:H3	1:A:661:A:N6	1.68	0.91
34:a:543:U:N3	34:a:544:G:C2	2.25	0.91
34:a:600:A:H2'	34:a:601:G:H5''	1.52	0.91
34:a:1386:G:H2'	34:a:1387:G:H5'	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:668:G:H21	48:o:45:HIS:HE1	1.21	0.88
34:a:369:G:H2'	34:a:393:A:C2	2.09	0.88
1:A:271:G:N2	1:A:366:C:O2	2.07	0.87
1:A:714:U:P	48:o:88:ARG:NH1	2.47	0.87
1:A:362:A:O3'	1:A:363:G:O4'	1.93	0.86
34:a:969:A:N6	42:i:129:ARG:NH1	2.22	0.86
34:a:514:C:C2	34:a:538:G:N2	2.37	0.86
34:a:374:A:N1	34:a:391:G:H1'	1.91	0.86
55:w:58:A:O3'	55:w:60:U:H5	1.60	0.85
1:A:714:U:P	48:o:88:ARG:HH11	2.00	0.84
1:A:2638:G:HO2'	1:A:2639:A:H8	0.90	0.84
42:i:45:MET:O	42:i:48:ARG:N	2.09	0.84
48:o:44:GLU:HG2	48:o:45:HIS:CD2	2.08	0.84
1:A:225:C:N3	1:A:231:A:H2	1.76	0.84
1:A:231:A:N7	1:A:232:G:C5	2.45	0.83
34:a:600:A:H2'	34:a:601:G:H5'	1.61	0.83
34:a:604:G:H2'	34:a:605:U:O4'	1.79	0.83
1:A:2028:U:H2'	1:A:2029:G:C8	2.14	0.82
1:A:1422:G:N2	1:A:1498:C:O2	2.13	0.82
1:A:362:A:N7	1:A:363:G:C6	2.48	0.82
34:a:142:G:O6	34:a:221:C:C4	2.33	0.81
1:A:1216:G:OP1	17:Q:10:ARG:NH2	2.14	0.81
34:a:437:U:C4	34:a:495:A:C6	2.68	0.81
53:t:8:LYS:O	53:t:11:ILE:HG12	1.80	0.81
34:a:437:U:N3	34:a:495:A:N6	2.28	0.81
1:A:271:G:N2	1:A:366:C:C2	2.49	0.80
34:a:969:A:N6	42:i:129:ARG:HH11	1.78	0.80
1:A:406:G:N2	1:A:421:C:O2	2.15	0.80
1:A:2658:C:OP1	7:G:157:LYS:NZ	2.13	0.80
34:a:83:C:O2	34:a:85:U:C5	2.35	0.80
1:A:2791:G:N2	1:A:2805:C:O2	2.15	0.79
34:a:437:U:C4	34:a:495:A:N6	2.51	0.79
34:a:58:C:N3	34:a:354:G:O6	2.16	0.78
1:A:710:U:O2	1:A:721:A:N1	2.16	0.78
1:A:711:G:O6	1:A:720:U:N3	2.15	0.78
55:w:58:A:O3'	55:w:60:U:C5	2.36	0.78
34:a:515:G:O2'	34:a:537:G:N1	2.15	0.78
1:A:2013:A:N1	1:A:2613:U:C4	2.53	0.77
1:A:272:A:C2	1:A:366:C:C2	2.72	0.77
34:a:600:A:C2'	34:a:601:G:C5'	2.60	0.76
1:A:2028:U:C4	1:A:2029:G:C6	2.74	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2638:G:O2'	1:A:2639:A:C8	2.30	0.76
34:a:1386:G:C2'	34:a:1387:G:H5'	2.15	0.76
34:a:502:A:N1	34:a:544:G:N3	2.32	0.76
34:a:870:U:C2	34:a:872:A:N6	2.55	0.75
11:K:98:ARG:NH2	34:a:339:C:OP2	2.20	0.75
1:A:270:A:N7	1:A:369:U:O2'	2.19	0.75
1:A:225:C:N3	1:A:231:A:C2	2.55	0.74
1:A:1496:A:C2	1:A:1498:C:N3	2.56	0.74
1:A:2788:C:H2'	1:A:2789:C:C6	2.22	0.74
4:D:153:GLY:O	4:D:154:LYS:HB3	1.86	0.74
34:a:502:A:C6	34:a:544:G:N2	2.56	0.74
34:a:827:U:C4	34:a:872:A:N6	2.56	0.74
34:a:668:G:H21	48:o:45:HIS:CE1	2.05	0.73
34:a:112:G:H21	34:a:354:G:C4'	2.01	0.73
34:a:223:A:H2'	34:a:224:U:C6	2.23	0.73
34:a:74:A:C2	34:a:97:G:N2	2.56	0.73
1:A:1245:G:OP1	12:L:13:LYS:NZ	2.21	0.73
1:A:40:U:H2'	1:A:41:C:H5'	1.70	0.73
34:a:219:U:H2'	34:a:220:G:C5'	2.09	0.72
1:A:40:U:C2'	1:A:41:C:H5'	2.19	0.72
34:a:85:U:H4'	34:a:86:G:O5'	1.89	0.72
1:A:1048:A:N7	1:A:1049:C:C5	2.58	0.71
34:a:543:U:N3	34:a:544:G:N3	2.38	0.71
34:a:83:C:O2	34:a:85:U:H5	1.71	0.71
1:A:2013:A:C2	1:A:2613:U:O4	2.43	0.71
34:a:148:G:N2	34:a:1446:A:C2	2.59	0.70
34:a:1409:C:N3	34:a:1491:G:O6	2.23	0.70
34:a:378:G:N2	34:a:386:C:O2	2.25	0.70
39:f:38:ARG:CG	39:f:63:ASN:HB3	2.22	0.70
48:o:44:GLU:O	48:o:46:LYS:N	2.25	0.70
1:A:51:G:HO2'	1:A:52:A:P	2.13	0.70
1:A:231:A:N6	1:A:232:G:N1	2.39	0.69
34:a:518:C:C4	34:a:530:G:N7	2.60	0.69
1:A:568:U:H1'	1:A:2030:6MZ:H9C1	1.72	0.69
34:a:1178:G:C8	42:i:98:ARG:NH2	2.60	0.69
1:A:2030:6MZ:H4'	1:A:2030:6MZ:OP2	1.92	0.69
1:A:686:U:O4	29:2:12:ARG:HG2	1.93	0.69
34:a:112:G:N2	34:a:354:G:O4'	2.25	0.69
34:a:605:U:O2	34:a:633:G:O6	2.11	0.69
34:a:500:G:N2	34:a:501:C:O2	2.25	0.68
34:a:113:G:N3	34:a:353:A:O2'	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:i:45:MET:O	42:i:47:VAL:N	2.27	0.67
1:A:2013:A:N6	1:A:2613:U:N3	2.43	0.67
42:i:45:MET:O	42:i:46:VAL:C	2.38	0.66
34:a:517:G:C6	34:a:531:U:O4'	2.49	0.66
1:A:749:A:C8	1:A:1618:6MZ:N6	2.64	0.66
1:A:362:A:O5'	1:A:363:G:OP2	2.14	0.66
1:A:365:U:O2'	1:A:366:C:O4'	2.06	0.66
1:A:1422:G:N2	1:A:1498:C:H1'	2.11	0.66
52:s:48:ILE:HD11	52:s:70:LEU:HD22	1.77	0.66
1:A:271:G:N1	1:A:366:C:N3	2.44	0.65
1:A:627:A:H5''	12:L:78:ARG:HH12	1.60	0.65
34:a:502:A:N1	34:a:544:G:C2	2.63	0.65
1:A:1062:G:N2	9:I:131:THR:O	2.30	0.65
1:A:931:U:OP1	26:Z:29:ARG:NH1	2.30	0.65
1:A:714:U:OP2	48:o:88:ARG:CZ	2.44	0.65
34:a:126:G:OP1	34:a:605:U:O2'	2.14	0.64
1:A:749:A:O2'	1:A:1618:6MZ:OP1	2.15	0.64
34:a:437:U:N3	34:a:495:A:C6	2.64	0.64
1:A:517:C:OP1	27:0:12:ARG:NH2	2.30	0.64
34:a:142:G:O6	34:a:221:C:N3	2.31	0.64
1:A:362:A:C3'	1:A:363:G:O4'	2.45	0.64
34:a:776:G:N2	34:a:802:A:OP2	2.31	0.64
55:w:59:A:P	55:w:60:U:C5	2.85	0.64
1:A:271:G:C6	1:A:367:G:N1	2.67	0.63
34:a:601:G:N2	34:a:638:U:C2	2.67	0.63
3:C:131:MET:HE2	3:C:173:LEU:HD21	1.80	0.63
34:a:603:U:O2	34:a:635:A:N1	2.32	0.63
1:A:1528:A:N6	1:A:1543:G:O2'	2.32	0.63
1:A:1048:A:C8	1:A:1049:C:C5	2.86	0.63
34:a:78:A:H2'	34:a:79:G:O4'	1.98	0.63
34:a:500:G:H1'	34:a:547:A:N7	2.14	0.62
1:A:406:G:H2'	1:A:407:G:O4'	1.99	0.62
34:a:113:G:H21	34:a:353:A:H2'	1.64	0.62
1:A:230:G:N1	1:A:231:A:N3	2.46	0.62
1:A:1479:G:O2'	1:A:1560:G:O2'	2.17	0.62
36:c:96:VAL:HB	36:c:97:PRO:HD3	1.82	0.62
34:a:73:C:H2'	34:a:74:A:C8	2.35	0.62
34:a:437:U:O4	34:a:495:A:C5	2.53	0.61
34:a:500:G:C8	34:a:500:G:H5''	2.35	0.61
53:t:16:ALA:O	53:t:20:ASN:HB2	2.00	0.61
1:A:272:A:C2	1:A:366:C:N3	2.69	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:185:U:C4	34:a:186:C:N4	2.68	0.61
34:a:591:U:O4	34:a:648:A:N1	2.33	0.61
34:a:186:C:N4	34:a:187:G:O6	2.33	0.61
58:z:220:ILE:HD12	58:z:226:VAL:HG21	1.82	0.61
1:A:2013:A:N6	1:A:2613:U:H3	1.98	0.61
1:A:2793:C:N3	1:A:2803:G:O6	2.34	0.61
1:A:272:A:N1	1:A:366:C:N3	2.49	0.61
1:A:714:U:H2'	1:A:716:A:N7	2.16	0.60
43:j:57:VAL:HG12	43:j:58:ASN:H	1.66	0.60
43:j:88:MET:C	43:j:90:LEU:H	1.97	0.60
53:t:11:ILE:CG1	53:t:12:GLN:N	2.64	0.60
1:A:1795:C:H2'	1:A:1796:U:O4'	2.00	0.60
1:A:368:A:H5''	1:A:368:A:H8	1.65	0.60
1:A:406:G:H2'	1:A:407:G:C8	2.36	0.60
5:E:46:GLN:HB3	5:E:83:VAL:HG11	1.83	0.60
34:a:544:G:H2'	34:a:545:C:O4'	2.02	0.60
1:A:1747:U:H2'	1:A:1748:C:C6	2.36	0.60
34:a:75:G:N2	34:a:96:U:C4	2.70	0.60
34:a:372:C:N4	34:a:389:A:N7	2.50	0.60
3:C:153:LEU:HD13	3:C:175:LEU:HD21	1.84	0.60
34:a:26:A:N6	34:a:558:G:H1'	2.17	0.60
34:a:325:A:H2'	34:a:326:G:O4'	2.01	0.60
34:a:532:A:N6	34:a:1206:G:O2'	2.35	0.59
34:a:1258:G:H2'	34:a:1259:C:C6	2.37	0.59
34:a:84:U:O5'	34:a:84:U:H6	1.85	0.59
42:i:126:PHE:CE1	42:i:128:LYS:HG3	2.27	0.59
64:a:2122:HOH:O	52:s:69:LYS:HD3	2.02	0.59
1:A:1492:G:C2	1:A:1499:C:C2	2.90	0.59
39:f:38:ARG:O	39:f:62:MET:O	2.19	0.59
42:i:44:ARG:O	42:i:47:VAL:HG22	2.02	0.59
1:A:563:A:OP1	17:Q:40:LYS:NZ	2.25	0.59
1:A:1141:U:OP1	10:J:27:ARG:NH1	2.36	0.59
1:A:1271:G:O2'	1:A:1618:6MZ:H8	2.03	0.59
34:a:827:U:N3	34:a:872:A:C6	2.59	0.59
1:A:803:U:H2'	1:A:804:A:H5'	1.84	0.58
39:f:38:ARG:HG3	39:f:63:ASN:HB3	1.83	0.58
34:a:1346:A:C6	40:g:9:ARG:NH2	2.72	0.58
1:A:2357:G:OP1	23:W:16:ARG:NH2	2.37	0.58
34:a:17:U:H2'	34:a:18:C:C6	2.38	0.58
1:A:1422:G:H22	1:A:1498:C:H1'	1.69	0.58
1:A:771:G:H8	1:A:771:G:H5''	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2638:G:O2'	1:A:2639:A:O5'	2.22	0.58
34:a:246:A:N1	34:a:278:G:O2'	2.34	0.58
34:a:1256:A:N6	34:a:1278:G:O4'	2.37	0.58
46:m:15:VAL:HG23	46:m:16:ILE:HD12	1.85	0.58
1:A:585:G:N7	17:Q:5:ARG:NH1	2.51	0.58
9:I:91:LYS:O	9:I:95:ASP:N	2.37	0.58
34:a:827:U:H2'	34:a:870:U:O4	2.04	0.58
34:a:500:G:N2	34:a:501:C:C2	2.73	0.57
1:A:231:A:N7	1:A:232:G:C6	2.73	0.57
23:W:15:LYS:HB3	23:W:17:LEU:HG	1.86	0.57
38:e:93:VAL:HG13	38:e:110:MET:HE3	1.86	0.57
50:q:63:CYS:SG	50:q:64:ARG:N	2.78	0.57
55:w:18:G:C2	55:w:58:A:C5	2.92	0.57
1:A:709:U:O4	1:A:721:A:N6	2.37	0.57
55:w:18:G:O2'	55:w:19:G:O5'	2.21	0.57
1:A:160:A:N3	1:A:2208:C:O2'	2.37	0.57
1:A:362:A:N7	1:A:363:G:O6	2.36	0.57
34:a:29:U:O4	34:a:554:A:N1	2.37	0.57
34:a:406:G:C2	34:a:495:A:N6	2.72	0.57
34:a:437:U:O4	34:a:495:A:C6	2.56	0.57
34:a:149:A:O2'	34:a:1446:A:N3	2.31	0.57
1:A:715:A:H2'	1:A:716:A:O4'	2.04	0.57
53:t:59:ARG:O	53:t:63:LYS:HD3	2.04	0.57
1:A:287:G:N7	1:A:352:A:N1	2.52	0.57
1:A:1216:G:H5''	17:Q:10:ARG:NH2	2.20	0.57
34:a:500:G:N1	34:a:501:C:N3	2.53	0.57
43:j:88:MET:C	43:j:90:LEU:N	2.60	0.57
1:A:1615:C:H2'	1:A:1617:C:C5	2.40	0.56
23:W:71:LYS:HB2	23:W:73:ARG:HG3	1.86	0.56
39:f:29:ILE:HG21	39:f:64:VAL:HG21	1.87	0.56
1:A:406:G:H2'	1:A:407:G:H8	1.70	0.56
1:A:597:G:C6	1:A:661:A:N6	2.73	0.56
1:A:1492:G:C2	1:A:1499:C:O2	2.59	0.56
2:B:39:A:O2'	2:B:46:A:N1	2.37	0.56
1:A:362:A:C8	1:A:363:G:C6	2.93	0.56
1:A:78:U:C2	1:A:108:G:O6	2.55	0.56
34:a:515:G:O2'	34:a:516:PSU:OP1	2.21	0.56
1:A:1919:A:N1	34:a:1495:U:O2'	2.30	0.56
53:t:11:ILE:HG12	53:t:12:GLN:H	1.71	0.56
34:a:515:G:H3'	34:a:515:G:N3	2.20	0.56
55:w:19:G:O2'	55:w:20:H2U:H62	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:143:A:C2	34:a:220:G:C6	2.74	0.55
34:a:500:G:C2	34:a:501:C:C2	2.93	0.55
34:a:513:C:O2	34:a:514:C:C2	2.59	0.55
34:a:553:A:H2'	34:a:554:A:C8	2.41	0.55
1:A:12:U:H2'	1:A:12:U:O2	2.07	0.55
1:A:230:G:C2	1:A:231:A:N3	2.75	0.55
24:X:3:VAL:HG22	24:X:10:ARG:HG3	1.88	0.55
42:i:94:ARG:O	42:i:98:ARG:HB2	2.06	0.55
55:w:59:A:OP1	55:w:60:U:H5	1.89	0.55
34:a:502:A:OP1	45:l:113:ARG:N	2.38	0.55
1:A:2531:A:N3	1:A:2659:G:H5'	2.21	0.55
34:a:437:U:H2'	34:a:437:U:O2	2.07	0.55
1:A:2327:A:H2'	1:A:2328:A:C8	2.42	0.55
34:a:66:A:O4'	34:a:173:U:N3	2.39	0.55
34:a:864:A:H2'	34:a:865:A:C8	2.41	0.55
53:t:11:ILE:CG1	53:t:12:GLN:H	2.19	0.55
34:a:85:U:C5'	34:a:86:G:OP1	2.54	0.55
1:A:2038:G:H2'	1:A:2039:U:O4'	2.07	0.55
34:a:976:G:C8	34:a:1358:U:O2	2.60	0.55
34:a:1235:U:H2'	34:a:1236:A:O4'	2.06	0.55
1:A:271:G:C5	1:A:367:G:C2	2.94	0.55
1:A:1063:G:N2	9:I:134:SER:O	2.39	0.55
1:A:406:G:C2'	1:A:407:G:O4'	2.54	0.54
1:A:1153:C:OP1	17:Q:91:ARG:NH2	2.36	0.54
1:A:1715:G:H8	1:A:1715:G:H5''	1.72	0.54
34:a:149:A:O2'	34:a:1446:A:C2	2.58	0.54
1:A:710:U:H3	1:A:721:A:H61	1.55	0.54
1:A:1466:U:O2'	1:A:1546:G:O2'	2.24	0.54
34:a:852:G:H5''	34:a:852:G:H8	1.72	0.54
29:2:12:ARG:HE	29:2:44:VAL:HG21	1.71	0.54
34:a:74:A:C2	34:a:97:G:C2	2.94	0.54
16:P:59:THR:HG22	16:P:72:VAL:HG22	1.89	0.54
1:A:362:A:C8	1:A:363:G:C5	2.95	0.54
34:a:1346:A:N6	40:g:9:ARG:NH2	2.56	0.54
55:w:59:A:OP1	55:w:60:U:C5	2.60	0.54
1:A:710:U:O2	1:A:721:A:C2	2.61	0.54
1:A:2638:G:O2'	1:A:2639:A:P	2.66	0.54
34:a:515:G:N3	34:a:515:G:C5'	2.70	0.54
34:a:1241:G:H2'	34:a:1242:G:C8	2.43	0.54
1:A:406:G:O2'	1:A:407:G:O4'	2.25	0.54
34:a:113:G:H21	34:a:353:A:C2'	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:219:U:C3'	34:a:220:G:H5'	2.35	0.54
34:a:1218:C:H2'	34:a:1219:A:C8	2.43	0.54
1:A:78:U:O2	1:A:108:G:C6	2.61	0.54
34:a:97:G:H2'	34:a:98:A:O4'	2.08	0.54
34:a:442:G:C5	34:a:443:C:C5	2.95	0.54
1:A:1062:G:H4'	9:I:77:VAL:HG13	1.90	0.53
34:a:322:C:C2'	34:a:323:U:H5'	2.38	0.53
34:a:601:G:H2'	34:a:602:A:O4'	2.08	0.53
1:A:710:U:C2	1:A:721:A:N1	2.76	0.53
1:A:1048:A:N1	1:A:1111:A:C6	2.75	0.53
1:A:597:G:C2	1:A:661:A:C6	2.96	0.53
1:A:1061:U:H2'	1:A:1061:U:O2	2.09	0.53
1:A:465:G:H2'	1:A:466:A:C8	2.44	0.53
34:a:136:C:C2'	34:a:137:U:H5'	2.38	0.53
1:A:286:U:C2	1:A:354:A:N6	2.77	0.53
1:A:1181:U:H2'	1:A:1182:G:C8	2.44	0.53
13:M:50:ARG:HD3	13:M:65:ILE:HD11	1.90	0.53
34:a:543:U:C4	34:a:544:G:N1	2.44	0.53
1:A:1107:G:OP1	32:5:59:LEU:N	2.42	0.53
34:a:367:U:O2	34:a:367:U:C2'	2.57	0.53
1:A:2795:C:N3	1:A:2801:G:O6	2.42	0.53
1:A:1062:G:C2	1:A:1063:G:N2	2.77	0.53
1:A:1466:U:HO2'	1:A:1546:G:HO2'	1.54	0.53
1:A:1741:C:C5	1:A:1742:U:C5	2.97	0.53
1:A:362:A:H4'	1:A:363:G:OP2	2.09	0.53
1:A:1737:G:H2'	1:A:1738:G:H1'	1.92	0.53
1:A:1081:U:O2'	9:I:123:ALA:HB1	2.09	0.52
1:A:1809:A:H2'	1:A:1810:A:C8	2.44	0.52
1:A:290:U:C2	1:A:291:G:C8	2.96	0.52
10:J:35:ARG:HB2	10:J:54:ILE:HD11	1.91	0.52
1:A:1688:U:O2'	1:A:1700:A:N7	2.40	0.52
34:a:602:A:N6	34:a:635:A:N6	2.57	0.52
34:a:72:A:N7	34:a:73:C:C5	2.78	0.52
34:a:442:G:C6	34:a:443:C:C4	2.98	0.52
1:A:82:U:O2	1:A:82:U:O4'	2.28	0.52
1:A:910:A:N3	1:A:2264:C:O2'	2.40	0.52
34:a:545:C:C5	34:a:546:A:N7	2.78	0.52
1:A:272:A:C2	1:A:366:C:O2	2.62	0.52
1:A:1874:C:H2'	1:A:1875:G:O4'	2.09	0.52
34:a:1:A:H5'	34:a:2:A:OP2	2.10	0.52
34:a:518:C:O4'	34:a:518:C:O2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:G:C2	1:A:366:C:N3	2.77	0.52
34:a:760:G:H5''	34:a:760:G:H8	1.75	0.52
1:A:2031:A:C6	1:A:2498:OMC:H1'	2.45	0.51
34:a:600:A:O2'	34:a:601:G:H5''	2.10	0.51
24:X:10:ARG:HG2	24:X:11:PRO:CD	2.40	0.51
57:y:18:G:O2'	57:y:57:G:N2	2.43	0.51
1:A:1496:A:C2	1:A:1498:C:C2	2.97	0.51
24:X:10:ARG:HG2	24:X:11:PRO:HD2	1.92	0.51
34:a:171:A:H2'	34:a:172:A:C8	2.45	0.51
34:a:136:C:H2'	34:a:137:U:H5'	1.93	0.51
1:A:27:G:N2	1:A:512:G:H1'	2.25	0.51
1:A:780:G:OP1	3:C:216:ARG:NH2	2.44	0.51
1:A:1721:G:O2'	1:A:1739:A:N6	2.44	0.51
34:a:513:C:H2'	34:a:514:C:C6	2.46	0.51
34:a:539:A:N6	34:a:540:G:N1	2.59	0.51
1:A:1741:C:H6	1:A:1741:C:C5'	2.24	0.51
1:A:2028:U:C2'	1:A:2029:G:C8	2.92	0.51
9:I:109:ALA:HA	9:I:128:ILE:HG21	1.93	0.51
34:a:136:C:O2'	34:a:137:U:H5'	2.11	0.51
1:A:427:U:O2	1:A:427:U:H5''	2.10	0.51
1:A:1980:G:O2'	1:A:1982:U:OP2	2.24	0.51
34:a:83:C:N3	34:a:85:U:O4	2.43	0.51
1:A:2262:U:P	23:W:15:LYS:NZ	2.83	0.51
55:w:18:G:O2'	55:w:19:G:P	2.68	0.51
48:o:44:GLU:CG	48:o:45:HIS:HD2	2.04	0.51
1:A:1363:C:O2'	1:A:1809:A:N3	2.39	0.50
1:A:1794:A:H2'	1:A:1795:C:C6	2.45	0.50
1:A:2028:U:H2'	1:A:2029:G:H8	1.70	0.50
18:R:51:VAL:HG12	18:R:52:PRO:HD3	1.94	0.50
1:A:212:G:H2'	1:A:213:A:O4'	2.11	0.50
1:A:1492:G:N2	1:A:1499:C:C2	2.79	0.50
1:A:2757:A:N1	7:G:66:THR:OG1	2.43	0.50
1:A:2405:G:O2'	1:A:2411:A:N6	2.44	0.50
34:a:1389:C:H2'	34:a:1390:U:O4'	2.11	0.50
37:d:72:ARG:HG2	37:d:72:ARG:HH21	1.76	0.50
1:A:231:A:N6	1:A:232:G:C2	2.79	0.50
34:a:322:C:H2'	34:a:323:U:H5'	1.94	0.50
34:a:946:A:H2'	34:a:947:G:C8	2.47	0.50
1:A:1615:C:H2'	1:A:1617:C:H5	1.77	0.50
34:a:509:A:N7	34:a:510:A:C6	2.79	0.50
1:A:1076:C:N4	1:A:1077:A:N1	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2734:A:C3'	1:A:2735:G:H5'	2.42	0.50
23:W:16:ARG:HD3	23:W:16:ARG:N	2.27	0.50
1:A:1642:G:H2'	1:A:1643:G:O4'	2.11	0.49
1:A:2780:G:O6	10:J:99:ARG:NH2	2.45	0.49
34:a:675:A:H2'	34:a:676:A:O4'	2.11	0.49
1:A:230:G:C6	1:A:231:A:C2	3.00	0.49
1:A:2029:G:H8	1:A:2029:G:O5'	1.95	0.49
1:A:2805:C:H2'	1:A:2806:C:O4'	2.11	0.49
34:a:459:A:H2'	34:a:460:A:O4'	2.13	0.49
34:a:515:G:N3	34:a:515:G:H5'	2.26	0.49
42:i:128:LYS:O	42:i:129:ARG:HB2	2.11	0.49
34:a:437:U:C2	34:a:495:A:N6	2.80	0.49
1:A:215:G:H4'	1:A:216:A:H4'	1.94	0.49
1:A:2572:A:P	4:D:151:THR:HG1	2.35	0.49
34:a:331:G:C2	53:t:4:LYS:NZ	2.80	0.49
34:a:530:G:N2	57:y:35:A:C2	2.80	0.49
34:a:876:C:H1'	41:h:11:THR:HG21	1.93	0.49
53:t:26:MET:HE3	53:t:56:ILE:HG12	1.94	0.49
54:u:9:GLU:HB2	54:u:10:PRO:HD3	1.94	0.49
34:a:331:G:N2	53:t:4:LYS:NZ	2.60	0.49
34:a:1305:G:O2'	34:a:1306:A:OP2	2.24	0.49
41:h:77:VAL:HG11	41:h:124:ILE:HD12	1.95	0.49
34:a:220:G:H2'	34:a:221:C:C6	2.47	0.49
1:A:1049:C:H2'	1:A:1050:A:H5'	1.93	0.49
1:A:1914:C:O2	1:A:1914:C:O4'	2.27	0.49
12:L:77:ILE:CD1	12:L:108:ALA:HB1	2.43	0.49
34:a:226:G:N2	34:a:227:G:H1'	2.27	0.49
53:t:11:ILE:HG13	53:t:12:GLN:N	2.27	0.49
1:A:283:G:N2	1:A:359:G:N2	2.61	0.49
1:A:348:A:H2'	1:A:349:U:O4'	2.13	0.49
19:S:15:GLN:OE1	27:0:16:ARG:CZ	2.60	0.49
52:s:10:ILE:HD12	52:s:40:PHE:CE2	2.48	0.49
34:a:362:G:OP1	45:l:57:THR:OG1	2.31	0.48
1:A:1747:U:H2'	1:A:1748:C:H6	1.78	0.48
1:A:2020:A:N7	27:0:5:ASN:ND2	2.60	0.48
14:N:71:ARG:HA	14:N:71:ARG:HD2	1.70	0.48
1:A:2838:G:H2'	1:A:2839:G:O4'	2.13	0.48
34:a:927:G:O2'	34:a:1503:A:N7	2.46	0.48
1:A:749:A:C8	1:A:1618:6MZ:C6	2.97	0.48
1:A:2886:A:N1	27:0:39:ARG:HD3	2.28	0.48
1:A:1737:G:H2'	1:A:1738:G:C1'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:23:ILE:HD13	7:G:71:LEU:HD21	1.96	0.48
11:K:19:VAL:HB	11:K:41:ILE:HG23	1.96	0.48
15:O:63:LYS:HG3	15:O:64:TYR:N	2.28	0.48
34:a:711:G:OP2	39:f:53:LYS:NZ	2.47	0.48
34:a:1162:C:H2'	34:a:1163:A:C8	2.48	0.48
53:t:11:ILE:O	53:t:14:GLU:N	2.47	0.48
34:a:218:U:H2'	34:a:219:U:O4'	2.14	0.48
34:a:533:A:N3	34:a:535:A:OP2	2.46	0.48
34:a:778:G:H2'	34:a:779:C:O4'	2.14	0.48
34:a:1456:A:H2'	34:a:1457:G:O4'	2.14	0.48
34:a:140:U:H3	34:a:223:A:H2	1.61	0.48
34:a:219:U:O2'	34:a:220:G:H5'	2.10	0.48
1:A:1271:G:HO2'	1:A:1618:6MZ:H8	1.79	0.48
1:A:1744:A:C4	1:A:1745:A:H1'	2.49	0.48
1:A:2031:A:C5	1:A:2498:OMC:HM23	2.49	0.48
34:a:1023:U:C2	34:a:1024:G:C8	3.01	0.48
1:A:771:G:H5''	1:A:771:G:C8	2.49	0.48
1:A:1060:U:H5'	9:I:74:PRO:HB3	1.95	0.48
1:A:1061:U:H4'	1:A:1070:A:C4	2.49	0.48
23:W:70:PRO:C	23:W:72:ASN:H	2.22	0.48
55:w:18:G:C6	55:w:58:A:C6	3.01	0.48
34:a:369:G:H2'	34:a:393:A:H2	1.72	0.47
42:i:45:MET:C	42:i:47:VAL:N	2.72	0.47
55:w:48:C:C4	55:w:59:A:C8	3.02	0.47
1:A:271:G:C6	1:A:367:G:C6	3.02	0.47
34:a:513:C:O2'	34:a:514:C:O4'	2.30	0.47
34:a:1391:U:H2'	34:a:1392:G:C8	2.49	0.47
36:c:148:ILE:O	36:c:148:ILE:HG23	2.15	0.47
1:A:271:G:C6	1:A:367:G:C2	3.02	0.47
1:A:1106:G:N3	32:5:81:LEU:HD12	2.30	0.47
34:a:72:A:H2'	34:a:72:A:N3	2.30	0.47
34:a:109:A:C6	34:a:326:G:C6	3.02	0.47
34:a:1486:G:H2'	34:a:1487:G:O4'	2.14	0.47
34:a:1490:U:H2'	34:a:1491:G:H5'	1.97	0.47
1:A:214:G:HO2'	1:A:216:A:HO2'	1.57	0.47
1:A:1064:C:C5'	9:I:87:SER:HA	2.44	0.47
34:a:75:G:C2	34:a:96:U:C4	3.03	0.47
34:a:440:C:H2'	34:a:440:C:O2	2.13	0.47
34:a:456:A:H2'	34:a:457:G:O4'	2.13	0.47
34:a:515:G:N3	34:a:515:G:C3'	2.77	0.47
34:a:547:A:H1'	34:a:548:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:G:N2	1:A:1452:G:O6	2.43	0.47
34:a:211:G:N3	34:a:211:G:H2'	2.29	0.47
34:a:759:A:H3'	34:a:760:G:H5''	1.96	0.47
52:s:10:ILE:HD12	52:s:40:PHE:CD2	2.49	0.47
1:A:273:G:C8	1:A:365:U:C4	3.03	0.47
1:A:1076:C:O2	9:I:92:PRO:HD2	2.14	0.47
1:A:1272:A:C2	1:A:1618:6MZ:C2	2.98	0.47
