



Full wwPDB EM Validation Report ⓘ

May 4, 2026 – 12:05 PM EDT

PDB ID : 9PIJ / pdb_00009pij
EMDB ID : EMD-71669
Title : E. coli 70S ribosome bound to Minocycline
Authors : Devarkar, S.C.; Lomakin, I.B.; Bunick, C.G.
Deposited on : 2025-07-10
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

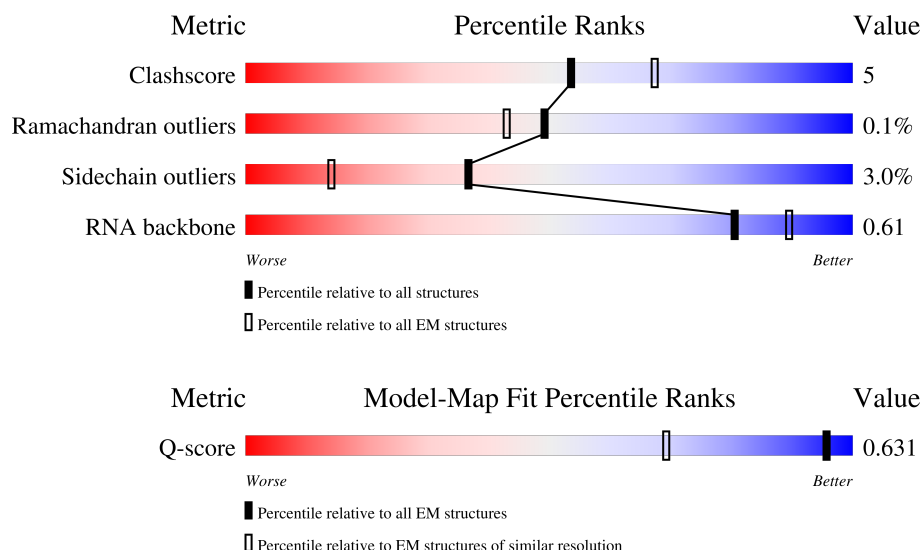
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









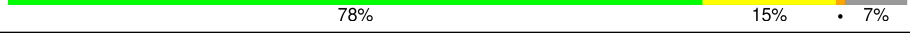

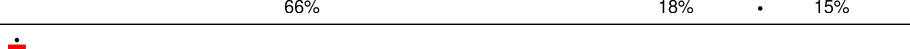
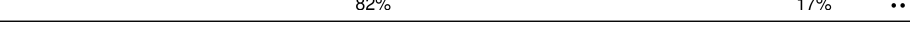
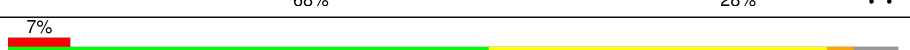

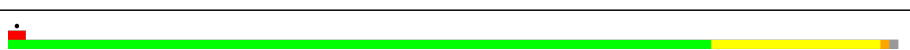

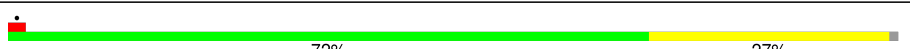





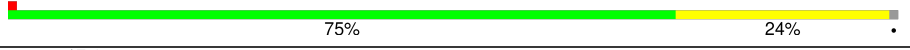
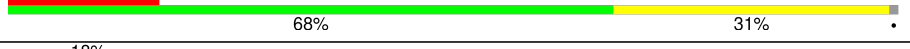



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3184 (1.71 - 2.70)

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

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	





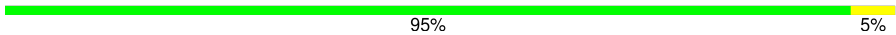




















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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	1542	
7	B	241	
8	C	233	
9	D	206	
10	E	167	
11	F	135	
12	G	179	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	X	22	
28	Z	75	

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Mol	Chain	Length	Quality of chain
29	a	2904	 71% 22% 5%
30	b	120	 83% 15% ..
31	c	273	 92% 7% .
32	d	209	 90% 9% .
33	e	201	 95% 5%
34	f	179	 74% 24% ..
35	g	177	 74% 23% ..
36	h	149	 21% 5% 72%
37	i	142	 87% 11% .
38	j	123	 83% 16% .
39	k	144	 90% 10%
40	l	136	 79% 21%
41	m	127	 83% 10% 7%
42	n	117	 85% 13% ...
43	o	115	 86% 13% .
44	p	118	 88% 11% .
45	q	103	 81% 18% .
46	r	110	 92% 8%
47	s	100	 78% 15% 7%
48	t	104	 88% 10% .
49	u	94	 81% 18% .
50	v	85	 85% 7% 8%
51	w	78	 87% 12% .
52	x	63	 89% 10% .
53	y	59	 5% 80% 15% ...