1:A:2811:G:O6	1:A:2889:C:N3	2.48	0.47
6:F:134:GLN:HB3	6:F:140:ILE:HD13	1.97	0.47
32:5:59:LEU:O	32:5:61:ARG:N	2.47	0.47
34:a:125:U:O3'	34:a:633:G:N2	2.48	0.47
34:a:600:A:C3'	34:a:601:G:C5'	2.92	0.47
34:a:1125:U:H2'	34:a:1126:U:H2'	1.96	0.47
1:A:715:A:H2'	1:A:716:A:C8	2.49	0.47
1:A:2030:6MZ:OP2	1:A:2031:A:C8	2.68	0.47
1:A:2405:G:O2'	1:A:2412:A:N6	2.48	0.47
34:a:473:U:C2	34:a:474:G:C8	3.02	0.47
3:C:203:VAL:O	3:C:205:GLY:N	2.48	0.47
34:a:57:G:H2'	34:a:58:C:O4'	2.14	0.47
34:a:331:G:O2'	53:t:3:ILE:HD12	2.15	0.47
34:a:668:G:N2	48:o:45:HIS:HE1	2.01	0.47
53:t:3:ILE:HG22	53:t:4:LYS:HD2	1.95	0.47
34:a:26:A:H61	34:a:558:G:H1'	1.80	0.46
34:a:182:A:N7	34:a:223:A:O2'	2.49	0.46
34:a:442:G:N2	34:a:493:A:C2	2.83	0.46
34:a:651:C:H3'	34:a:652:U:C6	2.49	0.46
42:i:83:THR:HG21	42:i:102:PHE:HB3	1.96	0.46
34:a:868:C:H2'	34:a:869:G:O4'	2.15	0.46
1:A:1182:G:H2'	1:A:1183:U:O4'	2.15	0.46
58:z:140:VAL:HG11	58:z:145:LEU:HD22	1.97	0.46
1:A:287:G:O4'	1:A:354:A:C6	2.68	0.46
1:A:529:A:OP2	10:J:113:PRO:HD3	2.16	0.46
1:A:2663:G:C6	1:A:2664:G:C5	3.03	0.46
1:A:2788:C:H2'	1:A:2789:C:H6	1.78	0.46
20:T:61:LEU:HG	20:T:82:LYS:HG2	1.97	0.46
34:a:72:A:C5	34:a:73:C:C6	3.04	0.46
58:z:84:ALA:HB3	58:z:87:TYR:CD2	2.50	0.46
34:a:77:A:C6	34:a:78:A:N6	2.84	0.46
1:A:804:A:H2'	1:A:806:C:C4	2.51	0.46
6:F:97:GLU:HG2	33:6:25:ARG:HG2	1.96	0.46
34:a:515:G:N1	34:a:517:G:C6	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:G:H2'	1:A:554:U:O4'	2.15	0.46
1:A:571:U:C4	1:A:2030:6MZ:C6	2.99	0.46
1:A:1432:G:H2'	1:A:1433:A:C8	2.50	0.46
1:A:2070:A:H2'	1:A:2071:A:O4'	2.15	0.46
34:a:143:A:N1	34:a:220:G:O6	2.43	0.46
49:p:12:LYS:HG2	49:p:13:LYS:HG2	1.97	0.46
54:u:9:GLU:HB2	54:u:10:PRO:CD	2.45	0.46
1:A:271:G:C2	1:A:367:G:C4	3.04	0.46
34:a:126:G:H5'	34:a:633:G:N2	2.31	0.46
34:a:518:C:C5	34:a:530:G:N7	2.84	0.46
34:a:1442:G:H2'	34:a:1443:C:C6	2.51	0.46
1:A:282:A:C6	1:A:359:G:N2	2.84	0.46
1:A:471:A:OP1	5:E:79:ARG:NH2	2.49	0.46
1:A:1027:A:O5'	1:A:1027:A:H8	1.98	0.46
1:A:1050:A:H2'	1:A:1051:G:O4'	2.16	0.46
1:A:1595:C:H2'	1:A:1596:A:O4'	2.16	0.46
1:A:2262:U:OP1	23:W:15:LYS:NZ	2.49	0.46
22:V:30:ILE:HG23	22:V:72:VAL:HG11	1.98	0.46
34:a:246:A:H4'	34:a:247:G:OP1	2.14	0.46
34:a:510:A:N3	34:a:543:U:H1'	2.31	0.46
1:A:362:A:H3'	1:A:363:G:O4'	2.16	0.46
1:A:2212:A:C2	1:A:2214:C:N4	2.84	0.46
11:K:98:ARG:HB3	11:K:98:ARG:HH11	1.81	0.46
11:K:110:GLU:C	11:K:112:PHE:H	2.24	0.46
34:a:340:U:C4	34:a:341:C:N3	2.84	0.46
51:r:20:ILE:HG21	51:r:54:LEU:HA	1.98	0.46
1:A:2773:C:P	4:D:169:ARG:NH1	2.89	0.45
38:e:12:GLU:HB2	38:e:38:VAL:HG12	1.97	0.45
9:I:91:LYS:N	9:I:92:PRO:HD3	2.30	0.45
34:a:504:C:H2'	34:a:511:C:H5	1.81	0.45
1:A:573:U:O4	1:A:2029:G:O2'	2.32	0.45
4:D:25:THR:HG21	4:D:193:VAL:HG22	1.99	0.45
34:a:126:G:H2'	34:a:127:G:O4'	2.15	0.45
34:a:136:C:H2'	34:a:137:U:C5'	2.47	0.45
34:a:1002:G:H2'	34:a:1003:G:O4'	2.16	0.45
37:d:72:ARG:HH21	37:d:72:ARG:CG	2.29	0.45
1:A:362:A:N7	1:A:363:G:C5	2.85	0.45
1:A:2031:A:C8	1:A:2498:OMC:HM21	2.51	0.45
6:F:91:ARG:HA	6:F:95:MET:HB2	1.98	0.45
46:m:94:LEU:HD22	46:m:101:THR:HG21	1.99	0.45
1:A:466:A:OP1	29:2:34:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1618:6MZ:H2'	1:A:1618:6MZ:N3	2.30	0.45
1:A:2273:A:H2'	1:A:2274:A:C8	2.51	0.45
11:K:34:GLY:O	11:K:36:GLY:N	2.49	0.45
34:a:77:A:N1	34:a:78:A:N6	2.64	0.45
34:a:499:A:O2'	34:a:547:A:N6	2.49	0.45
34:a:1127:G:H1'	34:a:1280:A:C6	2.51	0.45
1:A:1049:C:H5''	1:A:1049:C:H6	1.82	0.45
9:I:74:PRO:HG2	9:I:77:VAL:HG22	1.98	0.45
19:S:5:ALA:HB3	19:S:54:ALA:HB2	1.99	0.45
34:a:112:G:N2	34:a:354:G:OP2	2.45	0.45
34:a:129:A:N1	34:a:232:G:C6	2.84	0.45
34:a:633:G:H2'	34:a:634:C:O4'	2.17	0.45
34:a:890:G:O2'	34:a:906:A:N6	2.49	0.45
1:A:735:A:C8	1:A:736:C:C5	3.05	0.45
1:A:2514:U:H2'	1:A:2515:C:C6	2.52	0.45
1:A:803:U:C2'	1:A:804:A:H5'	2.47	0.45
1:A:1430:G:H2'	1:A:1431:A:O4'	2.16	0.45
1:A:2883:A:H5'	1:A:2884:U:H5'	1.98	0.45
11:K:111:LYS:HB3	11:K:111:LYS:HE3	1.47	0.45
18:R:51:VAL:HB	18:R:52:PRO:CD	2.47	0.45
34:a:600:A:C3'	34:a:601:G:H5''	2.47	0.45
1:A:1061:U:N3	9:I:53:PRO:HB2	2.31	0.45
6:F:94:ARG:HD3	33:6:9:TYR:CE2	2.51	0.45
12:L:78:ARG:HG2	12:L:113:ALA:CB	2.47	0.45
34:a:61:G:H2'	34:a:62:U:O4'	2.16	0.44
34:a:203:G:N2	34:a:204:G:O6	2.50	0.44
1:A:2028:U:C4	1:A:2029:G:C5	3.06	0.44
34:a:2:A:C6	34:a:3:A:N1	2.85	0.44
34:a:367:U:O2	34:a:367:U:H2'	2.16	0.44
1:A:157:C:C4	1:A:169:G:O6	2.70	0.44
1:A:749:A:H1'	1:A:1618:6MZ:OP1	2.17	0.44
8:H:90:LEU:CD2	8:H:94:ILE:HD11	2.48	0.44
34:a:167:A:H2'	34:a:168:G:O4'	2.17	0.44
34:a:827:U:N3	34:a:874:G:C2	2.86	0.44
1:A:1057:A:N6	1:A:1080:A:N1	2.65	0.44
1:A:1062:G:H1'	9:I:76:ALA:HB3	1.99	0.44
1:A:1111:A:H2'	1:A:1112:G:H4'	2.00	0.44
1:A:1447:C:O2'	1:A:1544:A:N3	2.44	0.44
4:D:151:THR:CB	4:D:152:PRO:HD3	2.48	0.44
34:a:369:G:C2	34:a:393:A:C5	3.05	0.44
1:A:563:A:OP2	18:R:79:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1509:A:H2'	1:A:1510:G:C8	2.52	0.44
34:a:129:A:C2	34:a:233:C:O2	2.71	0.44
34:a:187:G:N2	34:a:191:G:C5	2.85	0.44
34:a:1177:G:H2'	34:a:1178:G:O4'	2.18	0.44
42:i:115:VAL:HG21	43:j:62:ARG:HB2	2.00	0.44
43:j:88:MET:HB3	43:j:89:ARG:H	1.50	0.44
1:A:2078:C:H2'	1:A:2079:U:O4'	2.18	0.44
9:I:92:PRO:HG3	9:I:136:GLY:HA3	1.99	0.44
14:N:98:LEU:HB3	27:O:42:ILE:HD11	1.99	0.44
34:a:603:U:C2	34:a:635:A:N1	2.86	0.44
1:A:265:A:H4'	1:A:266:G:OP1	2.16	0.44
1:A:538:A:H2'	1:A:539:G:O4'	2.18	0.44
1:A:597:G:C2	1:A:661:A:C5	3.05	0.44
1:A:710:U:H3	1:A:721:A:N6	2.14	0.44
1:A:1548:A:H2'	1:A:1549:A:C8	2.53	0.44
34:a:85:U:H5''	34:a:86:G:OP1	2.17	0.44
34:a:369:G:C2	34:a:393:A:C6	3.06	0.44
1:A:1076:C:O2	9:I:92:PRO:HG2	2.17	0.44
1:A:1615:C:OP2	1:A:1617:C:N4	2.31	0.44
1:A:1717:A:C8	1:A:1744:A:C6	3.05	0.44
1:A:2791:G:N1	1:A:2805:C:N3	2.58	0.44
34:a:1244:G:C6	34:a:1293:C:N4	2.85	0.44
37:d:72:ARG:NH2	37:d:203:TYR:CD1	2.86	0.44
12:L:108:ALA:HB3	12:L:125:LEU:HD11	1.99	0.43
34:a:222:C:O2	34:a:222:C:H2'	2.18	0.43
34:a:651:C:H2'	34:a:652:U:O4'	2.18	0.43
1:A:1059:G:H1'	9:I:116:MET:HE1	1.99	0.43
34:a:706:A:H2'	34:a:707:U:O4'	2.18	0.43
34:a:1356:G:H2'	34:a:1357:A:C8	2.52	0.43
1:A:2800:A:H3'	1:A:2801:G:C5'	2.48	0.43
34:a:1476:A:H2'	34:a:1477:U:O4'	2.18	0.43
51:r:10:CYS:SG	51:r:11:ARG:N	2.84	0.43
1:A:1086:A:H2'	1:A:1086:A:N3	2.33	0.43
1:A:1582:C:O2'	1:A:1585:C:N3	2.51	0.43
34:a:129:A:N1	34:a:233:C:C2	2.87	0.43
35:b:56:LEU:HD13	35:b:216:VAL:HG13	2.01	0.43
34:a:112:G:H21	34:a:354:G:H4'	1.78	0.43
36:c:63:ILE:HD13	36:c:94:ALA:HB1	2.00	0.43
1:A:1044:C:O2	1:A:1044:C:O4'	2.36	0.43
5:E:146:VAL:HG12	5:E:185:LYS:HB2	2.01	0.43
9:I:132:ALA:O	9:I:133:ARG:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:325:A:N6	34:a:326:G:C6	2.86	0.43
1:A:2323:G:H2'	1:A:2324:U:O4'	2.19	0.43
34:a:602:A:H61	34:a:636:U:H3	1.63	0.43
34:a:749:A:H2'	34:a:750:C:O4'	2.18	0.43
34:a:1498:UR3:H3U2	56:x:17:U:H4'	2.00	0.43
58:z:103:LEU:N	58:z:131:ILE:O	2.52	0.43
34:a:539:A:OP1	45:l:110:LYS:HD2	2.19	0.43
1:A:709:U:C4	1:A:710:U:C4	3.07	0.43
1:A:1491:G:C5	1:A:1500:G:C2	3.07	0.43
1:A:1715:G:H5''	1:A:1715:G:C8	2.51	0.43
1:A:1741:C:H6	1:A:1741:C:H5''	1.83	0.43
1:A:684:G:C2	1:A:794:A:C2	3.07	0.43
1:A:1327:A:N6	1:A:1328:A:C2	2.87	0.43
11:K:110:GLU:C	11:K:112:PHE:N	2.77	0.43
34:a:84:U:O5'	34:a:84:U:C6	2.71	0.43
34:a:946:A:O2'	34:a:1333:A:N3	2.42	0.43
53:t:60:GLN:HA	53:t:63:LYS:HG2	2.01	0.43
1:A:1328:A:H2'	1:A:1330:C:C5	2.54	0.42
11:K:110:GLU:O	11:K:112:PHE:N	2.52	0.42
34:a:127:G:O6	34:a:234:C:N3	2.52	0.42
1:A:631:A:N3	1:A:2415:G:O2'	2.44	0.42
1:A:987:C:O2'	1:A:1000:A:N3	2.49	0.42
1:A:1009:A:N3	1:A:1153:C:O2'	2.48	0.42
34:a:43:C:H2'	34:a:44:A:O4'	2.18	0.42
43:j:83:THR:HG22	43:j:87:LEU:HD11	2.01	0.42
1:A:273:G:O6	1:A:364:C:N3	2.51	0.42
1:A:362:A:C5	1:A:363:G:N7	2.87	0.42
1:A:1075:C:O2'	9:I:91:LYS:HA	2.19	0.42
1:A:1751:U:H2'	1:A:1752:C:C6	2.53	0.42
1:A:1802:A:H2'	1:A:1803:A:C8	2.55	0.42
21:U:33:VAL:HG13	21:U:66:VAL:HG22	2.00	0.42
34:a:673:A:H2'	34:a:674:G:C8	2.54	0.42
34:a:1244:G:H2'	34:a:1245:C:C6	2.55	0.42
56:x:19:C:O2	56:x:19:C:H2'	2.18	0.42
1:A:1021:A:N6	1:A:1141:U:H3	2.17	0.42
1:A:1149:G:H2'	1:A:1150:C:C6	2.54	0.42
1:A:2330:G:C2	1:A:2386:A:C2	3.08	0.42
2:B:37:C:C5	2:B:38:C:C5	3.07	0.42
34:a:59:A:H1'	34:a:354:G:C2	2.54	0.42
34:a:175:C:H2'	34:a:176:C:C6	2.55	0.42
34:a:345:C:O2	34:a:345:C:O4'	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:546:A:H2'	34:a:546:A:N3	2.34	0.42
34:a:782:A:H4'	34:a:1514:G:O2'	2.19	0.42
34:a:1248:A:HO2'	42:i:32:ARG:HH22	1.64	0.42
34:a:1434:A:H2'	34:a:1435:G:O4'	2.20	0.42
1:A:1482:G:O2'	1:A:1509:A:N1	2.52	0.42
34:a:37:U:H2'	34:a:38:G:O4'	2.20	0.42
34:a:401:C:H2'	34:a:402:G:C8	2.54	0.42
34:a:500:G:C2	34:a:501:C:N3	2.87	0.42
34:a:220:G:H2'	34:a:221:C:H6	1.84	0.42
17:Q:35:PHE:CZ	17:Q:39:ILE:HD11	2.55	0.42
34:a:602:A:N6	34:a:636:U:H3	2.16	0.42
44:k:108:ASN:HB3	54:u:6:ARG:HG2	2.01	0.42
1:A:215:G:C4'	1:A:216:A:H4'	2.50	0.42
1:A:2567:G:H2'	1:A:2568:U:C6	2.54	0.42
1:A:2849:U:O4	16:P:20:ARG:NH2	2.51	0.42
34:a:369:G:N2	34:a:393:A:C5	2.88	0.42
34:a:537:G:H2'	34:a:538:G:C8	2.55	0.42
34:a:1098:C:O2'	54:u:66:ARG:HD2	2.19	0.42
48:o:88:ARG:HD3	48:o:88:ARG:N	2.35	0.42
1:A:1357:C:H2'	1:A:1358:G:O4'	2.20	0.42
18:R:40:MET:HG3	18:R:48:LYS:HG2	2.00	0.42
21:U:3:LYS:HB2	21:U:4:ILE:HD12	2.02	0.42
34:a:1292:G:C6	34:a:1293:C:N4	2.88	0.42
42:i:34:LEU:HD11	42:i:47:VAL:HG21	2.01	0.42
1:A:45:G:H2'	1:A:215:G:C5	2.55	0.42
1:A:281:C:H2'	1:A:282:A:C8	2.54	0.42
1:A:715:A:C6	1:A:716:A:C6	3.08	0.42
1:A:1433:A:H2'	1:A:1434:A:C8	2.55	0.42
1:A:1469:A:H2'	1:A:1470:A:C8	2.55	0.42
1:A:1851:U:O3'	55:w:71:C:O2'	2.38	0.42
9:I:91:LYS:N	9:I:92:PRO:CD	2.83	0.42
1:A:362:A:C4'	1:A:363:G:OP2	2.68	0.41
1:A:1471:G:O6	1:A:1520:U:O4	2.38	0.41
1:A:2883:A:C5'	1:A:2884:U:H5'	2.50	0.41
23:W:67:VAL:HG12	23:W:72:ASN:OD1	2.20	0.41
29:2:35:ARG:HG3	29:2:42:LEU:HD11	2.02	0.41
34:a:537:G:H8	34:a:537:G:H5''	1.85	0.41
34:a:827:U:C2	34:a:874:G:N2	2.88	0.41
55:v:18:G:C6	55:v:57:A:N6	2.88	0.41
1:A:2645:G:OP2	1:A:2645:G:N2	2.47	0.41
34:a:141:G:O2'	34:a:142:G:O4'	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1304:G:C6	34:a:1305:G:N1	2.88	0.41
1:A:1496:A:N1	1:A:1498:C:N3	2.68	0.41
1:A:1505:A:H2'	1:A:1506:U:O4'	2.20	0.41
1:A:2615:U:C2	27:0:3:GLN:HA	2.55	0.41
3:C:159:THR:HG23	3:C:176:ARG:HG3	2.02	0.41
34:a:1243:C:N3	34:a:1294:G:O6	2.53	0.41
34:a:1244:G:N1	34:a:1293:C:N4	2.68	0.41
40:g:107:ALA:HB1	40:g:115:MET:HE1	2.01	0.41
1:A:784:G:H5'	1:A:785:G:OP1	2.20	0.41
1:A:1028:A:N6	1:A:1125:G:H2'	2.35	0.41
19:S:23:LEU:HD11	27:0:21:LEU:HD11	2.02	0.41
34:a:529:G:O6	45:l:45:ASN:HA	2.20	0.41
34:a:969:A:H62	42:i:129:ARG:HD2	1.84	0.41
34:a:1295:U:H2'	34:a:1296:C:O4'	2.20	0.41
2:B:79:G:H2'	2:B:80:U:O4'	2.21	0.41
10:J:4:PHE:O	17:Q:63:ARG:NH2	2.53	0.41
19:S:24:ILE:HD11	19:S:36:LEU:HG	2.03	0.41
32:5:64:VAL:HG12	32:5:64:VAL:O	2.20	0.41
34:a:953:G:H2'	34:a:954:G:O4'	2.20	0.41
44:k:87:GLY:O	44:k:92:ARG:NH1	2.54	0.41
52:s:49:ALA:HB1	52:s:56:HIS:HB3	2.03	0.41
1:A:639:U:H2'	1:A:640:C:C6	2.56	0.41
1:A:756:A:H2'	1:A:757:G:O4'	2.20	0.41
5:E:21:ARG:HD3	5:E:106:LYS:HB3	2.02	0.41
17:Q:93:ILE:HD13	18:R:4:VAL:HG13	2.02	0.41
1:A:308:G:H2'	1:A:309:A:C8	2.55	0.41
9:I:21:PRO:HA	57:y:56:C:C1'	2.50	0.41
34:a:27:G:C6	34:a:557:G:C2	3.09	0.41
34:a:219:U:C2'	34:a:220:G:C5'	2.69	0.41
34:a:299:G:H2'	34:a:300:A:C8	2.56	0.41
34:a:540:G:H2'	34:a:541:G:C8	2.56	0.41
34:a:760:G:H8	34:a:760:G:C5'	2.33	0.41
38:e:108:GLY:O	38:e:109:ALA:HB3	2.21	0.41
39:f:29:ILE:HG21	39:f:64:VAL:CG2	2.49	0.41
48:o:46:LYS:HB3	48:o:47:LYS:H	1.48	0.41
54:u:12:ASP:O	54:u:14:ALA:N	2.54	0.41
1:A:289:G:C2	1:A:290:U:H1'	2.56	0.41
1:A:1048:A:N7	1:A:1049:C:H5	2.13	0.41
1:A:2313:C:H5''	6:F:87:LYS:HD2	2.03	0.41
14:N:58:ASP:OD1	14:N:63:ARG:NH1	2.54	0.41
16:P:91:VAL:HG11	16:P:96:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:49:ASP:OD1	25:Y:52:ARG:NH2	2.54	0.41
34:a:46:G:O2'	34:a:365:U:H1'	2.21	0.41
34:a:346:G:N3	34:a:346:G:H3'	2.36	0.41
34:a:635:A:H2'	34:a:636:U:O4'	2.20	0.41
34:a:909:A:H2'	34:a:910:C:O4'	2.20	0.41
34:a:1265:C:H3'	34:a:1266:G:H5''	2.03	0.41
35:b:183:PHE:HB3	35:b:197:PHE:HB2	2.03	0.41
45:l:98:ARG:HB2	45:l:116:TYR:HA	2.02	0.41
1:A:157:C:C4	1:A:169:G:C6	3.09	0.41
1:A:819:A:C4	1:A:1189:A:C2	3.09	0.41
1:A:974:G:N3	1:A:974:G:H2'	2.36	0.41
1:A:1320:C:N3	1:A:1331:G:O6	2.53	0.41
1:A:1779:U:H5	1:A:1784:A:N7	2.19	0.41
1:A:2734:A:H3'	1:A:2735:G:H5'	2.02	0.41
11:K:38:ILE:HD13	11:K:61:VAL:HG13	2.03	0.41
34:a:180:U:O2	34:a:195:A:N7	2.53	0.41
34:a:376:G:OP1	49:p:5:ARG:HB2	2.21	0.41
54:u:36:PHE:O	54:u:38:GLU:N	2.54	0.41
58:z:337:VAL:HG11	58:z:366:ILE:HD12	2.03	0.41
1:A:232:G:H22	1:A:420:C:H5'	1.86	0.41
1:A:596:U:N3	1:A:661:A:N6	2.41	0.41
1:A:714:U:H5''	1:A:714:U:C6	2.55	0.41
11:K:24:VAL:HG13	11:K:33:ALA:HB2	2.03	0.41
11:K:98:ARG:HB3	11:K:98:ARG:NH1	2.36	0.41
12:L:78:ARG:HG2	12:L:113:ALA:HB2	2.02	0.41
23:W:55:LEU:HD12	23:W:76:ILE:HD12	2.03	0.41
34:a:53:A:H2'	34:a:54:C:O4'	2.21	0.41
1:A:2570:G:H2'	1:A:2571:U:O4'	2.21	0.40
1:A:2884:U:C5	27:0:49:ARG:HG2	2.55	0.40
34:a:392:C:H2'	34:a:393:A:C8	2.56	0.40
34:a:605:U:N3	34:a:606:G:N7	2.69	0.40
42:i:98:ARG:HG3	42:i:103:VAL:HG21	2.02	0.40
6:F:30:VAL:HG12	6:F:95:MET:CE	2.52	0.40
34:a:186:C:N4	34:a:187:G:C6	2.89	0.40
34:a:397:A:H3'	34:a:397:A:N3	2.36	0.40
1:A:1327:A:H2'	1:A:1328:A:O4'	2.20	0.40
1:A:1727:A:C2	1:A:1728:C:C2	3.08	0.40
1:A:1964:G:H4'	1:A:1965:C:OP2	2.22	0.40
1:A:2029:G:C8	1:A:2029:G:O5'	2.73	0.40
34:a:75:G:N2	34:a:97:G:N1	2.70	0.40
34:a:187:G:C2	34:a:191:G:C6	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:219:U:C4	34:a:220:G:N7	2.89	0.40
34:a:603:U:H3	34:a:635:A:N6	2.19	0.40
1:A:80:G:C6	1:A:106:C:N3	2.89	0.40
1:A:597:G:C5	1:A:661:A:N6	2.90	0.40
1:A:1248:G:OP1	5:E:44:ARG:NH1	2.55	0.40
1:A:1528:A:H2'	1:A:1529:G:O4'	2.20	0.40
1:A:1591:A:H2'	1:A:1592:C:C6	2.57	0.40
1:A:1881:C:H2'	1:A:1882:U:O4'	2.22	0.40
1:A:2500:U:O2	1:A:2504:PSU:C2	2.74	0.40
3:C:131:MET:HE1	3:C:173:LEU:HD11	2.02	0.40
34:a:504:C:H2'	34:a:511:C:C5	2.56	0.40
34:a:1125:U:O2	34:a:1125:U:C2'	2.69	0.40
37:d:23:GLY:HA2	37:d:108:ALA:HB1	2.04	0.40
1:A:38:A:H2'	1:A:39:G:O4'	2.21	0.40
1:A:1061:U:O4	9:I:74:PRO:HD3	2.22	0.40
1:A:1720:U:O2	1:A:1740:G:O6	2.39	0.40
1:A:1853:A:H2'	1:A:1854:A:O4'	2.21	0.40
3:C:143:VAL:HB	3:C:153:LEU:HB2	2.03	0.40
5:E:145:ASP:HA	5:E:166:LYS:HB3	2.04	0.40
15:O:12:THR:HG23	15:O:16:ARG:NH2	2.37	0.40
34:a:499:A:C6	34:a:547:A:C8	3.09	0.40
34:a:1255:G:C5	34:a:1279:G:C2	3.10	0.40
34:a:1370:G:C2	34:a:1371:G:C8	3.10	0.40
52:s:38:THR:HA	52:s:69:LYS:HG3	2.04	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
3	C	269/271 (99%)	241 (90%)	26 (10%)	2 (1%)	18 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	206/208 (99%)	187 (91%)	15 (7%)	4 (2%)	6	33
5	E	198/200 (99%)	181 (91%)	13 (7%)	4 (2%)	6	32
6	F	175/177 (99%)	158 (90%)	17 (10%)	0	100	100
7	G	172/174 (99%)	156 (91%)	15 (9%)	1 (1%)	21	54
8	H	147/149 (99%)	126 (86%)	18 (12%)	3 (2%)	6	32
9	I	139/141 (99%)	110 (79%)	24 (17%)	5 (4%)	2	22
10	J	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
11	K	120/122 (98%)	104 (87%)	12 (10%)	4 (3%)	3	24
12	L	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	4	26
13	M	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	5	30
14	N	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	7	35
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	14	46
16	P	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
17	Q	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
18	R	100/102 (98%)	83 (83%)	13 (13%)	4 (4%)	2	20
19	S	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	14	46
20	T	90/92 (98%)	77 (86%)	11 (12%)	2 (2%)	5	30
21	U	100/102 (98%)	84 (84%)	12 (12%)	4 (4%)	2	20
22	V	90/92 (98%)	84 (93%)	5 (6%)	1 (1%)	11	43
23	W	73/75 (97%)	65 (89%)	7 (10%)	1 (1%)	9	38
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
25	Y	58/60 (97%)	55 (95%)	2 (3%)	1 (2%)	7	35
26	Z	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
27	0	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	6	33
28	1	49/51 (96%)	41 (84%)	6 (12%)	2 (4%)	2	19
29	2	43/45 (96%)	42 (98%)	1 (2%)	0	100	100
30	3	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
31	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
32	5	129/131 (98%)	98 (76%)	21 (16%)	10 (8%)	1	8
33	6	64/66 (97%)	54 (84%)	9 (14%)	1 (2%)	7	36
35	b	216/218 (99%)	187 (87%)	25 (12%)	4 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	c	204/206 (99%)	184 (90%)	14 (7%)	6 (3%)	3	26
37	d	203/205 (99%)	181 (89%)	20 (10%)	2 (1%)	12	45
38	e	155/157 (99%)	129 (83%)	23 (15%)	3 (2%)	6	33
39	f	98/100 (98%)	84 (86%)	12 (12%)	2 (2%)	6	32
40	g	149/151 (99%)	132 (89%)	12 (8%)	5 (3%)	3	23
41	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
42	i	125/127 (98%)	96 (77%)	24 (19%)	5 (4%)	2	20
43	j	96/98 (98%)	73 (76%)	16 (17%)	7 (7%)	1	10
44	k	114/116 (98%)	100 (88%)	9 (8%)	5 (4%)	2	18
45	l	119/121 (98%)	98 (82%)	14 (12%)	7 (6%)	1	13
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	6	34
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	1	15
48	o	86/88 (98%)	79 (92%)	3 (4%)	4 (5%)	2	17
49	p	80/82 (98%)	69 (86%)	8 (10%)	3 (4%)	2	21
50	q	78/80 (98%)	71 (91%)	4 (5%)	3 (4%)	2	21
51	r	63/65 (97%)	52 (82%)	7 (11%)	4 (6%)	1	12
52	s	77/79 (98%)	68 (88%)	8 (10%)	1 (1%)	9	39
53	t	83/85 (98%)	73 (88%)	7 (8%)	3 (4%)	2	22
54	u	63/65 (97%)	41 (65%)	13 (21%)	9 (14%)	0	3
58	z	391/393 (100%)	348 (89%)	32 (8%)	11 (3%)	4	26
All	All	6218/6322 (98%)	5461 (88%)	605 (10%)	152 (2%)	7	29

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	31	GLY
18	R	51	VAL
20	T	37	ASP
21	U	6	ARG
32	5	123	ILE
36	c	96	VAL
36	c	156	LEU
42	i	90	ASP
43	j	57	VAL
43	j	89	ARG

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Mol	Chain	Res	Type
44	k	88	PRO
48	o	45	HIS
48	o	47	LYS
53	t	39	GLU
54	u	13	VAL
54	u	14	ALA
54	u	37	TYR
4	D	58	ASN
5	E	8	ALA
5	E	83	VAL
7	G	60	GLY
9	I	24	GLY
11	K	89	ASN
18	R	49	ILE
18	R	54	VAL
18	R	55	ASP
20	T	6	ARG
32	5	60	LEU
38	e	77	ASN
40	g	20	GLU
40	g	64	ALA
40	g	129	ASN
42	i	46	VAL
42	i	57	VAL
42	i	108	ARG
43	j	29	ALA
44	k	51	PHE
44	k	94	SER
45	l	42	LYS
45	l	75	GLU
45	l	88	ASP
46	m	7	ASN
47	n	2	LYS
47	n	22	LYS
47	n	38	ASP
47	n	90	ARG
49	p	64	GLY
51	r	10	CYS
51	r	17	VAL
54	u	36	PHE
58	z	180	GLY
58	z	222	GLY

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Mol	Chain	Res	Type
3	C	13	ARG
4	D	31	ALA
4	D	154	LYS
9	I	64	ARG
11	K	110	GLU
11	K	111	LYS
12	L	15	ALA
14	N	59	SER
14	N	117	ASP
22	V	58	SER
23	W	72	ASN
27	0	2	VAL
28	1	5	ARG
32	5	88	HIS
35	b	73	ARG
37	d	191	SER
39	f	63	ASN
42	i	124	PRO
43	j	35	GLN
44	k	13	LYS
45	l	35	ARG
47	n	55	SER
49	p	81	ALA
50	q	69	THR
53	t	5	SER
54	u	9	GLU
54	u	24	LYS
54	u	30	GLU
58	z	249	GLU
3	C	204	LEU
5	E	122	GLU
8	H	15	LEU
8	H	41	LYS
9	I	38	CYS
12	L	29	LYS
13	M	58	LYS
13	M	69	PRO
15	O	100	HIS
19	S	65	ASP
21	U	75	ALA
21	U	97	SER
25	Y	24	GLU

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Mol	Chain	Res	Type
32	5	48	ALA
32	5	55	VAL
32	5	118	ILE
33	6	4	ASP
36	c	147	GLY
37	d	166	LYS
40	g	19	SER
40	g	112	ASP
43	j	41	PRO
45	l	43	LYS
45	l	46	SER
45	l	77	SER
46	m	102	LYS
48	o	2	LEU
48	o	13	GLU
50	q	17	GLU
51	r	46	THR
52	s	36	ARG
53	t	44	ALA
4	D	149	ASN
5	E	69	ARG
8	H	3	VAL
12	L	91	ASP
13	M	6	ARG
32	5	51	TYR
32	5	80	THR
32	5	113	PHE
35	b	11	ALA
35	b	192	PRO
38	e	93	VAL
43	j	75	ASP
49	p	49	GLY
50	q	79	GLU
51	r	70	THR
54	u	11	PHE
54	u	22	CYS
58	z	207	ASP
58	z	248	LYS
58	z	332	PHE
11	K	35	VAL
21	U	38	ILE
32	5	108	VAL

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Mol	Chain	Res	Type
35	b	18	GLN
36	c	95	GLY
36	c	148	ILE
38	e	89	THR
39	f	33	GLU
43	j	6	ILE
44	k	103	GLY
58	z	9	LYS
58	z	126	GLY
58	z	137	CYS
28	l	4	ILE
36	c	144	GLY
9	I	90	GLY
58	z	82	PRO
9	I	48	ILE
58	z	52	ALA

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	
3	C	216/216 (100%)	205 (95%)	11 (5%)	21	49
4	D	163/163 (100%)	152 (93%)	11 (7%)	15	42
5	E	164/164 (100%)	156 (95%)	8 (5%)	22	49
6	F	148/148 (100%)	141 (95%)	7 (5%)	23	50
7	G	135/135 (100%)	132 (98%)	3 (2%)	45	65
8	H	114/114 (100%)	111 (97%)	3 (3%)	40	62
9	I	109/109 (100%)	102 (94%)	7 (6%)	16	43
10	J	115/115 (100%)	107 (93%)	8 (7%)	14	41
11	K	103/103 (100%)	93 (90%)	10 (10%)	8	31
12	L	102/102 (100%)	96 (94%)	6 (6%)	18	45
13	M	109/109 (100%)	104 (95%)	5 (5%)	24	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	99/99 (100%)	96 (97%)	3 (3%)	36	59
15	O	86/86 (100%)	83 (96%)	3 (4%)	32	57
16	P	99/99 (100%)	95 (96%)	4 (4%)	28	54
17	Q	88/88 (100%)	85 (97%)	3 (3%)	32	57
18	R	84/84 (100%)	81 (96%)	3 (4%)	31	56
19	S	92/92 (100%)	86 (94%)	6 (6%)	15	43
20	T	79/79 (100%)	74 (94%)	5 (6%)	16	44
21	U	83/83 (100%)	78 (94%)	5 (6%)	17	45
22	V	77/77 (100%)	75 (97%)	2 (3%)	40	62
23	W	57/57 (100%)	52 (91%)	5 (9%)	9	33
24	X	67/67 (100%)	67 (100%)	0	100	100
25	Y	55/55 (100%)	54 (98%)	1 (2%)	51	68
26	Z	47/47 (100%)	46 (98%)	1 (2%)	47	65
27	0	46/46 (100%)	46 (100%)	0	100	100
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	37/37 (100%)	33 (89%)	4 (11%)	6	28
30	3	51/51 (100%)	49 (96%)	2 (4%)	28	54
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	99 (99%)	1 (1%)	68	75
33	6	59/59 (100%)	53 (90%)	6 (10%)	7	30
35	b	180/180 (100%)	177 (98%)	3 (2%)	53	69
36	c	170/170 (100%)	169 (99%)	1 (1%)	78	79
37	d	172/172 (100%)	168 (98%)	4 (2%)	44	64
38	e	119/119 (100%)	113 (95%)	6 (5%)	22	49
39	f	87/87 (100%)	84 (97%)	3 (3%)	32	57
40	g	124/124 (100%)	117 (94%)	7 (6%)	19	47
41	h	104/104 (100%)	99 (95%)	5 (5%)	23	50
42	i	105/105 (100%)	102 (97%)	3 (3%)	37	60
43	j	86/86 (100%)	83 (96%)	3 (4%)	32	57
44	k	89/89 (100%)	81 (91%)	8 (9%)	9	33
45	l	102/102 (100%)	96 (94%)	6 (6%)	18	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	m	93/93 (100%)	86 (92%)	7 (8%)	12	39
47	n	83/83 (100%)	76 (92%)	7 (8%)	10	35
48	o	76/76 (100%)	74 (97%)	2 (3%)	40	62
49	p	65/65 (100%)	63 (97%)	2 (3%)	35	59
50	q	74/74 (100%)	68 (92%)	6 (8%)	11	36
51	r	56/56 (100%)	52 (93%)	4 (7%)	13	40
52	s	70/70 (100%)	65 (93%)	5 (7%)	13	40
53	t	65/65 (100%)	57 (88%)	8 (12%)	4	23
54	u	55/55 (100%)	50 (91%)	5 (9%)	9	33
58	z	325/325 (100%)	322 (99%)	3 (1%)	70	76
All	All	5164/5164 (100%)	4933 (96%)	231 (4%)	26	51

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	12	ARG
3	C	35	LYS
3	C	42	ARG
3	C	69	ASN
3	C	131	MET
3	C	164	VAL
3	C	183	VAL
3	C	241	LYS
3	C	249	VAL
3	C	263	ASP
3	C	268	ARG
4	D	12	THR
4	D	13	ARG
4	D	39	ASP
4	D	77	ARG
4	D	99	GLU
4	D	148	GLN
4	D	150	GLN
4	D	151	THR
4	D	157	LYS
4	D	169	ARG
4	D	200	ASP
5	E	21	ARG

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Mol	Chain	Res	Type
5	E	47	LYS
5	E	80	SER
5	E	88	ARG
5	E	117	ARG
5	E	139	LYS
5	E	141	MET
5	E	193	VAL
6	F	16	MET
6	F	32	LYS
6	F	70	ARG
6	F	87	LYS
6	F	94	ARG
6	F	112	ASP
6	F	132	ARG
7	G	59	ASP
7	G	113	ASP
7	G	165	ASP
8	H	18	GLN
8	H	35	LYS
8	H	101	ASP
9	I	11	GLN
9	I	30	GLN
9	I	92	PRO
9	I	95	ASP
9	I	117	THR
9	I	126	ARG
9	I	135	MET
10	J	3	THR
10	J	50	THR
10	J	61	LYS
10	J	70	THR
10	J	80	HIS
10	J	85	LYS
10	J	90	GLU
10	J	99	ARG
11	K	40	LYS
11	K	52	VAL
11	K	58	LEU
11	K	59	LYS
11	K	61	VAL
11	K	67	LYS
11	K	84	CYS

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Mol	Chain	Res	Type
11	K	97	THR
11	K	109	SER
11	K	111	LYS
12	L	1	MET
12	L	13	LYS
12	L	14	LYS
12	L	79	LEU
12	L	126	ARG
12	L	129	LYS
13	M	57	VAL
13	M	59	ARG
13	M	110	GLU
13	M	118	LYS
13	M	134	THR
14	N	17	ARG
14	N	71	ARG
14	N	117	ASP
15	O	28	VAL
15	O	76	LYS
15	O	100	HIS
16	P	38	ARG
16	P	47	ILE
16	P	79	VAL
16	P	88	ARG
17	Q	29	ARG
17	Q	74	SER
17	Q	84	LYS
18	R	66	HIS
18	R	80	ARG
18	R	95	ASP
19	S	19	LEU
19	S	29	VAL
19	S	57	ASN
19	S	62	ASP
19	S	72	THR
19	S	101	SER
20	T	5	GLU
20	T	12	ARG
20	T	69	ARG
20	T	70	HIS
20	T	93	LEU
21	U	3	LYS

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Mol	Chain	Res	Type
21	U	16	LYS
21	U	18	LYS
21	U	34	ILE
21	U	65	GLN
22	V	35	GLU
22	V	42	LEU
23	W	7	ARG
23	W	8	ASN
23	W	15	LYS
23	W	58	LYS
23	W	68	LYS
25	Y	54	LYS
26	Z	56	VAL
29	2	11	LYS
29	2	25	LYS
29	2	41	ARG
29	2	43	THR
30	3	51	LYS
30	3	61	LEU
32	5	34	THR
33	6	1	MET
33	6	3	LYS
33	6	8	LYS
33	6	26	SER
33	6	37	CYS
33	6	56	ARG
35	b	67	LEU
35	b	71	THR
35	b	188	THR
36	c	156	LEU
37	d	72	ARG
37	d	120	LYS
37	d	189	ASP
37	d	190	LEU
38	e	9	GLU
38	e	11	GLN
38	e	12	GLU
38	e	45	VAL
38	e	111	ARG
38	e	136	VAL
39	f	38	ARG
39	f	39	LEU

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Mol	Chain	Res	Type
39	f	91	ARG
40	g	9	ARG
40	g	11	ILE
40	g	20	GLU
40	g	47	GLU
40	g	55	LYS
40	g	76	SER
40	g	124	SER
41	h	59	GLU
41	h	79	ARG
41	h	106	SER
41	h	110	MET
41	h	120	LEU
42	i	41	GLU
42	i	42	THR
42	i	44	ARG
43	j	67	ILE
43	j	87	LEU
43	j	88	MET
44	k	12	ARG
44	k	28	ASN
44	k	54	SER
44	k	58	THR
44	k	71	ASP
44	k	118	ASN
44	k	120	CYS
44	k	126	ARG
45	l	13	ARG
45	l	14	LYS
45	l	38	THR
45	l	61	GLU
45	l	85	ARG
45	l	88	ASP
46	m	15	VAL
46	m	45	SER
46	m	47	LEU
46	m	54	THR
46	m	75	SER
46	m	84	CYS
46	m	89	ARG
47	n	10	VAL
47	n	15	LEU