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Mol	Chain	Length	Quality of chain
54	z	57	<div><div></div><div>88%</div><div>11%</div><div></div></div>

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 141677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1500	Total	C	N	O	P	0	0
			32211	14373	5919	10419	1500		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 26 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 27 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	10	Total	C	N	O	P	0	0
			211	95	35	71	10		

- Molecule 28 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	75	Total	C	N	O	P	S	
			1605	716	291	522	75	1	
								0	0

- Molecule 29 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	2753	Total	C	N	O	P		
			59130	26384	10897	19096	2753		
								0	0

- Molecule 30 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	119	Total	C	N	O	P		
			2549	1135	466	829	119		
								0	0

- Molecule 31 is a protein called 50S ribosomal protein L2.

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

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	209	Total	C	N	O	S		
			1566	980	288	294	4		
								0	0

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 36 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 37 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 42 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called Ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	t	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 49 is a protein called Large ribosomal subunit protein bL25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 53 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 54 is a protein called 50S ribosomal protein L32.

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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	Zn	0
			1	1	

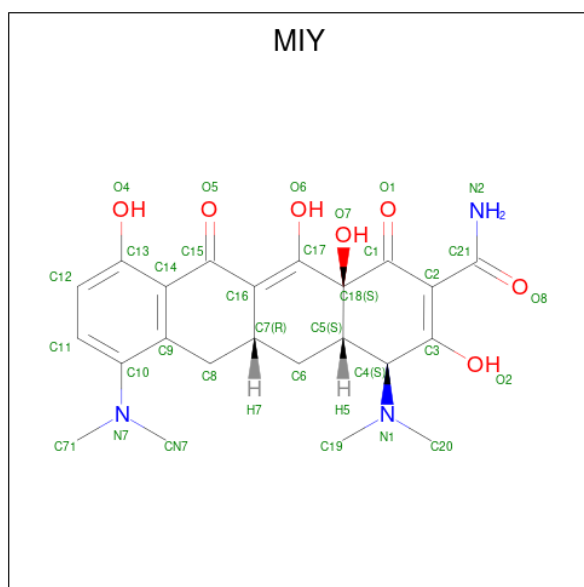
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	85	Total	Mg	0
			85	85	
56	a	248	Total	Mg	0
			248	248	
56	b	5	Total	Mg	0
			5	5	
56	p	2	Total	Mg	0
			2	2	

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	A	37	Total	K	0
			37	37	
57	a	109	Total	K	0
			109	109	
57	b	1	Total	K	0
			1	1	
57	c	1	Total	K	0
			1	1	

- Molecule 58 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: MIY) (formula: C₂₃H₂₇N₃O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
58	A	1	Total	C	N	O	0
			33	23	3	7	
58	a	1	Total	C	N	O	0
			33	23	3	7	

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		AltConf
59	0	1	Total	O	0
			1	1	
59	1	8	Total	O	0
			8	8	
59	3	2	Total	O	0
			2	2	
59	A	119	Total	O	0
			119	119	
59	O	1	Total	O	0
			1	1	
59	U	1	Total	O	0
			1	1	
59	a	1450	Total	O	0
			1450	1450	
59	b	10	Total	O	0
			10	10	
59	c	6	Total	O	0
			6	6	
59	d	3	Total	O	0
			3	3	
59	e	4	Total	O	0
			4	4	
59	h	1	Total	O	0
			1	1	
59	i	2	Total	O	0
			2	2	
59	j	1	Total	O	0
			1	1	
59	k	7	Total	O	0
			7	7	
59	l	1	Total	O	0
			1	1	
59	m	6	Total	O	0
			6	6	
59	p	5	Total	O	0
			5	5	

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Mol	Chain	Residues	Atoms		AltConf
59	q	5	Total 5	O 5	0
59	r	2	Total 2	O 2	0
59	s	2	Total 2	O 2	0
59	t	1	Total 1	O 1	0
59	u	2	Total 2	O 2	0
59	v	2	Total 2	O 2	0
59	w	2	Total 2	O 2	0
59	y	1	Total 1	O 1	0
59	z	4	Total 4	O 4	0