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Mol	Chain	Res	Type
47	n	23	ARG
47	n	37	SER
47	n	56	SER
47	n	63	ARG
47	n	75	ARG
48	o	46	LYS
48	o	88	ARG
49	p	31	ARG
49	p	34	GLU
50	q	3	LYS
50	q	4	ILE
50	q	15	LYS
50	q	16	MET
50	q	52	CYS
50	q	66	LEU
51	r	13	THR
51	r	37	LYS
51	r	42	ARG
51	r	60	ARG
52	s	5	LYS
52	s	12	LEU
52	s	13	HIS
52	s	36	ARG
52	s	69	LYS
53	t	4	LYS
53	t	8	LYS
53	t	15	LYS
53	t	29	THR
53	t	43	LYS
53	t	56	ILE
53	t	63	LYS
53	t	68	LYS
54	u	17	ARG
54	u	34	ARG
54	u	43	GLU
54	u	62	GLU
54	u	66	ARG
58	z	22	HIS
58	z	167	THR
58	z	241	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	59	GLN
3	C	116	GLN
3	C	133	ASN
3	C	196	ASN
3	C	242	HIS
5	E	30	GLN
5	E	41	GLN
5	E	94	GLN
5	E	115	GLN
6	F	20	ASN
7	G	37	ASN
8	H	18	GLN
8	H	135	HIS
9	I	5	GLN
10	J	47	HIS
10	J	58	ASN
10	J	77	HIS
10	J	128	ASN
10	J	131	ASN
10	J	132	HIS
10	J	136	GLN
11	K	3	GLN
12	L	93	ASN
13	M	97	GLN
16	P	6	GLN
16	P	65	ASN
18	R	43	ASN
19	S	9	HIS
19	S	102	HIS
20	T	48	GLN
21	U	39	ASN
21	U	73	ASN
22	V	24	ASN
22	V	87	GLN
33	6	41	HIS
33	6	65	ASN
35	b	17	HIS
35	b	23	ASN
35	b	38	HIS
36	c	5	HIS
36	c	7	ASN
36	c	122	GLN
37	d	35	GLN

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Mol	Chain	Res	Type
37	d	70	GLN
37	d	119	HIS
38	e	96	GLN
38	e	121	ASN
39	f	14	GLN
39	f	37	HIS
40	g	96	ASN
41	h	66	GLN
42	i	30	ASN
42	i	125	GLN
43	j	58	ASN
44	k	63	GLN
45	l	71	HIS
45	l	111	GLN
48	o	19	ASN
48	o	27	GLN
48	o	36	ASN
48	o	45	HIS
50	q	49	ASN
51	r	18	GLN
51	r	53	GLN
52	s	56	HIS
53	t	47	GLN
53	t	69	ASN
53	t	81	GLN
54	u	63	ASN
58	z	97	GLN
58	z	301	HIS
58	z	355	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2903 (99%)	732 (25%)	74 (2%)
2	B	119/120 (99%)	25 (21%)	5 (4%)
34	a	1539/1540 (99%)	466 (30%)	0
55	v	76/77 (98%)	18 (23%)	0
55	w	76/77 (98%)	34 (44%)	0
56	x	11/12 (91%)	3 (27%)	0
57	y	75/76 (98%)	30 (40%)	0
All	All	4793/4805 (99%)	1308 (27%)	79 (1%)

All (1308) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	4	U
1	A	5	A
1	A	6	A
1	A	10	A
1	A	12	U
1	A	15	G
1	A	23	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	41	C
1	A	46	G
1	A	49	A
1	A	50	U
1	A	51	G
1	A	52	A
1	A	61	C
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	80	G
1	A	82	U
1	A	84	A
1	A	92	U
1	A	93	G
1	A	97	C
1	A	98	G
1	A	100	U
1	A	101	A
1	A	102	U
1	A	118	A
1	A	119	A
1	A	120	U
1	A	130	C
1	A	133	U
1	A	136	G
1	A	139	U
1	A	140	C
1	A	141	G

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Mol	Chain	Res	Type
1	A	143	C
1	A	153	U
1	A	155	A
1	A	156	A
1	A	157	C
1	A	159	G
1	A	162	U
1	A	163	C
1	A	165	A
1	A	166	U
1	A	168	G
1	A	170	U
1	A	173	A
1	A	181	A
1	A	186	G
1	A	188	G
1	A	196	A
1	A	205	G
1	A	214	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	226	A
1	A	228	C
1	A	230	G
1	A	234	U
1	A	239	C
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	265	A
1	A	266	G
1	A	267	C
1	A	272	A
1	A	273	G
1	A	274	C
1	A	275	C
1	A	276	U
1	A	279	A

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Mol	Chain	Res	Type
1	A	281	C
1	A	282	A
1	A	283	G
1	A	284	U
1	A	285	G
1	A	286	U
1	A	287	G
1	A	290	U
1	A	294	A
1	A	301	G
1	A	302	C
1	A	311	A
1	A	317	G
1	A	322	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	349	U
1	A	352	A
1	A	354	A
1	A	357	C
1	A	358	U
1	A	361	G
1	A	362	A
1	A	363	G
1	A	365	U
1	A	366	C
1	A	368	A
1	A	369	U
1	A	371	A
1	A	372	G
1	A	386	G
1	A	387	U
1	A	395	U
1	A	396	G
1	A	400	G
1	A	403	U
1	A	404	A
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A

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Mol	Chain	Res	Type
1	A	420	C
1	A	427	U
1	A	438	G
1	A	442	G
1	A	445	C
1	A	451	U
1	A	456	C
1	A	473	G
1	A	475	C
1	A	480	A
1	A	481	G
1	A	491	G
1	A	492	A
1	A	494	G
1	A	503	A
1	A	505	A
1	A	507	A
1	A	509	C
1	A	510	C
1	A	521	U
1	A	527	C
1	A	529	A
1	A	531	C
1	A	532	A
1	A	533	G
1	A	535	G
1	A	543	G
1	A	544	C
1	A	545	U
1	A	547	A
1	A	548	G
1	A	550	C
1	A	555	G
1	A	556	A
1	A	563	A
1	A	564	C
1	A	573	U
1	A	575	A
1	A	586	A
1	A	592	A
1	A	602	A
1	A	603	A

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Mol	Chain	Res	Type
1	A	610	C
1	A	612	G
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	622	G
1	A	627	A
1	A	633	A
1	A	636	G
1	A	637	A
1	A	640	C
1	A	645	C
1	A	646	U
1	A	653	U
1	A	654	A
1	A	655	A
1	A	659	G
1	A	660	C
1	A	661	A
1	A	685	A
1	A	686	U
1	A	694	U
1	A	695	G
1	A	696	G
1	A	711	G
1	A	715	A
1	A	717	C
1	A	730	A
1	A	738	G
1	A	746	PSU
1	A	747	5MC
1	A	764	A
1	A	771	G
1	A	774	G
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	804	A

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Mol	Chain	Res	Type
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	837	C
1	A	844	A
1	A	845	A
1	A	846	C
1	A	858	G
1	A	859	G
1	A	860	U
1	A	878	A
1	A	880	G
1	A	882	G
1	A	892	A
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	C
1	A	903	C
1	A	907	G
1	A	910	A
1	A	914	G
1	A	915	C
1	A	931	U
1	A	934	U
1	A	940	G
1	A	941	A
1	A	942	G
1	A	946	C
1	A	951	C
1	A	953	G
1	A	958	U
1	A	961	C
1	A	973	A
1	A	974	G
1	A	975	A
1	A	983	A
1	A	985	C

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Mol	Chain	Res	Type
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	1005	C
1	A	1006	C
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1019	U
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1026	G
1	A	1033	U
1	A	1036	G
1	A	1037	G
1	A	1038	G
1	A	1040	A
1	A	1044	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1050	A
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1075	C

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Mol	Chain	Res	Type
1	A	1076	C
1	A	1079	C
1	A	1084	A
1	A	1085	A
1	A	1087	G
1	A	1088	A
1	A	1089	A
1	A	1090	A
1	A	1097	U
1	A	1101	U
1	A	1104	C
1	A	1106	G
1	A	1108	U
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1115	G
1	A	1117	C
1	A	1119	U
1	A	1130	U
1	A	1132	U
1	A	1135	C
1	A	1139	G
1	A	1141	U
1	A	1142	A
1	A	1143	A
1	A	1150	C
1	A	1151	A
1	A	1155	A
1	A	1171	G
1	A	1172	C
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1180	U
1	A	1184	U
1	A	1193	G
1	A	1203	U
1	A	1210	G
1	A	1218	G

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Mol	Chain	Res	Type
1	A	1225	G
1	A	1227	G
1	A	1236	G
1	A	1238	G
1	A	1247	A
1	A	1248	G
1	A	1253	A
1	A	1256	G
1	A	1258	U
1	A	1262	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1300	G
1	A	1301	A
1	A	1305	C
1	A	1320	C
1	A	1332	G
1	A	1345	C
1	A	1352	U
1	A	1359	A
1	A	1365	A
1	A	1367	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1387	A
1	A	1395	A
1	A	1401	G
1	A	1403	A
1	A	1407	G
1	A	1410	G
1	A	1416	G
1	A	1418	G
1	A	1419	A
1	A	1420	A
1	A	1427	A
1	A	1428	C
1	A	1441	G
1	A	1450	G
1	A	1452	G

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Mol	Chain	Res	Type
1	A	1453	A
1	A	1455	G
1	A	1458	U
1	A	1461	C
1	A	1468	U
1	A	1475	G
1	A	1476	U
1	A	1478	G
1	A	1479	G
1	A	1482	G
1	A	1484	U
1	A	1485	U
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1498	C
1	A	1504	A
1	A	1507	C
1	A	1515	A
1	A	1516	G
1	A	1519	G
1	A	1520	U
1	A	1522	A
1	A	1523	U
1	A	1524	G
1	A	1533	C
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1542	U
1	A	1546	G
1	A	1555	G
1	A	1556	C
1	A	1558	C
1	A	1559	U
1	A	1565	C
1	A	1567	G
1	A	1569	A
1	A	1578	U
1	A	1579	A
1	A	1581	G
1	A	1582	C

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Mol	Chain	Res	Type
1	A	1584	U
1	A	1585	C
1	A	1587	G
1	A	1588	G
1	A	1590	A
1	A	1595	C
1	A	1605	C
1	A	1608	A
1	A	1610	A
1	A	1616	A
1	A	1617	C
1	A	1618	6MZ
1	A	1619	G
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1651	G
1	A	1654	A
1	A	1674	G
1	A	1675	C
1	A	1693	U
1	A	1694	C
1	A	1695	G
1	A	1710	G
1	A	1714	U
1	A	1715	G
1	A	1716	U
1	A	1721	G
1	A	1723	G
1	A	1724	G
1	A	1726	G
1	A	1728	C
1	A	1729	U
1	A	1731	G
1	A	1738	G
1	A	1741	C
1	A	1745	A
1	A	1746	A
1	A	1747	U
1	A	1750	G
1	A	1758	U
1	A	1764	C

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Mol	Chain	Res	Type
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1782	U
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1809	A
1	A	1816	C
1	A	1826	G
1	A	1833	C
1	A	1841	U
1	A	1842	G
1	A	1847	G
1	A	1858	A
1	A	1862	G
1	A	1866	A
1	A	1869	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1875	G
1	A	1876	A
1	A	1884	G
1	A	1885	A
1	A	1895	C
1	A	1903	G
1	A	1906	G
1	A	1907	G
1	A	1913	A
1	A	1914	C
1	A	1915	3TD
1	A	1917	PSU
1	A	1918	A
1	A	1919	A
1	A	1929	G
1	A	1930	G
1	A	1936	A
1	A	1937	A

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Mol	Chain	Res	Type
1	A	1938	A
1	A	1939	5MU
1	A	1940	U
1	A	1941	C
1	A	1942	C
1	A	1955	U
1	A	1962	5MC
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1982	U
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2004	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2029	G
1	A	2030	6MZ
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	7MG
1	A	2072	C
1	A	2077	A
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2096	C
1	A	2098	U
1	A	2100	G
1	A	2102	G
1	A	2104	C

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Mol	Chain	Res	Type
1	A	2106	U
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2118	U
1	A	2119	A
1	A	2121	G
1	A	2122	U
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2141	G
1	A	2145	C
1	A	2147	A
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2180	U
1	A	2186	G
1	A	2192	U
1	A	2198	A
1	A	2204	G
1	A	2206	C
1	A	2211	A
1	A	2213	U
1	A	2214	C
1	A	2221	G
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2278	A
1	A	2279	G
1	A	2283	C
1	A	2286	G

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Mol	Chain	Res	Type
1	A	2287	A
1	A	2288	A
1	A	2297	A
1	A	2305	U
1	A	2309	A
1	A	2311	A
1	A	2318	G
1	A	2319	G
1	A	2325	G
1	A	2326	C
1	A	2327	A
1	A	2332	C
1	A	2333	A
1	A	2335	A
1	A	2336	A
1	A	2342	C
1	A	2350	C
1	A	2357	G
1	A	2361	G
1	A	2373	G
1	A	2378	A
1	A	2379	G
1	A	2383	G
1	A	2385	C
1	A	2392	A
1	A	2399	G
1	A	2402	U
1	A	2403	C
1	A	2404	U
1	A	2406	A
1	A	2408	U
1	A	2423	U
1	A	2425	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2441	U
1	A	2445	2MG
1	A	2447	G
1	A	2448	A
1	A	2457	PSU

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Mol	Chain	Res	Type
1	A	2469	A
1	A	2470	G
1	A	2475	C
1	A	2476	A
1	A	2480	C
1	A	2481	G
1	A	2491	U
1	A	2494	G
1	A	2498	OMC
1	A	2499	C
1	A	2502	G
1	A	2503	2MA
1	A	2505	G
1	A	2506	U
1	A	2513	A
1	A	2518	A
1	A	2525	G
1	A	2529	G
1	A	2535	G
1	A	2542	A
1	A	2547	A
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2578	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2608	G
1	A	2609	U
1	A	2613	U
1	A	2623	G
1	A	2624	G
1	A	2629	U
1	A	2636	C
1	A	2639	A
1	A	2654	A
1	A	2656	U
1	A	2661	G

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Mol	Chain	Res	Type
1	A	2662	A
1	A	2663	G
1	A	2682	A
1	A	2685	G
1	A	2689	U
1	A	2690	U
1	A	2707	U
1	A	2713	U
1	A	2714	G
1	A	2716	C
1	A	2720	U
1	A	2724	U
1	A	2726	A
1	A	2728	U
1	A	2733	A
1	A	2734	A
1	A	2735	G
1	A	2742	G
1	A	2744	G
1	A	2746	U
1	A	2748	A
1	A	2752	C
1	A	2754	U
1	A	2758	A
1	A	2762	C
1	A	2764	A
1	A	2765	A
1	A	2778	A
1	A	2791	G
1	A	2794	U
1	A	2798	U
1	A	2799	G
1	A	2800	A
1	A	2801	G
1	A	2803	G
1	A	2805	C
1	A	2806	C
1	A	2807	U
1	A	2809	A
1	A	2811	G
1	A	2818	U
1	A	2820	A

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Mol	Chain	Res	Type
1	A	2833	U
1	A	2849	U
1	A	2850	A
1	A	2861	U
1	A	2863	C
1	A	2867	G
1	A	2868	A
1	A	2872	A
1	A	2873	A
1	A	2874	C
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2885	G
1	A	2886	A
1	A	2900	A
1	A	2901	C
1	A	2902	C
2	B	4	C
2	B	12	C
2	B	13	G
2	B	21	G
2	B	26	C
2	B	28	C
2	B	31	C
2	B	33	G
2	B	35	C
2	B	36	C
2	B	42	C
2	B	44	G
2	B	65	U
2	B	66	A
2	B	67	G
2	B	89	U
2	B	90	C
2	B	91	C
2	B	105	G
2	B	108	A
2	B	109	A
2	B	111	U
2	B	113	C
2	B	114	C

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Mol	Chain	Res	Type
2	B	118	C
34	a	2	A
34	a	3	A
34	a	4	U
34	a	5	U
34	a	6	G
34	a	8	A
34	a	9	G
34	a	22	G
34	a	27	G
34	a	29	U
34	a	32	A
34	a	38	G
34	a	39	G
34	a	40	C
34	a	44	A
34	a	47	C
34	a	48	C
34	a	49	U
34	a	50	A
34	a	51	A
34	a	52	C
34	a	57	G
34	a	64	G
34	a	66	A
34	a	69	G
34	a	70	U
34	a	71	A
34	a	72	A
34	a	73	C
34	a	74	A
34	a	76	G
34	a	77	A
34	a	78	A
34	a	80	A
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	87	C
34	a	94	G
34	a	95	C

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Mol	Chain	Res	Type
34	a	96	U
34	a	97	G
34	a	99	C
34	a	100	G
34	a	104	G
34	a	107	G
34	a	116	A
34	a	117	G
34	a	120	A
34	a	121	U
34	a	127	G
34	a	128	G
34	a	129	A
34	a	130	A
34	a	131	A
34	a	132	C
34	a	139	A
34	a	140	U
34	a	141	G
34	a	142	G
34	a	143	A
34	a	144	G
34	a	146	G
34	a	149	A
34	a	150	U
34	a	151	A
34	a	161	A
34	a	164	G
34	a	165	G
34	a	168	G
34	a	177	G
34	a	181	A
34	a	183	C
34	a	184	G
34	a	188	C
34	a	189	A
34	a	197	A
34	a	202	G
34	a	203	G
34	a	207	C
34	a	209	U
34	a	210	C

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Mol	Chain	Res	Type
34	a	211	G
34	a	212	G
34	a	213	G
34	a	215	C
34	a	220	G
34	a	222	C
34	a	223	A
34	a	224	U
34	a	225	C
34	a	226	G
34	a	227	G
34	a	230	G
34	a	244	U
34	a	245	U
34	a	246	A
34	a	247	G
34	a	251	G
34	a	254	G
34	a	259	G
34	a	266	G
34	a	267	C
34	a	281	G
34	a	289	G
34	a	300	A
34	a	305	G
34	a	306	A
34	a	317	U
34	a	321	A
34	a	323	U
34	a	325	A
34	a	328	C
34	a	329	A
34	a	330	C
34	a	335	C
34	a	339	C
34	a	340	U
34	a	341	C
34	a	342	C
34	a	344	A
34	a	345	C
34	a	347	G
34	a	348	G

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Mol	Chain	Res	Type
34	a	349	A
34	a	351	G
34	a	352	C
34	a	353	A
34	a	354	G
34	a	355	C
34	a	365	U
34	a	366	A
34	a	367	U
34	a	368	U
34	a	369	G
34	a	372	C
34	a	375	U
34	a	376	G
34	a	381	C
34	a	382	A
34	a	388	G
34	a	389	A
34	a	391	G
34	a	392	C
34	a	393	A
34	a	394	G
34	a	397	A
34	a	398	U
34	a	400	C
34	a	403	C
34	a	404	G
34	a	405	U
34	a	406	G
34	a	411	A
34	a	412	A
34	a	413	G
34	a	414	A
34	a	422	C
34	a	424	G
34	a	429	U
34	a	435	A
34	a	436	C
34	a	438	U
34	a	439	U
34	a	441	A
34	a	443	C

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Mol	Chain	Res	Type
34	a	446	G
34	a	449	G
34	a	457	G
34	a	458	U
34	a	459	A
34	a	464	U
34	a	467	U
34	a	468	A
34	a	484	G
34	a	485	U
34	a	486	U
34	a	495	A
34	a	496	A
34	a	497	G
34	a	499	A
34	a	501	C
34	a	503	C
34	a	505	G
34	a	506	G
34	a	509	A
34	a	511	C
34	a	512	U
34	a	513	C
34	a	514	C
34	a	515	G
34	a	516	PSU
34	a	517	G
34	a	518	C
34	a	521	G
34	a	524	G
34	a	525	C
34	a	527	7MG
34	a	528	C
34	a	531	U
34	a	532	A
34	a	533	A
34	a	534	U
34	a	535	A
34	a	537	G
34	a	538	G
34	a	541	G
34	a	542	G

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Mol	Chain	Res	Type
34	a	545	C
34	a	546	A
34	a	547	A
34	a	572	A
34	a	573	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	579	A
34	a	590	U
34	a	592	G
34	a	596	A
34	a	601	G
34	a	602	A
34	a	615	G
34	a	633	G
34	a	640	A
34	a	642	A
34	a	648	A
34	a	650	G
34	a	651	C
34	a	653	U
34	a	654	G
34	a	661	G
34	a	665	A
34	a	671	G
34	a	682	G
34	a	687	A
34	a	695	A
34	a	700	G
34	a	701	U
34	a	702	A
34	a	703	G
34	a	704	A
34	a	713	G
34	a	720	C
34	a	721	G
34	a	722	G
34	a	723	U
34	a	724	G
34	a	731	G
34	a	733	G

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Mol	Chain	Res	Type
34	a	742	G
34	a	747	A
34	a	748	G
34	a	749	A
34	a	754	C
34	a	755	G
34	a	758	C
34	a	760	G
34	a	761	G
34	a	769	G
34	a	777	A
34	a	793	U
34	a	794	A
34	a	802	A
34	a	814	A
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	832	G
34	a	836	G
34	a	838	G
34	a	843	U
34	a	844	G
34	a	846	G
34	a	851	G
34	a	852	G
34	a	870	U
34	a	872	A
34	a	885	G
34	a	902	G
34	a	905	U
34	a	906	A
34	a	914	A
34	a	934	C
34	a	935	A
34	a	939	G
34	a	945	G
34	a	960	U
34	a	961	U
34	a	965	U
34	a	966	2MG

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Mol	Chain	Res	Type
34	a	969	A
34	a	971	G
34	a	972	C
34	a	974	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	978	A
34	a	982	U
34	a	989	U
34	a	991	U
34	a	992	U
34	a	993	G
34	a	998	C
34	a	999	C
34	a	1001	C
34	a	1003	G
34	a	1004	A
34	a	1006	G
34	a	1016	A
34	a	1020	G
34	a	1027	C
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1033	G
34	a	1034	G
34	a	1035	A
34	a	1043	G
34	a	1045	C
34	a	1053	G
34	a	1056	U
34	a	1065	U
34	a	1070	U
34	a	1087	G
34	a	1088	G
34	a	1094	G
34	a	1095	U
34	a	1096	C
34	a	1101	A
34	a	1108	G
34	a	1113	C

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Mol	Chain	Res	Type
34	a	1124	G
34	a	1125	U
34	a	1126	U
34	a	1132	C
34	a	1133	G
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1142	G
34	a	1143	G
34	a	1146	A
34	a	1151	A
34	a	1152	A
34	a	1154	G
34	a	1155	A
34	a	1159	U
34	a	1160	G
34	a	1167	A
34	a	1168	U
34	a	1171	A
34	a	1174	G
34	a	1182	G
34	a	1184	G
34	a	1190	G
34	a	1191	A
34	a	1196	A
34	a	1197	A
34	a	1201	A
34	a	1202	U
34	a	1205	U
34	a	1206	G
34	a	1207	2MG
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1217	C
34	a	1219	A
34	a	1220	G
34	a	1225	A
34	a	1226	C

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Mol	Chain	Res	Type
34	a	1227	A
34	a	1228	C
34	a	1236	A
34	a	1238	A
34	a	1240	U
34	a	1245	C
34	a	1247	U
34	a	1248	A
34	a	1253	G
34	a	1256	A
34	a	1258	G
34	a	1260	G
34	a	1264	U
34	a	1266	G
34	a	1268	G
34	a	1269	A
34	a	1273	C
34	a	1274	A
34	a	1275	A
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1291	U
34	a	1293	C
34	a	1294	G
34	a	1296	C
34	a	1297	G
34	a	1298	U
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1304	G
34	a	1305	G
34	a	1306	A
34	a	1312	G
34	a	1313	U
34	a	1317	C
34	a	1320	C
34	a	1338	G

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Mol	Chain	Res	Type
34	a	1340	A
34	a	1345	U
34	a	1346	A
34	a	1348	U
34	a	1363	A
34	a	1368	A
34	a	1370	G
34	a	1371	G
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1387	G
34	a	1391	U
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1400	C
34	a	1402	4OC
34	a	1419	G
34	a	1429	A
34	a	1433	A
34	a	1434	A
34	a	1441	A
34	a	1442	G
34	a	1448	C
34	a	1449	C
34	a	1452	C
34	a	1454	G
34	a	1475	G
34	a	1487	G
34	a	1491	G
34	a	1492	A
34	a	1493	A
34	a	1497	G
34	a	1502	A
34	a	1503	A
34	a	1506	U
34	a	1517	G
34	a	1519	MA6
34	a	1529	G
34	a	1530	G
34	a	1534	A

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Mol	Chain	Res	Type
34	a	1535	C
34	a	1536	C
34	a	1537	U
34	a	1538	C
34	a	1539	C
55	v	4	G
55	v	6	G
55	v	7	4SU
55	v	8	G
55	v	13	A
55	v	15	C
55	v	17	U
55	v	18	G
55	v	20	H2U
55	v	21	A
55	v	22	G
55	v	25	C
55	v	42	G
55	v	47	U
55	v	64	G
55	v	70	G
55	v	72	A
55	v	76	A
55	w	3	C
55	w	5	G
55	w	7	G
55	w	8	4SU
55	w	9	G
55	w	14	A
55	w	16	C
55	w	17	C
55	w	117	U
55	w	18	G
55	w	19	G
55	w	20	H2U
55	w	21	A
55	w	22	G
55	w	24	U
55	w	25	C
55	w	28	C
55	w	30	G
55	w	34	C

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Mol	Chain	Res	Type
55	w	37	A
55	w	38	A
55	w	42	G
55	w	48	C
55	w	49	G
55	w	56	C
55	w	59	A
55	w	64	G
55	w	67	C
55	w	69	C
55	w	70	G
55	w	71	C
55	w	73	A
55	w	75	C
55	w	76	A
56	x	14	C
56	x	20	U
56	x	24	G
57	y	3	C
57	y	4	C
57	y	5	G
57	y	8	4SU
57	y	9	A
57	y	10	G
57	y	11	C
57	y	16	H2U
57	y	17	C
57	y	18	G
57	y	20	H2U
57	y	21	A
57	y	24	G
57	y	33	U
57	y	36	A
57	y	37	MIA
57	y	44	G
57	y	45	U
57	y	46	7MG
57	y	47	U
57	y	48	C
57	y	52	G
57	y	59	U
57	y	61	C

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Mol	Chain	Res	Type
57	y	65	G
57	y	68	C
57	y	69	G
57	y	72	C
57	y	73	A
57	y	76	A

All (79) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	141	G
1	A	162	U
1	A	177	G
1	A	199	A
1	A	204	A
1	A	242	G
1	A	265	A
1	A	301	G
1	A	341	C
1	A	362	A
1	A	404	A
1	A	446	G
1	A	500	G
1	A	534	U
1	A	537	G
1	A	555	G
1	A	613	A
1	A	641	U
1	A	653	U
1	A	746	PSU
1	A	764	A
1	A	774	G
1	A	775	G
1	A	784	G
1	A	827	U
1	A	859	G
1	A	884	U
1	A	1020	A
1	A	1022	G
1	A	1046	A
1	A	1064	C

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Mol	Chain	Res	Type
1	A	1070	A
1	A	1089	A
1	A	1111	A
1	A	1124	G
1	A	1140	C
1	A	1141	U
1	A	1190	G
1	A	1378	A
1	A	1399	C
1	A	1432	G
1	A	1475	G
1	A	1491	G
1	A	1523	U
1	A	1555	G
1	A	1558	C
1	A	1567	G
1	A	1608	A
1	A	1647	U
1	A	1730	U
1	A	1745	A
1	A	1818	U
1	A	1857	G
1	A	1913	A
1	A	1918	A
1	A	1939	5MU
1	A	1940	U
1	A	1976	U
1	A	2238	G
1	A	2296	U
1	A	2319	G
1	A	2326	C
1	A	2391	G
1	A	2401	U
1	A	2402	U
1	A	2407	A
1	A	2517	C
1	A	2566	A
1	A	2581	G
1	A	2638	G
1	A	2798	U
1	A	2849	U
1	A	2873	A

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Mol	Chain	Res	Type
2	B	34	A
2	B	56	G
2	B	66	A
2	B	89	U
2	B	108	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	1MG	A	745	1	23,26,27	1.41	3 (13%)	33,39,42	2.00	7 (21%)
1	PSU	A	955	1	18,21,22	1.42	2 (11%)	21,30,33	2.08	4 (19%)
1	5MU	A	1939	1	19,22,23	1.47	4 (21%)	27,32,35	2.10	8 (29%)
1	PSU	A	2604	60,1	18,21,22	1.43	2 (11%)	21,30,33	1.95	4 (19%)
55	4SU	w	8	55	18,21,22	1.82	5 (27%)	25,30,33	2.26	6 (24%)
34	UR3	a	1498	34	19,22,23	1.13	2 (10%)	26,32,35	1.97	5 (19%)
55	H2U	w	20	55	18,21,22	0.81	0	19,30,33	1.34	3 (15%)
55	5MU	v	54	55	19,22,23	1.49	4 (21%)	27,32,35	1.97	7 (25%)
1	3TD	A	1915	1	19,22,23	7.09	13 (68%)	23,32,35	1.95	5 (21%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.02	11 (40%)
57	PSU	y	55	57	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
1	6MZ	A	2030	60,1	22,25,26	1.53	4 (18%)	29,36,39	2.29	10 (34%)
1	5MC	A	1962	1	19,22,23	2.00	2 (10%)	26,32,35	1.52	4 (15%)
34	2MG	a	1207	34	23,26,27	1.27	3 (13%)	33,38,41	2.82	10 (30%)
57	MIA	y	37	57	28,31,32	2.39	8 (28%)	38,44,47	2.88	17 (44%)
1	OMU	A	2552	1	19,22,23	1.30	3 (15%)	25,31,34	2.03	8 (32%)
55	PSU	w	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.07	5 (23%)
1	5MC	A	747	1	19,22,23	1.97	2 (10%)	26,32,35	1.59	4 (15%)
57	H2U	y	20	57	18,21,22	0.85	1 (5%)	19,30,33	1.50	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	5MC	a	967	34	19,22,23	2.05	2 (10%)	26,32,35	1.51	4 (15%)
34	5MC	a	1407	34	19,22,23	1.98	2 (10%)	26,32,35	1.60	5 (19%)
1	2MG	A	1835	1	23,26,27	1.36	4 (17%)	33,38,41	2.24	7 (21%)
57	5MU	y	54	57	19,22,23	1.47	4 (21%)	27,32,35	2.04	8 (29%)
55	H2U	v	20	60,55	18,21,22	0.83	1 (5%)	19,30,33	1.57	3 (15%)
57	PSU	y	32	57	18,21,22	1.35	2 (11%)	21,30,33	2.10	5 (23%)
1	PSU	A	1917	1	18,21,22	1.44	2 (11%)	21,30,33	2.07	5 (23%)
57	PSU	y	39	57	18,21,22	1.41	2 (11%)	21,30,33	2.00	4 (19%)
34	PSU	a	516	34	18,21,22	1.36	2 (11%)	21,30,33	2.12	5 (23%)
55	4SU	v	7	55	18,21,22	1.81	4 (22%)	25,30,33	2.34	6 (24%)
1	H2U	A	2449	1	18,21,22	0.94	2 (11%)	19,30,33	1.61	4 (21%)
1	OMG	A	2251	55,1	23,26,27	1.26	3 (13%)	32,38,41	1.99	6 (18%)
1	PSU	A	1911	1	18,21,22	1.41	2 (11%)	21,30,33	2.15	5 (23%)
1	7MG	A	2069	1	23,26,27	1.46	3 (13%)	27,39,42	2.52	11 (40%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.40	3 (15%)
1	6MZ	A	1618	1	22,25,26	1.53	4 (18%)	29,36,39	2.30	11 (37%)
34	2MG	a	1516	34	23,26,27	1.26	4 (17%)	33,38,41	2.33	10 (30%)
34	MA6	a	1518	34	23,26,27	1.77	5 (21%)	33,38,41	2.37	11 (33%)
55	PSU	v	55	55	18,21,22	1.37	3 (16%)	21,30,33	2.00	4 (19%)
57	7MG	y	46	57	23,26,27	1.42	3 (13%)	27,39,42	2.48	7 (25%)
1	PSU	A	2580	1	18,21,22	1.44	2 (11%)	21,30,33	2.03	5 (23%)
1	OMC	A	2498	60,1	19,22,23	0.86	0	25,31,34	1.25	2 (8%)
1	2MG	A	2445	1	23,26,27	1.26	4 (17%)	33,38,41	2.35	10 (30%)
57	4SU	y	8	57	18,21,22	1.82	5 (27%)	25,30,33	2.37	7 (28%)
1	PSU	A	746	60,1	18,21,22	1.40	2 (11%)	21,30,33	2.05	5 (23%)
1	2MA	A	2503	60,1	22,25,26	1.59	5 (22%)	32,37,40	2.22	9 (28%)
34	7MG	a	527	34,60	23,26,27	1.42	3 (13%)	27,39,42	2.55	7 (25%)
34	MA6	a	1519	34	23,26,27	1.73	5 (21%)	33,38,41	2.49	16 (48%)
34	4OC	a	1402	34	20,23,24	0.84	0	25,32,35	1.33	5 (20%)
1	PSU	A	2504	1	18,21,22	1.39	2 (11%)	21,30,33	2.04	4 (19%)
34	2MG	a	966	34	23,26,27	1.30	4 (17%)	33,38,41	2.64	9 (27%)
1	PSU	A	2457	1	18,21,22	1.44	2 (11%)	21,30,33	2.12	5 (23%)
1	PSU	A	2605	1	18,21,22	1.39	2 (11%)	21,30,33	2.07	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
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2604	60,1	-	0/7/25/26	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
55	H2U	w	20	55	-	2/7/38/39	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
57	PSU	y	55	57	-	2/7/25/26	0/2/2/2
1	6MZ	A	2030	60,1	-	3/9/27/28	0/3/3/3
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	2/9/27/28	0/3/3/3
57	MIA	y	37	57	-	4/15/33/34	0/3/3/3
1	OMU	A	2552	1	-	2/9/27/28	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
55	H2U	v	20	60,55	-	0/7/38/39	0/2/2/2
57	PSU	y	32	57	-	1/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
34	PSU	a	516	34	-	3/7/25/26	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	OMG	A	2251	55,1	-	0/9/27/28	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	7MG	A	2069	1	-	2/7/37/38	0/3/3/3
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	6MZ	A	1618	1	-	5/9/27/28	0/3/3/3
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	MA6	a	1518	34	-	4/11/29/30	0/3/3/3
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2498	60,1	-	1/9/27/28	0/2/2/2
1	2MG	A	2445	1	-	2/9/27/28	0/3/3/3
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
1	PSU	A	746	60,1	-	1/7/25/26	0/2/2/2
1	2MA	A	2503	60,1	-	2/7/25/26	0/3/3/3
34	7MG	a	527	34,60	-	2/7/37/38	0/3/3/3
34	MA6	a	1519	34	-	4/11/29/30	0/3/3/3
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/9/27/28	0/3/3/3
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.59	1.66	1.43
1	A	1915	3TD	C6-C5	15.85	1.52	1.35
1	A	1915	3TD	C2'-C1'	-14.27	1.34	1.53
1	A	1915	3TD	C2-N1	8.55	1.47	1.37
34	a	967	5MC	C5-C4	7.75	1.50	1.44
1	A	1962	5MC	C5-C4	7.57	1.49	1.44
1	A	747	5MC	C5-C4	7.53	1.49	1.44
34	a	1407	5MC	C5-C4	7.45	1.49	1.44
57	y	37	MIA	C13-C14	6.87	1.53	1.32
1	A	1915	3TD	C2-N3	6.31	1.51	1.38
57	y	37	MIA	C2-S10	-6.30	1.70	1.75
1	A	1915	3TD	O4'-C4'	-6.02	1.31	1.45
34	a	1518	MA6	C5-C4	5.32	1.48	1.39
1	A	1915	3TD	C6-N1	5.22	1.44	1.36
57	y	37	MIA	C5-C4	5.10	1.48	1.39
34	a	1519	MA6	C5-C4	5.06	1.48	1.39
55	v	7	4SU	C4-S4	-4.97	1.59	1.68
55	w	8	4SU	C4-S4	-4.93	1.60	1.68
57	y	8	4SU	C4-S4	-4.89	1.60	1.68
1	A	1618	6MZ	C5-C4	4.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2030	6MZ	C5-C4	4.75	1.47	1.39
1	A	2503	2MA	C5-C4	4.61	1.47	1.39
57	y	39	PSU	C6-C5	4.44	1.40	1.35
1	A	2580	PSU	C6-C5	4.38	1.40	1.35
1	A	1911	PSU	C6-C5	4.33	1.40	1.35
1	A	2604	PSU	C6-C5	4.33	1.40	1.35
1	A	955	PSU	C6-C5	4.33	1.40	1.35
1	A	2457	PSU	C6-C5	4.33	1.40	1.35
1	A	1917	PSU	C6-C5	4.32	1.40	1.35
1	A	746	PSU	C6-C5	4.31	1.40	1.35
57	y	55	PSU	C6-C5	4.22	1.40	1.35
55	v	55	PSU	C6-C5	4.21	1.39	1.35
34	a	516	PSU	C6-C5	4.20	1.39	1.35
1	A	2605	PSU	C6-C5	4.18	1.39	1.35
57	y	32	PSU	C6-C5	4.13	1.39	1.35
1	A	2069	7MG	C4-N9	-4.07	1.32	1.37
1	A	2504	PSU	C6-C5	4.01	1.39	1.35
55	w	55	PSU	C6-C5	4.00	1.39	1.35
1	A	745	1MG	C2-N1	3.52	1.43	1.37
57	y	46	7MG	C5-C4	3.50	1.48	1.37
34	a	1518	MA6	C5-C6	3.50	1.50	1.41
34	a	527	7MG	C5-C4	3.48	1.48	1.37
34	a	1519	MA6	C5-C6	3.38	1.50	1.41
1	A	2251	OMG	C5-C4	3.32	1.47	1.38
1	A	1835	2MG	C5-C4	3.25	1.47	1.38
1	A	745	1MG	C5-C4	3.24	1.47	1.38
1	A	2069	7MG	C5-C4	3.23	1.47	1.37
55	v	54	5MU	C6-C5	3.19	1.39	1.34
34	a	1407	5MC	C6-C5	3.19	1.39	1.34
57	y	37	MIA	C5-C6	3.18	1.49	1.41
34	a	966	2MG	C5-C4	3.18	1.47	1.38
34	a	967	5MC	C6-C5	3.15	1.39	1.34
34	a	527	7MG	C4-N9	-3.15	1.34	1.37
57	y	54	5MU	C2-N1	3.14	1.43	1.38
55	w	54	5MU	C6-C5	3.14	1.39	1.34
34	a	1207	2MG	C5-C4	3.14	1.47	1.38
1	A	1939	5MU	C6-C5	3.13	1.39	1.34
1	A	1962	5MC	C6-C5	3.08	1.39	1.34
57	y	46	7MG	C4-N9	-3.07	1.34	1.37
34	a	1516	2MG	C5-C4	3.04	1.47	1.38
57	y	8	4SU	C2-N1	3.00	1.43	1.38
57	y	54	5MU	C6-C5	2.99	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	54	5MU	C2-N1	2.98	1.43	1.38
55	w	8	4SU	C2-N1	2.97	1.43	1.38
1	A	1915	3TD	O2'-C2'	2.96	1.50	1.43
55	w	8	4SU	C4-N3	-2.94	1.34	1.37
1	A	2552	OMU	C2-N1	2.93	1.43	1.38
1	A	2445	2MG	C5-C4	2.93	1.46	1.38
55	v	54	5MU	C2-N1	2.91	1.43	1.38
1	A	2503	2MA	C5-C6	2.90	1.49	1.41
1	A	747	5MC	C6-C5	2.90	1.39	1.34
1	A	1915	3TD	C10-N3	-2.89	1.41	1.47
57	y	8	4SU	C4-N3	-2.88	1.34	1.37
1	A	1915	3TD	C4-N3	2.88	1.46	1.40
1	A	2030	6MZ	C5-C6	2.82	1.48	1.41
1	A	1618	6MZ	C5-C6	2.82	1.48	1.41
55	v	7	4SU	C2-N1	2.78	1.42	1.38
1	A	1835	2MG	C2-N3	2.76	1.37	1.32
1	A	2552	OMU	C4-N3	-2.70	1.34	1.38
55	w	54	5MU	C4-C5	2.70	1.49	1.44
1	A	1939	5MU	C4-C5	2.68	1.49	1.44
55	v	7	4SU	C4-N3	-2.67	1.34	1.37
34	a	1498	UR3	C2-N1	2.65	1.42	1.38
55	v	54	5MU	C4-C5	2.65	1.49	1.44
1	A	1939	5MU	C2-N1	2.62	1.42	1.38
34	a	1519	MA6	C5-N7	-2.62	1.34	1.39
34	a	966	2MG	C2-N3	2.58	1.36	1.32
57	y	54	5MU	C4-C5	2.56	1.49	1.44
55	v	7	4SU	C5-C4	-2.54	1.39	1.42
57	y	8	4SU	C5-C4	-2.50	1.39	1.42
1	A	2457	PSU	C4-N3	-2.48	1.34	1.38
1	A	2503	2MA	C8-N7	2.48	1.36	1.31
1	A	1915	3TD	O2-C2	-2.47	1.18	1.23
1	A	1835	2MG	C5-N7	-2.46	1.34	1.39
1	A	2251	OMG	C5-N7	-2.46	1.34	1.39
1	A	1939	5MU	C4-N3	-2.46	1.34	1.38
1	A	2580	PSU	C4-N3	-2.45	1.34	1.38
1	A	2604	PSU	C4-N3	-2.44	1.34	1.38
1	A	2504	PSU	C4-N3	-2.44	1.34	1.38
1	A	2449	H2U	C2-N3	-2.43	1.33	1.38
1	A	2605	PSU	C4-N3	-2.43	1.34	1.38
34	a	1207	2MG	C2-N3	2.42	1.36	1.32
1	A	1917	PSU	C4-N3	-2.42	1.34	1.38
55	w	54	5MU	C4-N3	-2.41	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	y	37	MIA	C8-N7	2.40	1.36	1.31
55	v	54	5MU	C4-N3	-2.40	1.34	1.38
1	A	1618	6MZ	C8-N7	2.40	1.36	1.31
1	A	1915	3TD	O3'-C3'	-2.39	1.37	1.43
34	a	1519	MA6	C6-N6	2.38	1.43	1.36
1	A	1835	2MG	C6-N1	-2.38	1.34	1.38
55	w	8	4SU	C5-C4	-2.35	1.39	1.42
1	A	1915	3TD	C3'-C4'	2.35	1.58	1.53
1	A	2030	6MZ	C8-N7	2.35	1.36	1.31
1	A	2449	H2U	C4-N3	-2.34	1.33	1.37
1	A	2503	2MA	C5-N7	-2.31	1.34	1.39
57	y	37	MIA	C5-N7	-2.30	1.34	1.39
34	a	1518	MA6	C6-N6	2.30	1.43	1.36
34	a	1518	MA6	C5-N7	-2.30	1.34	1.39
1	A	745	1MG	C5-N7	-2.29	1.34	1.39
34	a	1516	2MG	C2-N3	2.28	1.36	1.32
1	A	2251	OMG	C6-N1	-2.28	1.34	1.38
1	A	1618	6MZ	C5-N7	-2.27	1.34	1.39
57	y	55	PSU	C4-N3	-2.27	1.34	1.38
57	y	54	5MU	C4-N3	-2.27	1.34	1.38
34	a	1518	MA6	C8-N7	2.26	1.36	1.31
34	a	1207	2MG	C5-N7	-2.25	1.34	1.39
57	y	39	PSU	C4-N3	-2.24	1.34	1.38
34	a	516	PSU	C4-N3	-2.24	1.34	1.38
1	A	2030	6MZ	C5-N7	-2.24	1.35	1.39
1	A	746	PSU	C4-N3	-2.22	1.34	1.38
1	A	2445	2MG	C5-N7	-2.22	1.34	1.39
34	a	1516	2MG	C5-N7	-2.22	1.34	1.39
34	a	966	2MG	C5-N7	-2.21	1.34	1.39
55	w	55	PSU	C4-N3	-2.21	1.34	1.38
1	A	2445	2MG	C2-N3	2.20	1.36	1.32
57	y	32	PSU	C4-N3	-2.19	1.34	1.38
55	v	55	PSU	C4-N3	-2.19	1.34	1.38
34	a	1519	MA6	C8-N7	2.19	1.35	1.31
1	A	2552	OMU	C6-C5	2.18	1.40	1.35
1	A	955	PSU	C4-N3	-2.16	1.34	1.38
1	A	2503	2MA	C4-N9	-2.16	1.33	1.37
34	a	527	7MG	C6-N1	-2.16	1.34	1.38
1	A	1911	PSU	C4-N3	-2.16	1.34	1.38
57	y	20	H2U	C2-N3	-2.14	1.34	1.38
1	A	2445	2MG	C6-N1	-2.12	1.34	1.38
57	y	16	H2U	C2-N3	-2.10	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	20	H2U	C2-N3	-2.09	1.34	1.38
57	y	37	MIA	C2-N1	2.09	1.37	1.34
57	y	46	7MG	C5-C6	2.09	1.48	1.43
34	a	1498	UR3	C6-C5	2.08	1.39	1.35
1	A	2069	7MG	C5-C6	2.06	1.48	1.43
55	w	8	4SU	C6-C5	2.05	1.39	1.35
34	a	1516	2MG	C4-N9	-2.04	1.32	1.38
57	y	8	4SU	C6-C5	2.03	1.39	1.35
57	y	37	MIA	C2-N3	2.01	1.37	1.34
55	v	55	PSU	C4-C5	2.01	1.49	1.44
34	a	966	2MG	C6-N1	-2.00	1.35	1.38

All (336) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1207	2MG	C2-N3-C4	8.47	122.60	112.00
34	a	527	7MG	N9-C4-N3	8.41	137.79	125.46
34	a	966	2MG	C2-N3-C4	8.32	122.41	112.00
57	y	37	MIA	C5-C4-N3	-8.20	118.54	127.18
57	y	46	7MG	N9-C4-N3	8.18	137.45	125.46
57	y	37	MIA	C12-C13-C14	-8.01	112.63	127.01
1	A	1835	2MG	C2-N3-C4	7.78	121.73	112.00
1	A	2445	2MG	C2-N3-C4	7.77	121.72	112.00
34	a	1516	2MG	C2-N3-C4	7.55	121.44	112.00
34	a	1207	2MG	N1-C2-N2	7.36	124.08	116.56
1	A	2069	7MG	N9-C4-N3	7.32	136.18	125.46
1	A	2503	2MA	C5-C4-N3	-7.28	119.51	127.18
34	a	1498	UR3	C4-N3-C2	-6.85	119.07	124.58
1	A	1835	2MG	C5-C4-N3	-6.49	118.06	128.39
57	y	8	4SU	C4-N3-C2	-6.42	121.16	127.31
55	v	7	4SU	C4-N3-C2	-6.41	121.17	127.31
34	a	966	2MG	C5-C4-N3	-6.41	118.19	128.39
1	A	2457	PSU	N1-C2-N3	6.39	121.91	115.17
1	A	2504	PSU	N1-C2-N3	6.38	121.90	115.17
34	a	1207	2MG	C5-C4-N3	-6.35	118.28	128.39
55	w	8	4SU	C4-N3-C2	-6.35	121.23	127.31
1	A	2251	OMG	C5-C4-N3	-6.34	118.30	128.39
57	y	55	PSU	N1-C2-N3	6.26	121.77	115.17
57	y	37	MIA	N3-C4-N9	6.22	134.89	126.99
57	y	32	PSU	N1-C2-N3	6.20	121.70	115.17
55	w	55	PSU	N1-C2-N3	6.17	121.68	115.17
55	v	55	PSU	N1-C2-N3	6.15	121.66	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	516	PSU	N1-C2-N3	6.13	121.64	115.17
1	A	1911	PSU	N1-C2-N3	6.11	121.61	115.17
1	A	1917	PSU	N1-C2-N3	6.10	121.60	115.17
57	y	39	PSU	N1-C2-N3	6.09	121.59	115.17
1	A	746	PSU	N1-C2-N3	6.09	121.59	115.17
1	A	2605	PSU	N1-C2-N3	6.05	121.55	115.17
1	A	955	PSU	N1-C2-N3	5.98	121.48	115.17
34	a	1519	MA6	C5-C4-N3	-5.98	118.48	126.72
1	A	2604	PSU	N1-C2-N3	5.98	121.47	115.17
1	A	2030	6MZ	C5-C4-N3	-5.87	118.63	126.72
1	A	1618	6MZ	C5-C4-N3	-5.84	118.67	126.72
34	a	1516	2MG	C5-C4-N3	-5.80	119.16	128.39
1	A	2445	2MG	C5-C4-N3	-5.79	119.18	128.39
34	a	966	2MG	N1-C2-N2	5.78	122.46	116.56
1	A	2580	PSU	N1-C2-N3	5.62	121.09	115.17
1	A	2503	2MA	N3-C4-N9	5.52	134.00	126.99
1	A	745	1MG	C5-C4-N3	-5.43	119.75	128.39
55	v	7	4SU	C5-C4-N3	5.43	119.80	114.75
34	a	1518	MA6	C5-C4-N3	-5.41	119.26	126.72
55	w	8	4SU	C5-C4-N3	5.40	119.77	114.75
57	y	8	4SU	C5-C4-N3	5.34	119.72	114.75
34	a	527	7MG	C5-C4-N3	-5.25	118.28	128.13
1	A	1915	3TD	N1-C2-N3	5.21	119.92	116.13
57	y	46	7MG	C5-C4-N3	-5.17	118.43	128.13
1	A	1939	5MU	N3-C2-N1	5.09	121.52	114.89
1	A	2251	OMG	C2-N3-C4	5.09	121.07	112.30
55	v	20	H2U	O4'-C1'-N1	5.04	116.16	109.30
1	A	2552	OMU	N3-C2-N1	5.02	121.43	114.89
1	A	2069	7MG	C5-C4-N3	-5.01	118.73	128.13
55	w	54	5MU	N3-C2-N1	4.93	121.31	114.89
34	a	1518	MA6	C2-N1-C6	4.90	123.81	111.83
1	A	2069	7MG	C2-N3-C4	4.89	120.73	112.30
55	v	54	5MU	N3-C2-N1	4.89	121.25	114.89
34	a	1519	MA6	C4-C5-N7	-4.88	105.00	110.58
34	a	1207	2MG	N2-C2-N3	-4.87	114.31	120.51
1	A	1835	2MG	N9-C4-N3	4.80	135.56	125.95
34	a	1519	MA6	C2-N1-C6	4.77	123.49	111.83
1	A	1939	5MU	C4-N3-C2	-4.76	121.10	127.34
57	y	8	4SU	N3-C2-N1	4.76	121.08	114.89
57	y	54	5MU	N3-C2-N1	4.74	121.06	114.89
1	A	2552	OMU	C4-N3-C2	-4.73	120.75	126.61
57	y	46	7MG	C2-N3-C4	4.71	120.41	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2251	OMG	N9-C4-N3	4.69	135.34	125.95
1	A	745	1MG	C2-N3-C4	4.68	122.50	111.98
1	A	2069	7MG	N9-C8-N7	-4.66	96.78	103.37
34	a	966	2MG	N9-C4-N3	4.65	135.24	125.95
1	A	2030	6MZ	N3-C4-N9	4.64	135.06	127.17
1	A	1618	6MZ	N3-C4-N9	4.62	135.03	127.17
55	w	8	4SU	N3-C2-N1	4.56	120.83	114.89
34	a	527	7MG	C2-N3-C4	4.55	120.14	112.30
55	v	7	4SU	C5-C4-S4	-4.55	119.11	124.31
1	A	1915	3TD	C4-N3-C2	-4.44	119.91	124.61
57	y	46	7MG	N9-C8-N7	-4.43	97.11	103.37
34	a	527	7MG	N9-C8-N7	-4.41	97.12	103.37
57	y	54	5MU	C4-N3-C2	-4.37	121.61	127.34
55	v	7	4SU	N3-C2-N1	4.33	120.53	114.89
1	A	1911	PSU	O2-C2-N1	-4.30	118.36	122.79
55	w	54	5MU	C4-N3-C2	-4.29	121.71	127.34
34	a	1518	MA6	C4-C5-N7	-4.25	105.72	110.58
1	A	1939	5MU	C5-C4-N3	4.18	118.96	115.32
34	a	1207	2MG	N9-C4-N3	4.17	134.29	125.95
34	a	1519	MA6	N3-C4-N9	4.16	134.25	127.17
1	A	2605	PSU	C4-N3-C2	-4.16	120.64	126.37
55	v	54	5MU	C4-N3-C2	-4.14	121.92	127.34
1	A	747	5MC	CM5-C5-C6	-4.12	117.28	122.85
57	y	54	5MU	C5-C4-N3	4.11	118.90	115.32
1	A	745	1MG	N9-C4-N3	4.08	134.12	125.95
1	A	1915	3TD	C1'-C5-C4	3.99	123.67	117.61
57	y	8	4SU	C5-C4-S4	-3.98	119.75	124.31
57	y	55	PSU	C4-N3-C2	-3.98	120.88	126.37
1	A	2504	PSU	C4-N3-C2	-3.97	120.90	126.37
1	A	955	PSU	C4-N3-C2	-3.97	120.90	126.37
57	y	37	MIA	C16-C14-C13	-3.96	110.77	122.66
34	a	1518	MA6	N1-C2-N3	-3.95	122.60	128.58
57	y	32	PSU	C4-N3-C2	-3.91	120.99	126.37
55	w	54	5MU	C5-C4-N3	3.90	118.71	115.32
57	y	37	MIA	C4-C5-N7	-3.90	106.12	110.58
1	A	2457	PSU	C4-N3-C2	-3.90	121.00	126.37
55	w	55	PSU	C4-N3-C2	-3.89	121.01	126.37
1	A	2445	2MG	C6-C5-N7	3.89	137.37	130.29
34	a	516	PSU	C4-N3-C2	-3.89	121.01	126.37
57	y	39	PSU	C4-N3-C2	-3.89	121.02	126.37
1	A	746	PSU	C4-N3-C2	-3.88	121.03	126.37
1	A	1911	PSU	C4-N3-C2	-3.87	121.03	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	955	PSU	C6-C5-C4	-3.87	115.56	118.17
55	v	54	5MU	C5-C4-N3	3.86	118.68	115.32
34	a	1407	5MC	C5-C4-N3	-3.86	117.80	121.75
55	v	55	PSU	C4-N3-C2	-3.82	121.11	126.37
34	a	1516	2MG	C6-C5-N7	3.82	137.24	130.29
34	a	1518	MA6	C2-N3-C4	3.80	121.12	111.83
57	y	20	H2U	O4'-C1'-N1	3.80	114.48	109.30
34	a	1407	5MC	CM5-C5-C6	-3.79	117.72	122.85
1	A	747	5MC	C5-C4-N3	-3.79	117.87	121.75
34	a	1518	MA6	N3-C4-N9	3.79	133.62	127.17
1	A	2445	2MG	N9-C4-N3	3.78	133.52	125.95
1	A	1962	5MC	CM5-C5-C6	-3.78	117.74	122.85
34	a	1519	MA6	C2-N3-C4	3.76	121.02	111.83
1	A	1917	PSU	C4-N3-C2	-3.76	121.19	126.37
34	a	967	5MC	CM5-C5-C6	-3.75	117.78	122.85
34	a	1516	2MG	N9-C4-N3	3.75	133.45	125.95
34	a	1518	MA6	C9-N6-C6	-3.72	111.05	120.52
1	A	1618	6MZ	C2-N3-C4	3.72	120.92	111.83
1	A	2030	6MZ	C2-N3-C4	3.72	120.92	111.83
1	A	2449	H2U	N3-C2-N1	3.72	120.39	116.65
1	A	2504	PSU	O2-C2-N1	-3.71	118.96	122.79
55	w	8	4SU	C5-C4-S4	-3.70	120.08	124.31
57	y	37	MIA	C15-C14-C13	-3.69	111.59	122.66
1	A	2503	2MA	C4-C5-N7	-3.68	106.37	110.58
1	A	2604	PSU	C4-N3-C2	-3.68	121.30	126.37
1	A	745	1MG	N2-C2-N1	3.64	121.71	118.79
1	A	746	PSU	O2-C2-N1	-3.60	119.08	122.79
57	y	37	MIA	C2-N3-C4	3.59	121.69	112.29
1	A	2457	PSU	O2-C2-N1	-3.58	119.10	122.79
55	w	55	PSU	O2-C2-N1	-3.57	119.11	122.79
34	a	967	5MC	C5-C4-N3	-3.56	118.11	121.75
34	a	1518	MA6	O4'-C1'-N9	3.56	114.93	108.09
1	A	1917	PSU	O2-C2-N1	-3.55	119.13	122.79
1	A	2445	2MG	N1-C2-N2	3.55	120.18	116.56
34	a	1207	2MG	C6-C5-N7	3.55	136.74	130.29
1	A	2552	OMU	C5-C4-N3	3.55	119.77	114.80
34	a	1519	MA6	N1-C2-N3	-3.55	123.22	128.58
1	A	2605	PSU	O2-C2-N1	-3.54	119.14	122.79
57	y	32	PSU	O2-C2-N1	-3.53	119.14	122.79
34	a	1519	MA6	C10-N6-C6	-3.53	111.54	120.52
34	a	516	PSU	O2-C2-N1	-3.52	119.16	122.79
57	y	55	PSU	O2-C2-N1	-3.52	119.16	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2580	PSU	C4-N3-C2	-3.49	121.56	126.37
57	y	54	5MU	O4-C4-C5	-3.49	120.92	124.92
57	y	39	PSU	O2-C2-N1	-3.49	119.19	122.79
1	A	2030	6MZ	C4-C5-N7	-3.48	106.60	110.58
34	a	1519	MA6	C5-N7-C8	3.47	108.91	103.45
1	A	1618	6MZ	C4-C5-N7	-3.47	106.61	110.58
1	A	2580	PSU	C6-C5-C4	-3.47	115.83	118.17
34	a	966	2MG	N2-C2-N3	-3.45	116.11	120.51
1	A	1962	5MC	C5-C4-N3	-3.42	118.25	121.75
55	v	55	PSU	O2-C2-N1	-3.41	119.27	122.79
1	A	955	PSU	O2-C2-N1	-3.39	119.29	122.79
1	A	1618	6MZ	C6-C5-N7	3.38	136.11	132.43
34	a	966	2MG	C6-C5-N7	3.36	136.40	130.29
1	A	2030	6MZ	C6-C5-N7	3.33	136.06	132.43
1	A	2449	H2U	C5-C4-N3	3.33	120.23	116.69
34	a	1516	2MG	N1-C2-N2	3.31	119.94	116.56
57	y	37	MIA	C6-C5-N7	3.31	136.03	132.43
1	A	2449	H2U	O4'-C1'-N1	3.30	113.80	109.30
57	y	37	MIA	N6-C6-N1	3.30	122.76	118.33
1	A	1911	PSU	C6-C5-C4	-3.27	115.96	118.17
34	a	1498	UR3	C1'-N1-C2	3.24	122.35	117.04
1	A	1618	6MZ	N1-C2-N3	-3.24	123.69	128.58
34	a	1498	UR3	C5-C4-N3	3.23	119.30	115.04
1	A	2030	6MZ	N1-C2-N3	-3.23	123.69	128.58
1	A	2604	PSU	O2-C2-N1	-3.21	119.48	122.79
1	A	1939	5MU	O4-C4-C5	-3.19	121.27	124.92
1	A	2498	OMC	O2-C2-N3	-3.19	117.31	122.33
57	y	32	PSU	C3'-C2'-C1'	3.15	105.41	101.69
57	y	54	5MU	C5M-C5-C4	3.15	122.14	118.78
55	w	54	5MU	C5M-C5-C4	3.14	122.13	118.78
1	A	1962	5MC	O2-C2-N3	-3.14	117.39	122.33
1	A	1618	6MZ	C9-N6-C6	-3.09	119.98	122.85
34	a	1498	UR3	C6-N1-C2	-3.08	119.28	121.80
1	A	2605	PSU	C6-C5-C4	-3.07	116.10	118.17
1	A	2030	6MZ	C9-N6-C6	-3.05	120.02	122.85
1	A	1915	3TD	C10-N3-C4	3.03	122.34	117.64
55	v	54	5MU	O4-C4-C5	-3.03	121.45	124.92
34	a	1407	5MC	O2-C2-N3	-2.98	117.63	122.33
57	y	37	MIA	C5-N7-C8	2.98	108.13	103.45
34	a	527	7MG	C5-C6-N1	2.98	116.18	110.94
57	y	46	7MG	C5-C6-N1	2.97	116.16	110.94
1	A	2503	2MA	C4-N9-C8	2.96	108.85	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1835	2MG	C6-C5-N7	2.96	135.67	130.29
1	A	1917	PSU	C6-C5-C4	-2.94	116.19	118.17
55	w	55	PSU	C3'-C2'-C1'	2.94	105.16	101.69
1	A	2069	7MG	C5-C6-N1	2.93	116.11	110.94
55	v	54	5MU	C5M-C5-C4	2.93	121.91	118.78
1	A	2503	2MA	C2-N1-C6	2.91	122.57	118.10
34	a	1516	2MG	C4-C5-N7	-2.91	106.06	110.67
1	A	1939	5MU	O4'-C1'-N1	2.91	114.95	108.36
57	y	8	4SU	C6-N1-C2	-2.91	117.46	121.00
1	A	2552	OMU	C1'-N1-C2	2.90	122.81	117.59
1	A	1939	5MU	C5-C6-N1	-2.90	120.17	123.31
34	a	516	PSU	C3'-C2'-C1'	2.88	105.09	101.69
34	a	1518	MA6	C5-N7-C8	2.88	107.97	103.45
55	w	54	5MU	O4-C4-C5	-2.87	121.64	124.92
1	A	2251	OMG	C6-C5-N7	2.87	135.51	130.29
57	y	20	H2U	C5-C4-N3	2.85	119.72	116.69
1	A	2445	2MG	C4-C5-N7	-2.83	106.19	110.67
57	y	37	MIA	N3-C2-N1	-2.79	121.90	127.00
57	y	37	MIA	C2-N1-C6	2.79	122.83	117.54
34	a	1207	2MG	C4-C5-N7	-2.78	106.27	110.67
1	A	2580	PSU	O2-C2-N1	-2.77	119.93	122.79
34	a	967	5MC	O2-C2-N3	-2.76	117.97	122.33
34	a	1402	4OC	C6-C5-C4	2.72	120.28	117.00
55	w	20	H2U	O4'-C1'-N1	2.71	112.99	109.30
1	A	2503	2MA	C5-N7-C8	2.68	107.67	103.45
1	A	2580	PSU	C3'-C2'-C1'	2.67	104.84	101.69
1	A	1618	6MZ	C4-N9-C8	2.65	108.52	105.74
57	y	16	H2U	C5-C4-N3	2.63	119.49	116.69
1	A	746	PSU	C6-C5-C4	-2.63	116.40	118.17
1	A	2503	2MA	C6-C5-N7	2.63	137.16	132.09
1	A	2030	6MZ	C4-N9-C8	2.60	108.47	105.74
1	A	747	5MC	C5-C6-N1	-2.58	120.51	123.31
34	a	966	2MG	C4-C5-N7	-2.58	106.58	110.67
1	A	1917	PSU	C3'-C2'-C1'	2.57	104.72	101.69
34	a	1519	MA6	C10-N6-C9	-2.57	107.92	116.18
1	A	1618	6MZ	C5-N7-C8	2.56	107.48	103.45
1	A	2552	OMU	O4-C4-C5	-2.56	120.75	125.16
34	a	1207	2MG	O6-C6-C5	-2.56	119.78	126.53
1	A	745	1MG	C4-C5-N7	-2.56	106.62	110.67
55	w	8	4SU	C6-N1-C2	-2.55	117.89	121.00
1	A	1939	5MU	C5M-C5-C4	2.55	121.50	118.78
55	v	20	H2U	C5-C4-N3	2.55	119.40	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1407	5MC	O4'-C1'-N1	2.55	114.13	108.36
1	A	2030	6MZ	C5-N7-C8	2.54	107.44	103.45
1	A	2552	OMU	C6-N1-C2	-2.54	117.91	121.00
1	A	745	1MG	C6-C5-N7	2.53	134.97	129.36
1	A	2498	OMC	O4'-C1'-N1	2.51	114.04	108.36
34	a	1402	4OC	C5-C4-N3	-2.49	118.70	122.60
34	a	1402	4OC	O4'-C1'-N1	2.47	113.96	108.36
1	A	2030	6MZ	C3'-C2'-C1'	2.47	106.13	101.46
1	A	2552	OMU	O2-C2-N3	-2.47	116.94	121.49
1	A	1618	6MZ	C3'-C2'-C1'	2.46	106.12	101.46
1	A	1915	3TD	C3'-C2'-C1'	2.46	104.59	101.69
57	y	39	PSU	C6-C5-C4	-2.43	116.53	118.17
34	a	1498	UR3	C3U-N3-C2	2.43	121.57	117.33
55	v	54	5MU	O4'-C1'-N1	2.42	113.85	108.36
1	A	2457	PSU	C3'-C2'-C1'	2.42	104.54	101.69
55	v	55	PSU	C6-C5-C4	-2.39	116.56	118.17
1	A	2457	PSU	C6-C5-C4	-2.38	116.57	118.17
34	a	1519	MA6	C9-N6-C6	-2.37	114.49	120.52
1	A	2069	7MG	N2-C2-N3	-2.36	115.06	119.67
34	a	1518	MA6	C6-C5-N7	2.36	137.19	133.43
34	a	1207	2MG	C2-N1-C6	-2.35	121.70	124.55
1	A	2604	PSU	C6-C5-C4	-2.35	116.59	118.17
1	A	2069	7MG	O4'-C1'-N9	2.35	112.50	109.30
1	A	2251	OMG	C4-C5-N7	-2.35	106.95	110.67
1	A	2503	2MA	N9-C8-N7	-2.34	110.62	113.94
1	A	2069	7MG	N2-C2-N1	2.33	121.68	116.76
57	y	16	H2U	O4'-C1'-N1	2.32	112.46	109.30
1	A	1835	2MG	C4-C5-N7	-2.30	107.02	110.67
1	A	1962	5MC	CM5-C5-C4	2.30	124.29	120.51
57	y	16	H2U	C3'-C2'-C1'	2.30	105.81	101.46
1	A	2503	2MA	N6-C6-N1	2.30	120.12	117.03
57	y	37	MIA	C4-N9-C8	2.28	108.14	105.74
34	a	1402	4OC	O2-C2-N3	-2.28	118.74	122.33
34	a	1518	MA6	C3'-C2'-C1'	2.28	105.77	101.46
34	a	966	2MG	O6-C6-C5	-2.26	120.56	126.53
1	A	746	PSU	C3'-C2'-C1'	2.26	104.36	101.69
55	w	20	H2U	C2'-C3'-C4'	2.26	106.97	102.61
34	a	527	7MG	O4'-C1'-N9	2.25	112.37	109.30
55	v	7	4SU	O4'-C1'-N1	2.25	113.45	108.36
34	a	967	5MC	CM5-C5-C4	2.24	124.19	120.51
55	w	54	5MU	C3'-C2'-C1'	2.24	105.69	101.46
57	y	37	MIA	O4'-C1'-N9	2.24	112.38	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1402	4OC	C2'-C1'-N1	-2.24	110.00	114.24
1	A	1939	5MU	O2-C2-N1	-2.23	119.89	122.80
55	w	55	PSU	C6-C5-C4	-2.23	116.67	118.17
55	v	7	4SU	C6-N1-C2	-2.22	118.29	121.00
55	v	20	H2U	C5-C6-N1	-2.22	104.79	111.52
1	A	2445	2MG	O6-C6-C5	-2.21	120.69	126.53
34	a	1519	MA6	N9-C8-N7	-2.21	110.80	113.94
34	a	1407	5MC	CM5-C5-C4	2.21	124.14	120.51
34	a	1516	2MG	O6-C6-C5	-2.20	120.72	126.53
34	a	1519	MA6	O4'-C1'-N9	2.20	112.32	108.09
34	a	1516	2MG	N2-C2-N3	-2.20	117.71	120.51
55	w	54	5MU	C5M-C5-C6	-2.20	119.88	122.85
34	a	1207	2MG	C5-C6-N1	2.19	118.82	113.25
34	a	966	2MG	C5-C6-N1	2.18	118.81	113.25
34	a	1519	MA6	C4-C5-C6	2.18	118.16	115.91
1	A	1835	2MG	O6-C6-C5	-2.18	120.78	126.53
34	a	1519	MA6	C4-N9-C8	2.18	108.03	105.74
1	A	2069	7MG	O6-C6-C5	-2.17	122.29	127.62
55	w	54	5MU	C6-N1-C2	-2.17	119.14	121.30
55	v	54	5MU	C6-N1-C2	-2.17	119.14	121.30
1	A	2504	PSU	C6-C5-C4	-2.17	116.71	118.17
57	y	8	4SU	O2-C2-N3	-2.17	117.49	121.49
1	A	745	1MG	O6-C6-C5	-2.16	119.02	124.59
1	A	2251	OMG	O6-C6-C5	-2.16	120.83	126.53
34	a	1516	2MG	C2-N1-C6	-2.15	121.94	124.55
34	a	1519	MA6	C2'-C1'-N9	-2.14	107.98	113.30
1	A	2069	7MG	C6-C5-C4	-2.14	118.63	122.40
34	a	527	7MG	O6-C6-C5	-2.14	122.38	127.62
34	a	1519	MA6	C6-C5-N7	2.13	136.84	133.43
57	y	54	5MU	C1'-N1-C2	2.13	121.42	117.59
55	w	20	H2U	C5-C4-N3	2.13	118.95	116.69
1	A	2445	2MG	C5-C6-N1	2.12	118.65	113.25
57	y	46	7MG	O6-C6-C5	-2.11	122.44	127.62
57	y	54	5MU	C6-N1-C2	-2.11	119.20	121.30
34	a	516	PSU	C6-C5-C4	-2.10	116.75	118.17
55	w	54	5MU	O2-C2-N3	-2.10	117.62	121.49
57	y	37	MIA	C11-S10-C2	2.09	103.82	102.25
1	A	2449	H2U	O4-C4-C5	-2.09	117.92	122.20
1	A	2069	7MG	C6-C5-N7	2.09	135.17	131.93
1	A	1835	2MG	C5-C6-N1	2.09	118.57	113.25
1	A	2445	2MG	N2-C2-N3	-2.08	117.85	120.51
57	y	32	PSU	C6-C5-C4	-2.08	116.77	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1911	PSU	C3'-C2'-C1'	2.08	104.14	101.69
1	A	2552	OMU	O4'-C1'-N1	2.08	113.07	108.36
57	y	8	4SU	C3'-C2'-C1'	2.07	105.37	101.46
57	y	54	5MU	C5M-C5-C6	-2.06	120.06	122.85
1	A	2445	2MG	C2-N1-C6	-2.06	122.06	124.55
57	y	46	7MG	C6-C5-C4	-2.06	118.78	122.40
57	y	37	MIA	C3'-C2'-C1'	2.06	105.36	101.46
1	A	747	5MC	O2-C2-N3	-2.05	119.09	122.33
57	y	55	PSU	C3'-C2'-C1'	2.05	104.11	101.69
57	y	37	MIA	N9-C8-N7	-2.04	111.04	113.94
34	a	1516	2MG	C5-C6-N1	2.02	118.39	113.25
55	w	8	4SU	O2-C2-N3	-2.02	117.77	121.49
55	w	54	5MU	O4'-C1'-N1	2.01	112.91	108.36
55	w	54	5MU	C5-C6-N1	-2.00	121.14	123.31
1	A	1618	6MZ	N9-C8-N7	-2.00	111.09	113.94

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1618	6MZ	C5-C6-N6-C9
1	A	1618	6MZ	N1-C6-N6-C9
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	O4'-C1'-C5-C6
1	A	1915	3TD	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C4'-C5'-O5'
1	A	1917	PSU	O4'-C4'-C5'-O5'
1	A	1962	5MC	O4'-C4'-C5'-O5'
1	A	2030	6MZ	C4'-C5'-O5'-P
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2445	2MG	O4'-C4'-C5'-O5'
1	A	2503	2MA	O4'-C4'-C5'-O5'
1	A	2552	OMU	O4'-C1'-N1-C2
1	A	2552	OMU	O4'-C1'-N1-C6
34	a	1402	4OC	O4'-C4'-C5'-O5'
34	a	1518	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-C6-N6-C10
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
55	w	8	4SU	C3'-C4'-C5'-O5'
55	w	8	4SU	O4'-C4'-C5'-O5'
57	y	20	H2U	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
57	y	20	H2U	O4'-C1'-N1-C6
57	y	37	MIA	O4'-C4'-C5'-O5'
57	y	37	MIA	C12-C13-C14-C15
57	y	37	MIA	C12-C13-C14-C16
34	a	1498	UR3	O4'-C1'-N1-C2
1	A	1939	5MU	O4'-C4'-C5'-O5'
1	A	1962	5MC	C3'-C4'-C5'-O5'
1	A	2069	7MG	C3'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
1	A	2457	PSU	O4'-C4'-C5'-O5'
34	a	516	PSU	O4'-C4'-C5'-O5'
34	a	966	2MG	O4'-C4'-C5'-O5'
34	a	966	2MG	C3'-C4'-C5'-O5'
57	y	37	MIA	C3'-C4'-C5'-O5'
1	A	2030	6MZ	O4'-C4'-C5'-O5'
1	A	2503	2MA	C3'-C4'-C5'-O5'
34	a	516	PSU	C3'-C4'-C5'-O5'
57	y	16	H2U	O4'-C4'-C5'-O5'
57	y	55	PSU	C3'-C4'-C5'-O5'
34	a	1518	MA6	O4'-C1'-N9-C4
34	a	966	2MG	C4'-C5'-O5'-P
34	a	1518	MA6	N1-C6-N6-C9
34	a	1519	MA6	N1-C6-N6-C10
1	A	1917	PSU	C3'-C4'-C5'-O5'
34	a	1207	2MG	C3'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
55	w	8	4SU	C2'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C6
1	A	1939	5MU	C3'-C4'-C5'-O5'
1	A	2069	7MG	O4'-C4'-C5'-O5'
1	A	2457	PSU	C3'-C4'-C5'-O5'
55	v	7	4SU	O4'-C4'-C5'-O5'
57	y	46	7MG	C3'-C4'-C5'-O5'
34	a	1518	MA6	O4'-C1'-N9-C8
1	A	2504	PSU	O4'-C4'-C5'-O5'
57	y	46	7MG	O4'-C4'-C5'-O5'
57	y	55	PSU	O4'-C4'-C5'-O5'
34	a	527	7MG	C3'-C4'-C5'-O5'
57	y	16	H2U	C3'-C4'-C5'-O5'
34	a	1207	2MG	O4'-C4'-C5'-O5'
57	y	46	7MG	C2'-C1'-N9-C8
55	w	8	4SU	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
55	w	8	4SU	C2'-C1'-N1-C2
55	w	8	4SU	O4'-C1'-N1-C2
1	A	1618	6MZ	C4'-C5'-O5'-P
34	a	527	7MG	C4'-C5'-O5'-P
57	y	32	PSU	O4'-C1'-C5-C4
55	v	7	4SU	C3'-C4'-C5'-O5'
1	A	1618	6MZ	C2'-C1'-N9-C8
1	A	1618	6MZ	C2'-C1'-N9-C4
1	A	2504	PSU	C3'-C4'-C5'-O5'
55	w	20	H2U	O4'-C4'-C5'-O5'
34	a	1519	MA6	C4'-C5'-O5'-P
1	A	746	PSU	O4'-C1'-C5-C6
34	a	516	PSU	O4'-C1'-C5-C6
55	w	55	PSU	O4'-C1'-C5-C6
57	y	46	7MG	O4'-C1'-N9-C8
34	a	1519	MA6	C5-C6-N6-C9
55	w	20	H2U	C3'-C4'-C5'-O5'
1	A	2498	OMC	C4'-C5'-O5'-P
57	y	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	1498	UR3	1	0
55	w	20	H2U	1	0
1	A	1915	3TD	1	0
1	A	2030	6MZ	4	0
34	a	516	PSU	1	0
1	A	1618	6MZ	8	0
1	A	2498	OMC	3	0
1	A	2504	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1488 ligands modelled in this entry, 1485 are monoatomic - leaving 3 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	$\# Z > 2$
59	FME	A	3001	-	8,9,10	0.51	0	8,9,11	0.97	0
63	GTP	z	402	-	33,34,34	1.21	3 (9%)	50,54,54	1.75	8 (16%)
62	PHE	z	401	-	10,11,12	0.46	0	8,13,15	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	A	3001	-	-	1/7/9/11	-
63	GTP	z	402	-	-	1/22/38/38	0/3/3/3
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GTP	C5-C4	3.30	1.47	1.38
63	z	402	GTP	C5-N7	-2.11	1.34	1.39
63	z	402	GTP	C6-N1	-2.06	1.35	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GTP	C5-C4-N3	-6.16	118.58	128.39
63	z	402	GTP	C2-N3-C4	5.19	121.24	112.30
63	z	402	GTP	N9-C4-N3	4.62	135.19	125.95
63	z	402	GTP	C6-C5-N7	3.31	136.31	130.29
63	z	402	GTP	C4-C5-N7	-2.60	106.55	110.67
63	z	402	GTP	C3'-C2'-C1'	2.30	105.82	101.46
63	z	402	GTP	O6-C6-C5	-2.22	120.67	126.53
63	z	402	GTP	C5-C6-N1	2.02	118.39	113.25

There are no chirality outliers.

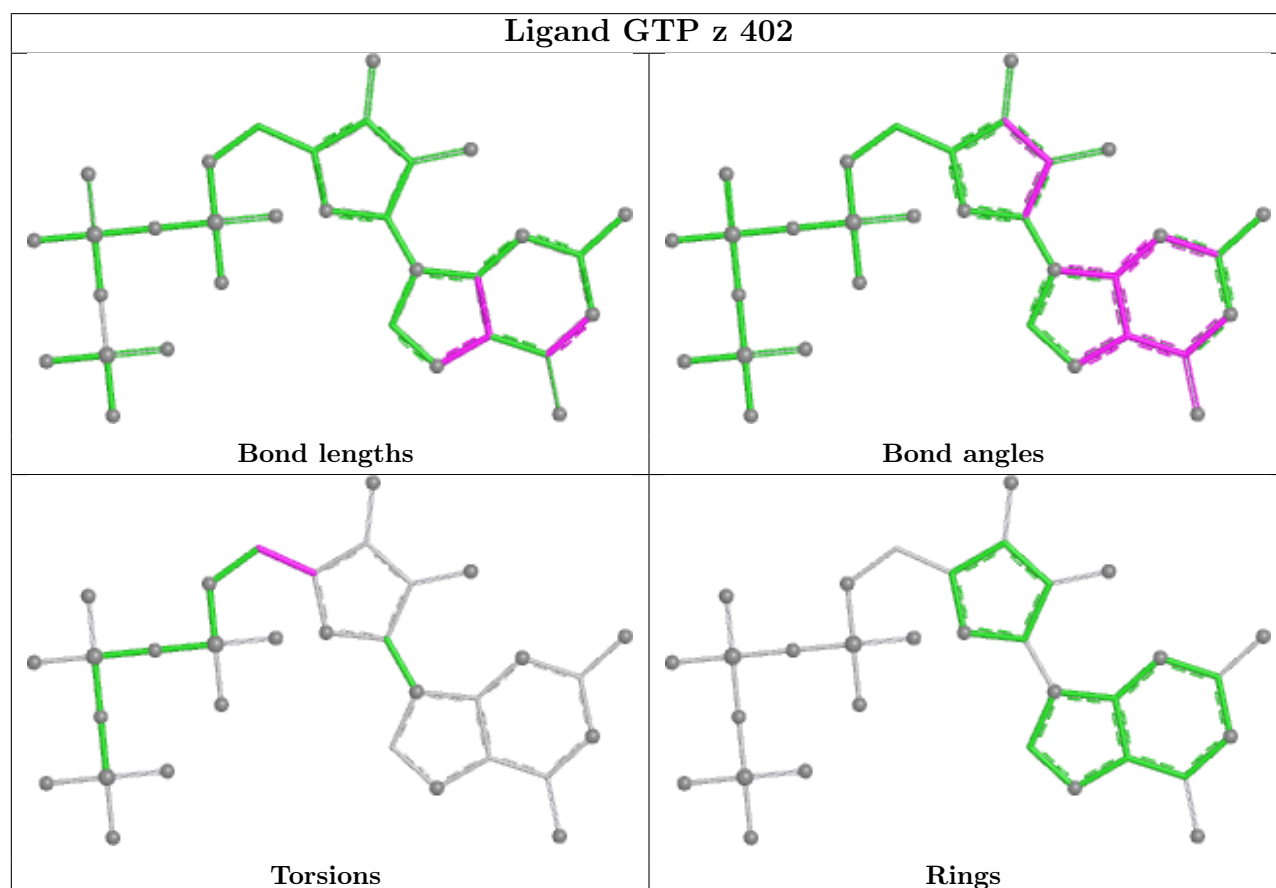
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	A	3001	FME	O-C-CA-CB
62	z	401	PHE	O-C-CA-CB
63	z	402	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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

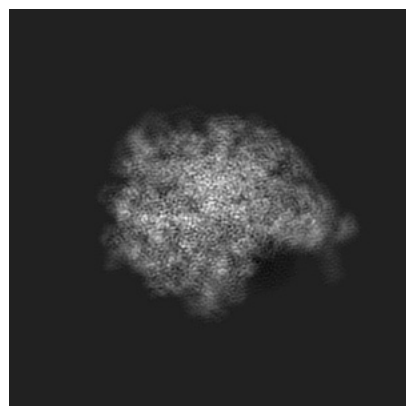
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8826. These allow visual inspection of the internal detail of the map and identification of artifacts.

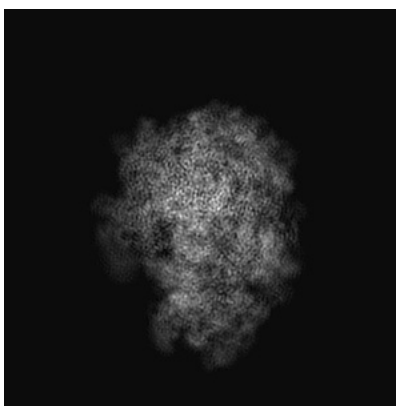
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

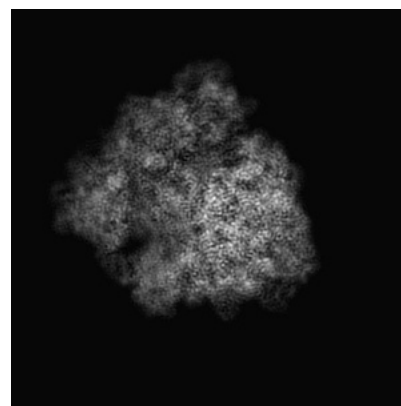
6.1.1 Primary map



X

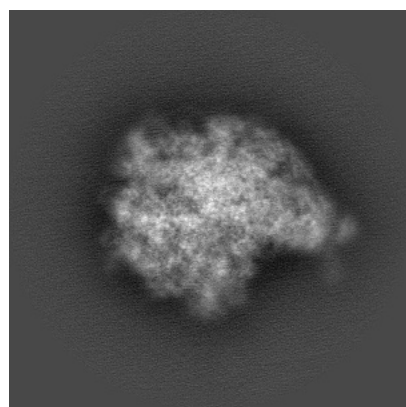


Y

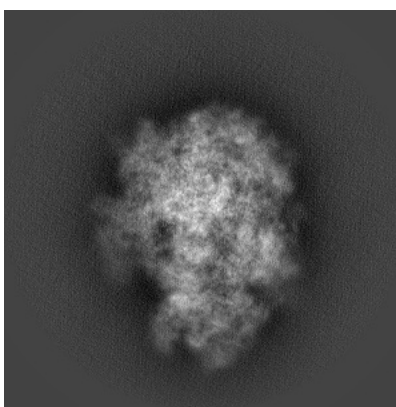


Z

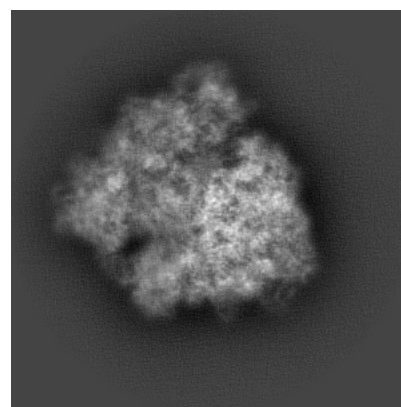
6.1.2 Raw map



X



Y

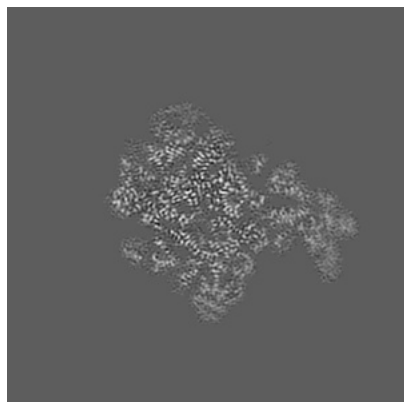


Z

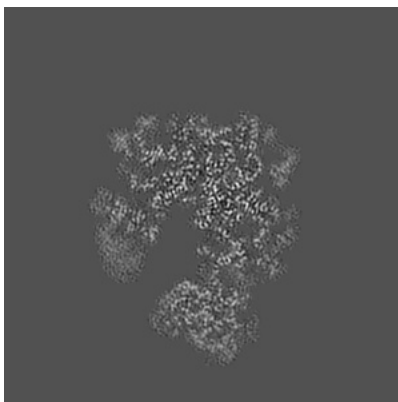
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

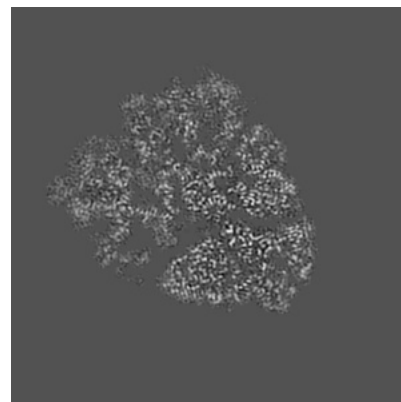
6.2.1 Primary map



X Index: 199

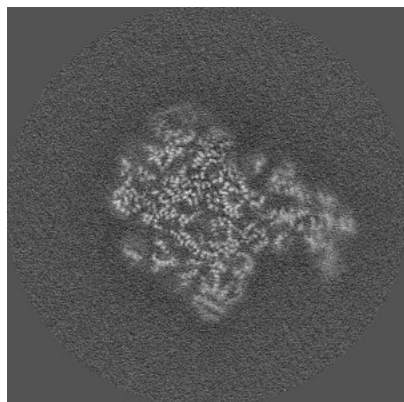


Y Index: 199

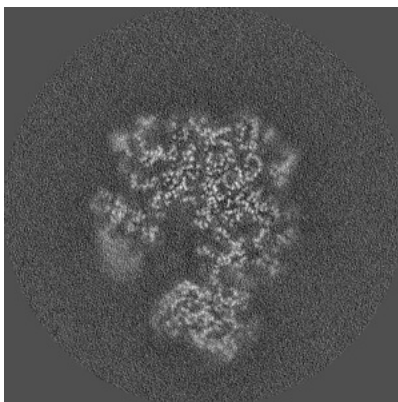


Z Index: 199

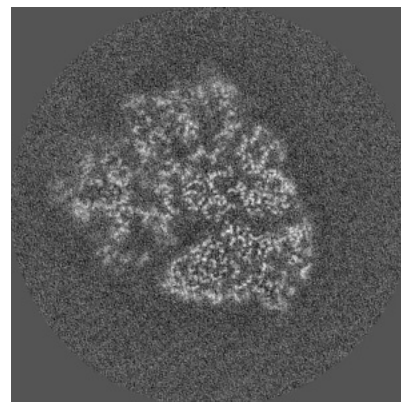
6.2.2 Raw map



X Index: 199



Y Index: 199

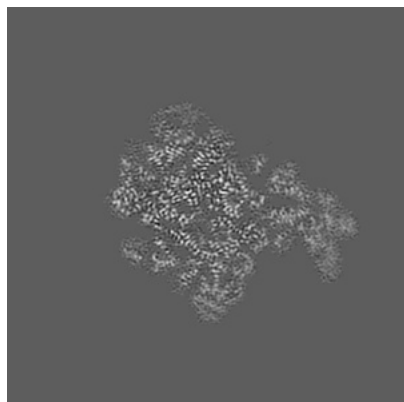


Z Index: 199

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

6.3 Largest variance slices [i](#)

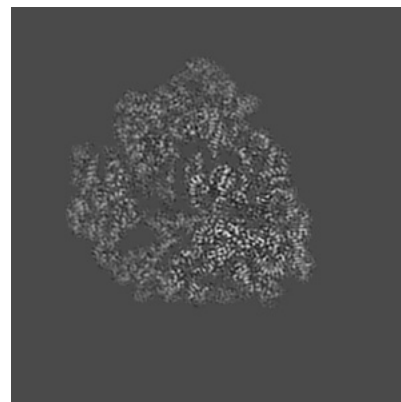
6.3.1 Primary map



X Index: 199

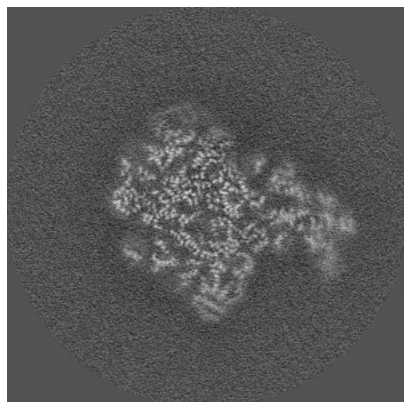


Y Index: 207

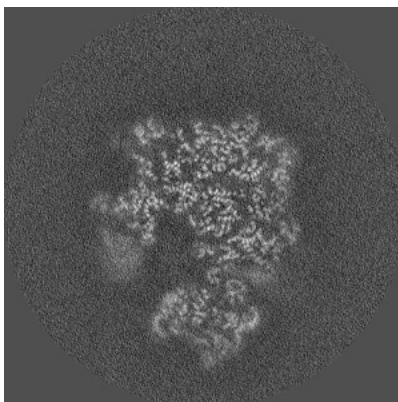


Z Index: 190

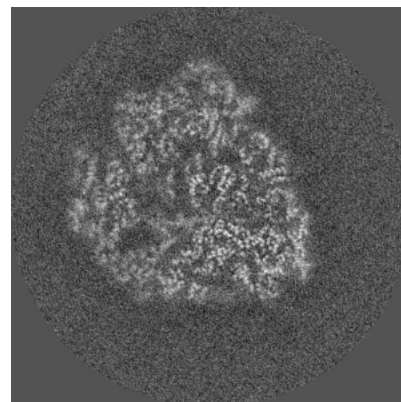
6.3.2 Raw map



X Index: 199



Y Index: 207

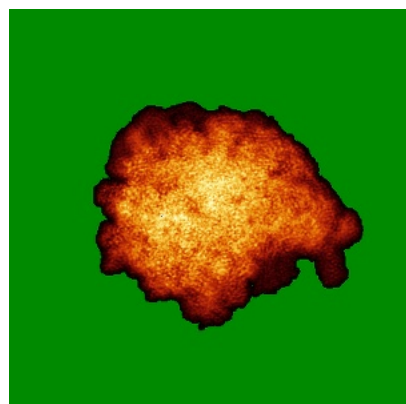


Z Index: 190

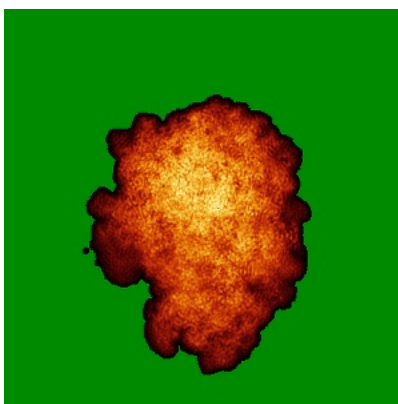
The images above show the largest variance slices of the map in three orthogonal directions.

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

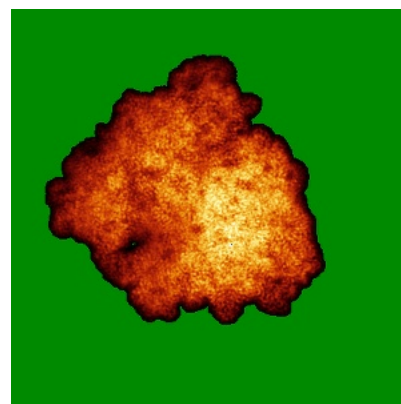
6.4.1 Primary map



X

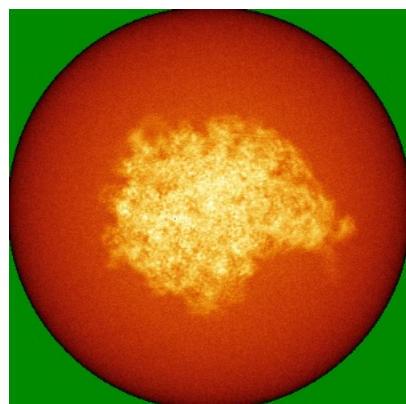


Y

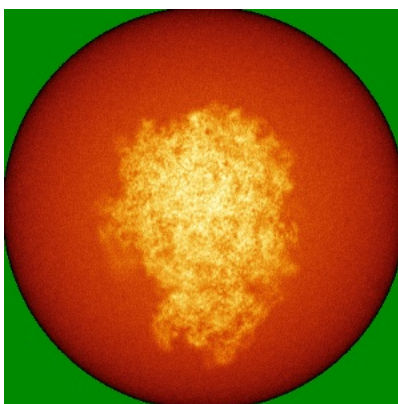


Z

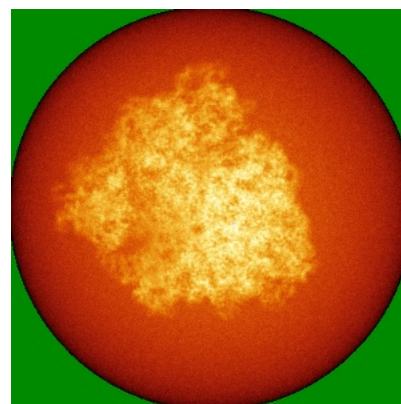
6.4.2 Raw map



X



Y

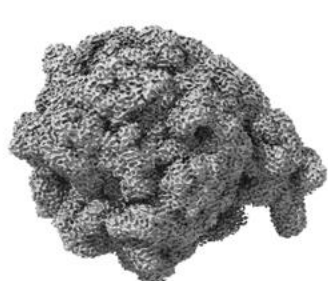


Z

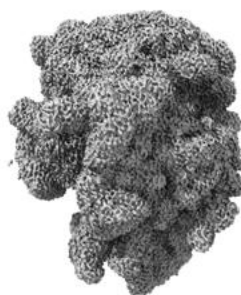
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

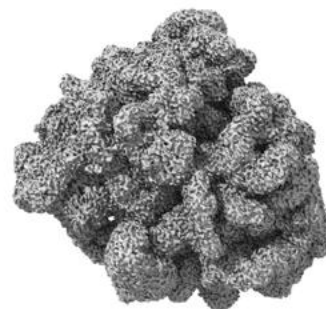
6.5.1 Primary map



X



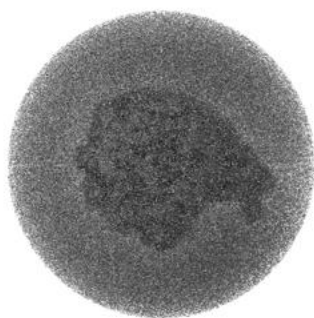
Y



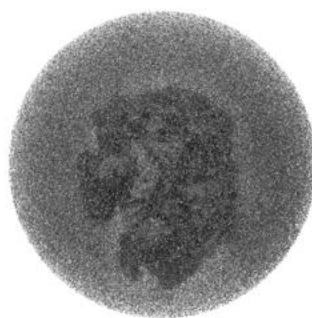
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00371. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

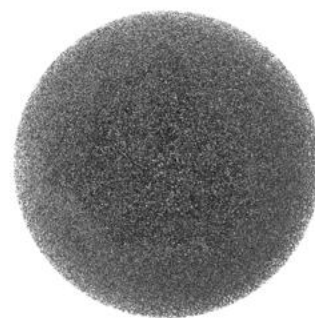
6.5.2 Raw map



X



Y



Z

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

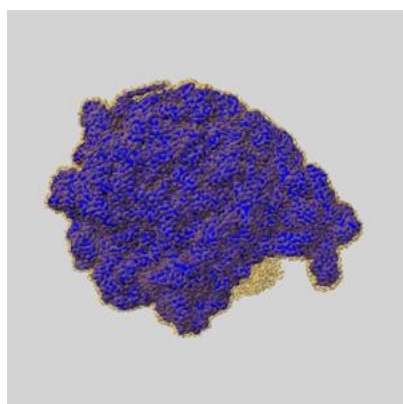
6.6 Mask visualisation [i](#)

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

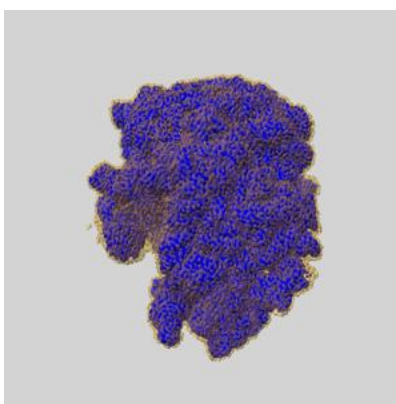
A mask typically either:

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

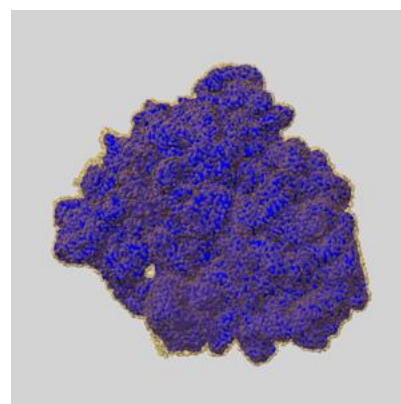
6.6.1 emd_8826_msk_1.map [i](#)



X



Y

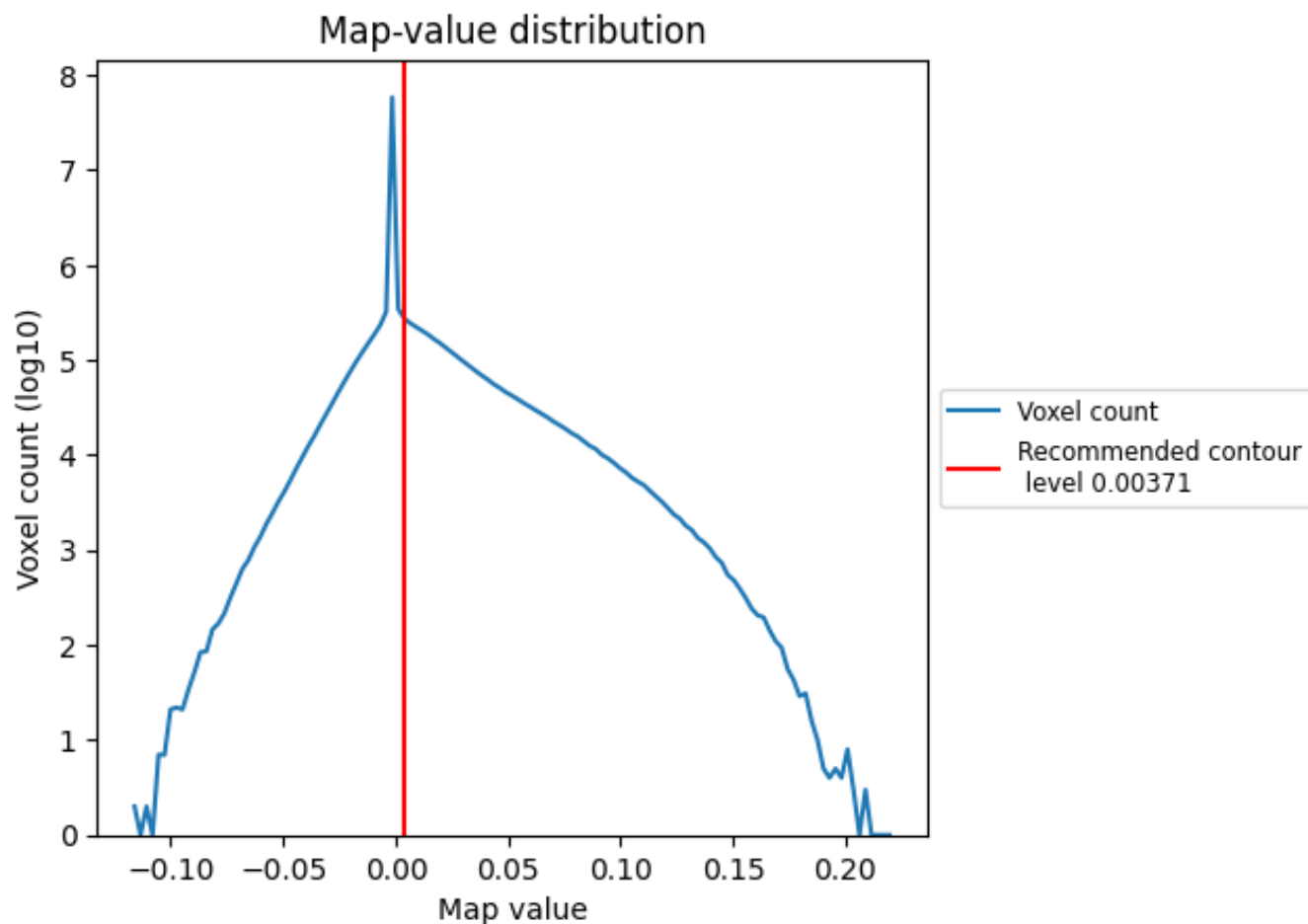


Z

7 Map analysis [i](#)

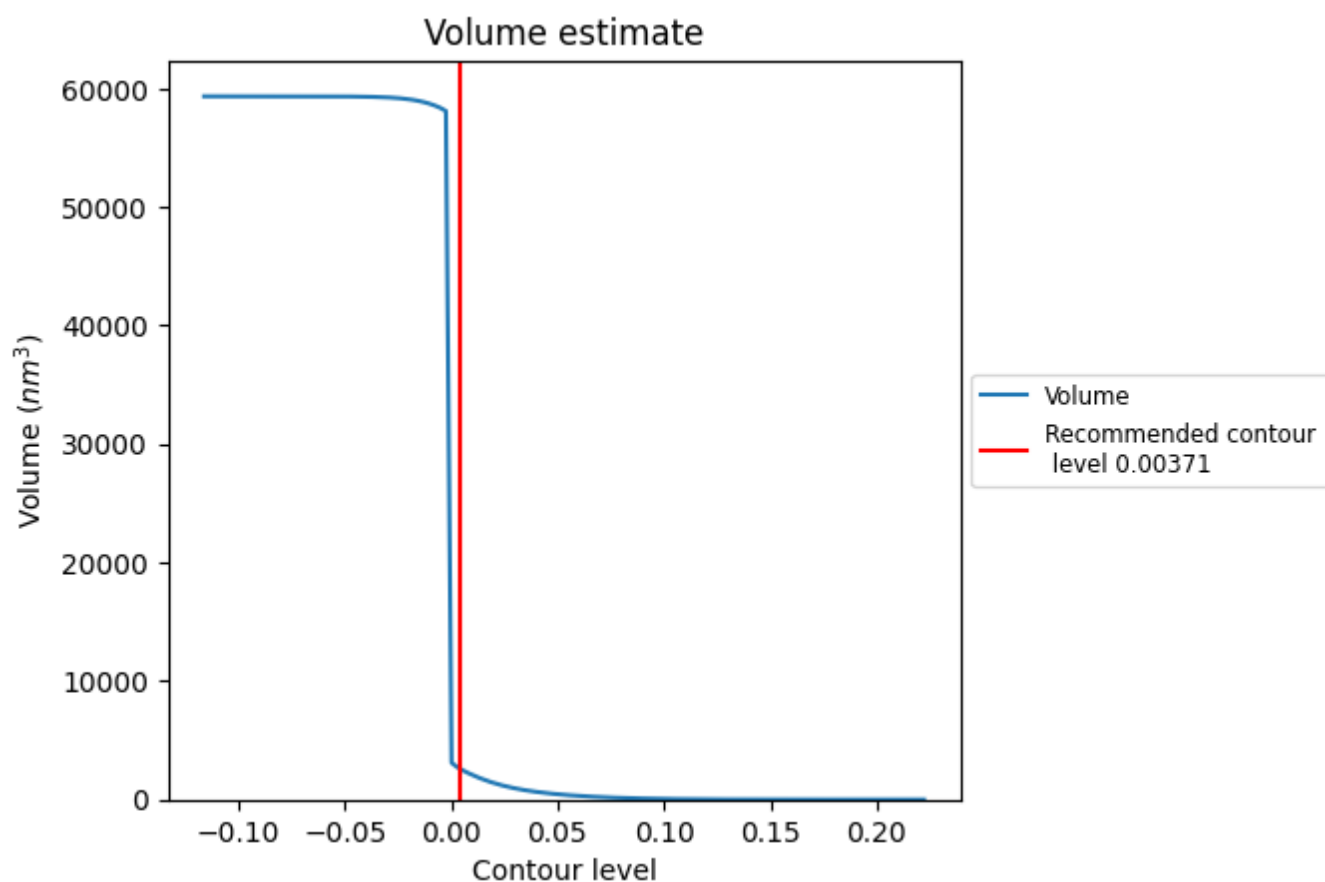
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

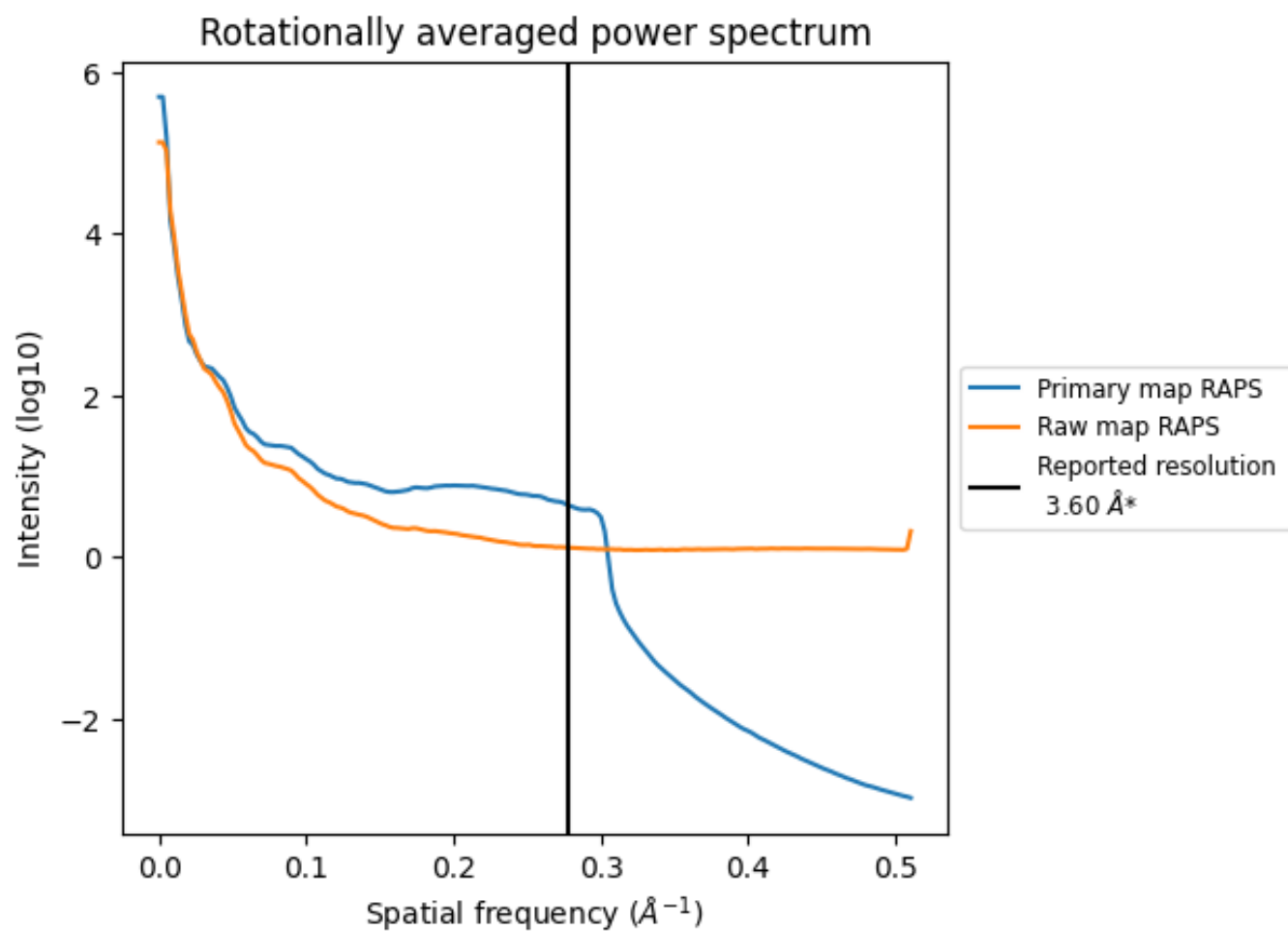
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2650 nm³; this corresponds to an approximate mass of 2393 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 ⓘ

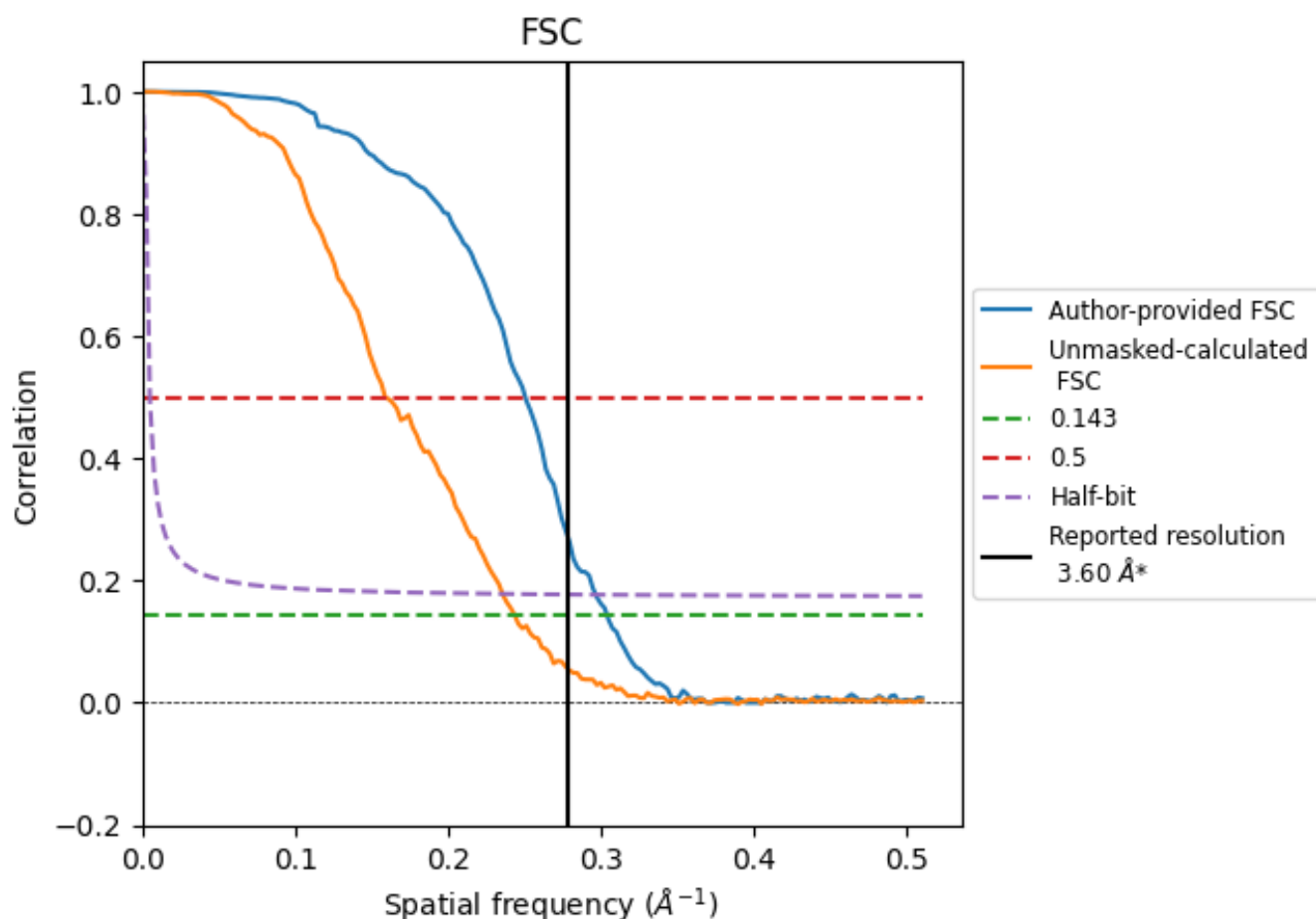


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

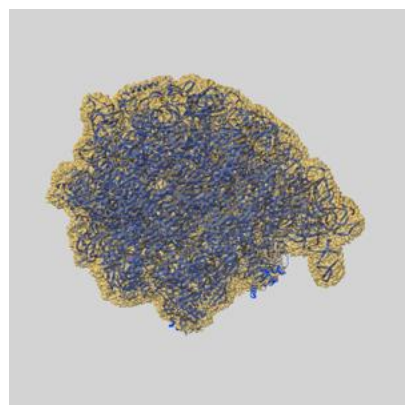
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.29	3.99	3.37
Unmasked-calculated*	4.10	6.29	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.10 differs from the reported value 3.6 by more than 10 %

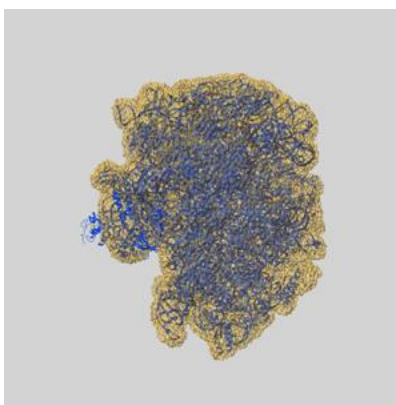
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8826 and PDB model 5WF0. Per-residue inclusion information can be found in section 3 on page 20.

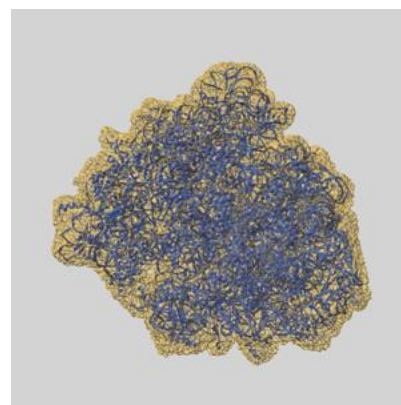
9.1 Map-model overlay [i](#)



X



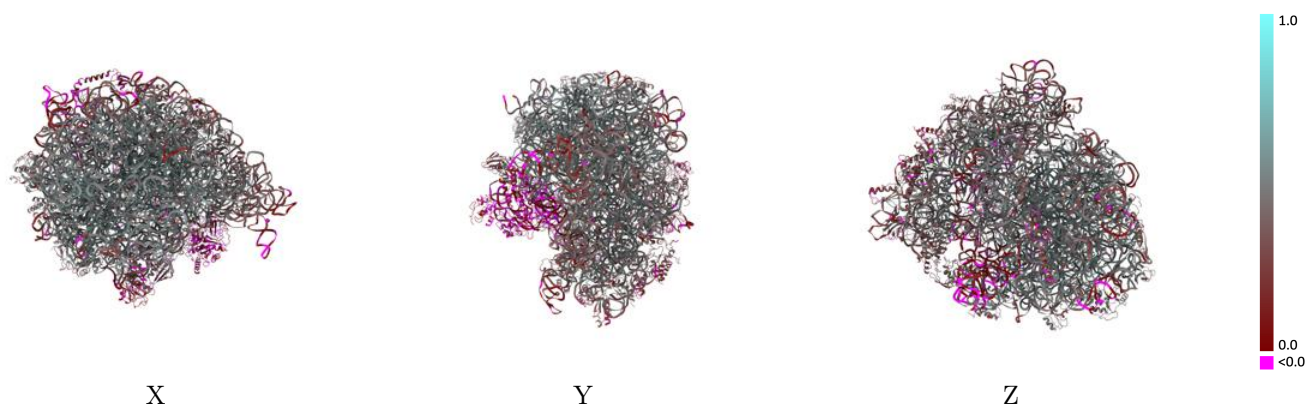
Y



Z

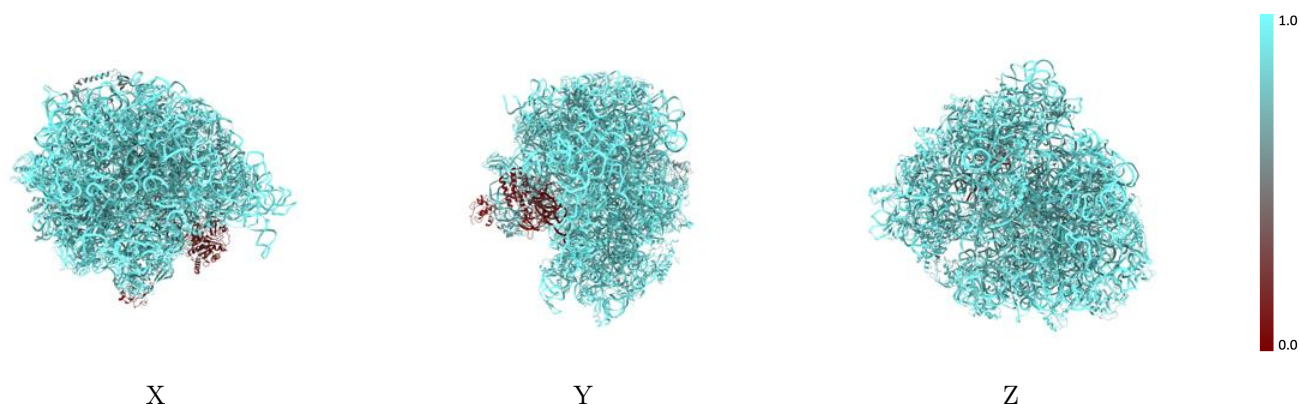
The images above show the 3D surface view of the map at the recommended contour level 0.00371 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



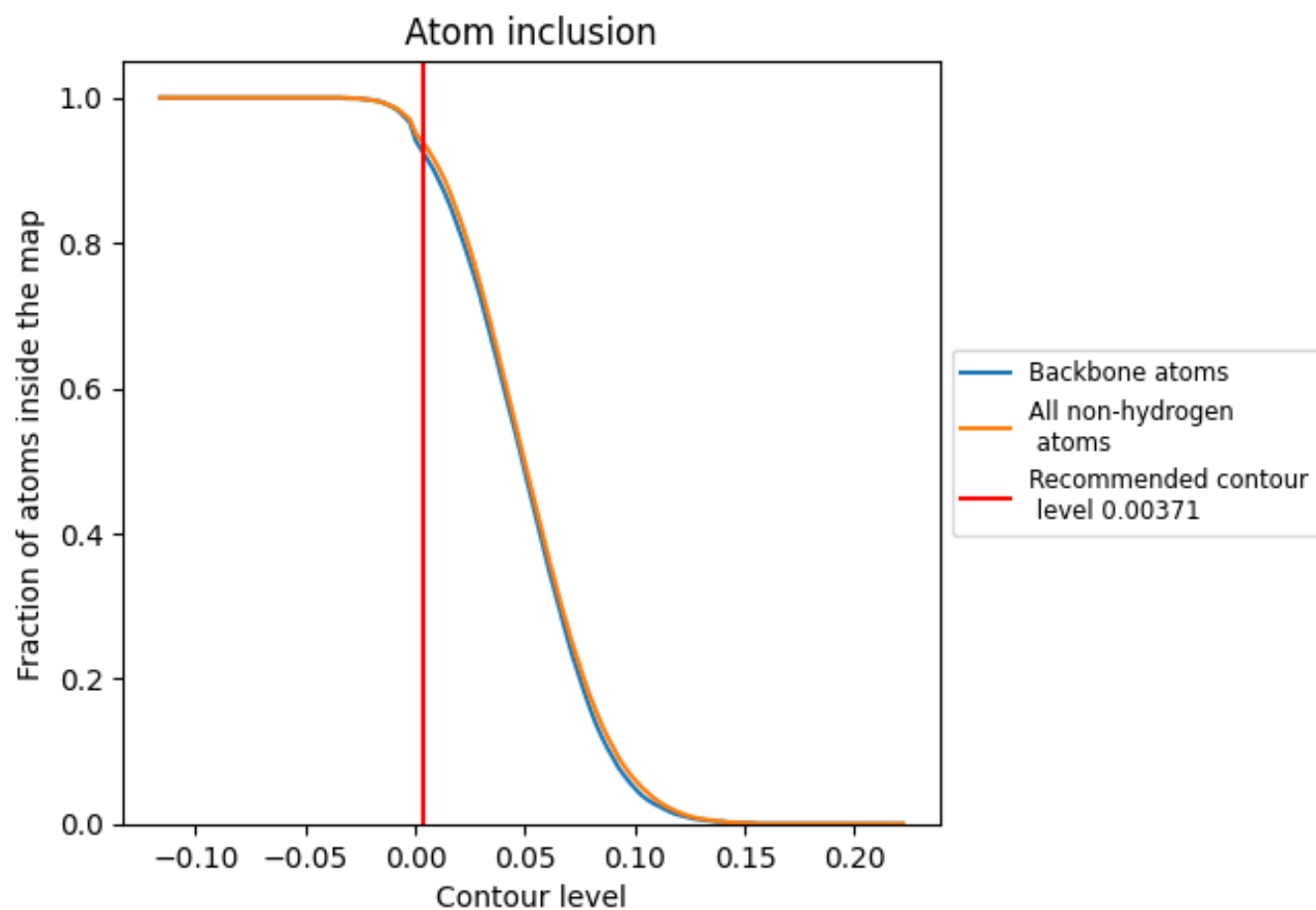
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00371).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 94% 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 (0.00371) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9370	 0.4130
0	 0.9550	 0.4680
1	 0.9630	 0.4550
2	 0.9800	 0.5340
3	 0.9740	 0.5360
4	 0.9690	 0.5040
5	 0.1960	 0.0000
6	 0.9060	 0.2600
A	 0.9840	 0.4570
B	 0.9920	 0.4280
C	 0.9600	 0.5020
D	 0.9620	 0.4850
E	 0.9550	 0.4560
F	 0.9420	 0.3720
G	 0.9410	 0.3460
H	 0.7500	 0.1730
I	 0.6790	 0.0210
J	 0.9630	 0.4730
K	 0.9550	 0.4780
L	 0.9670	 0.4740
M	 0.9640	 0.4860
N	 0.9730	 0.5000
O	 0.9700	 0.4120
P	 0.9610	 0.4690
Q	 0.9780	 0.5090
R	 0.9550	 0.4510
S	 0.9640	 0.4960
T	 0.9610	 0.4470
U	 0.9750	 0.4220
V	 0.9420	 0.4060
W	 0.9590	 0.5090
X	 0.9690	 0.4850
Y	 0.9340	 0.3890
Z	 0.9670	 0.4970
a	 0.9880	 0.4270



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.9110	 0.3010
c	 0.9370	 0.3800
d	 0.9380	 0.3590
e	 0.9590	 0.4440
f	 0.9370	 0.3760
g	 0.9200	 0.3330
h	 0.9510	 0.4390
i	 0.9350	 0.3430
j	 0.9330	 0.3240
k	 0.9550	 0.4270
l	 0.9380	 0.4240
m	 0.9340	 0.3490
n	 0.9490	 0.3720
o	 0.9570	 0.4110
p	 0.9300	 0.3780
q	 0.9380	 0.4060
r	 0.9260	 0.3890
s	 0.9440	 0.3650
t	 0.9480	 0.3790
u	 0.8260	 0.2460
v	 0.9690	 0.3980
w	 0.8240	 0.0890
x	 0.9250	 0.3220
y	 0.1160	 -0.0070
z	 0.1170	 -0.0010