3 Residue-property plots [i](#)


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

• Molecule 1: 50S ribosomal protein L33

Chain 0:  87% 5% 7%




• Molecule 2: 50S ribosomal protein L34

Chain 1:  89% 11%




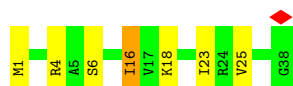
• Molecule 3: 50S ribosomal protein L35

Chain 2:  86% 12%



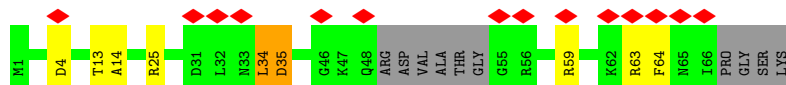
• Molecule 4: 50S ribosomal protein L36

Chain 3:  82% 16%

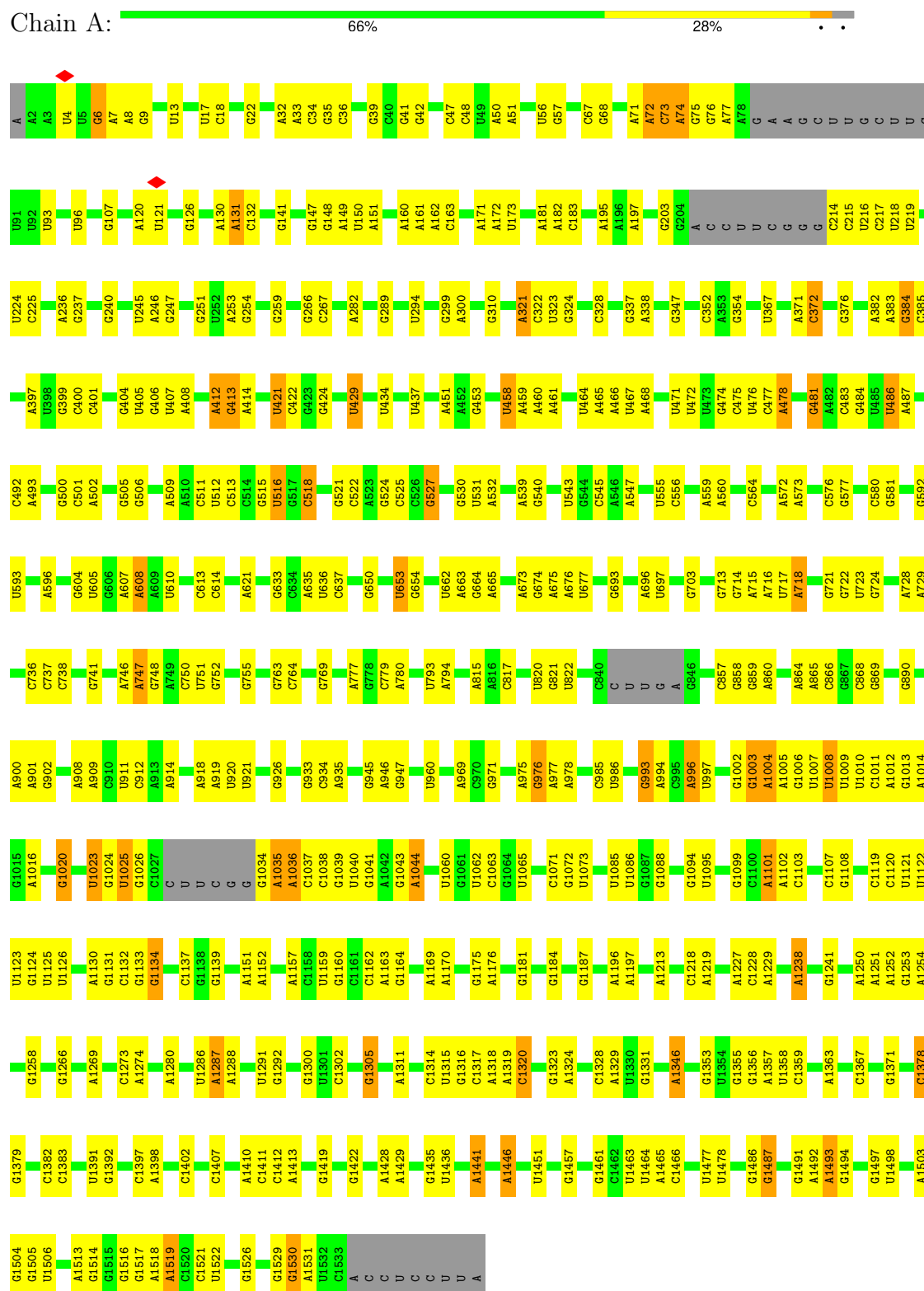


• Molecule 5: 50S ribosomal protein L31

Chain 4:  20% 73% 10% 14%

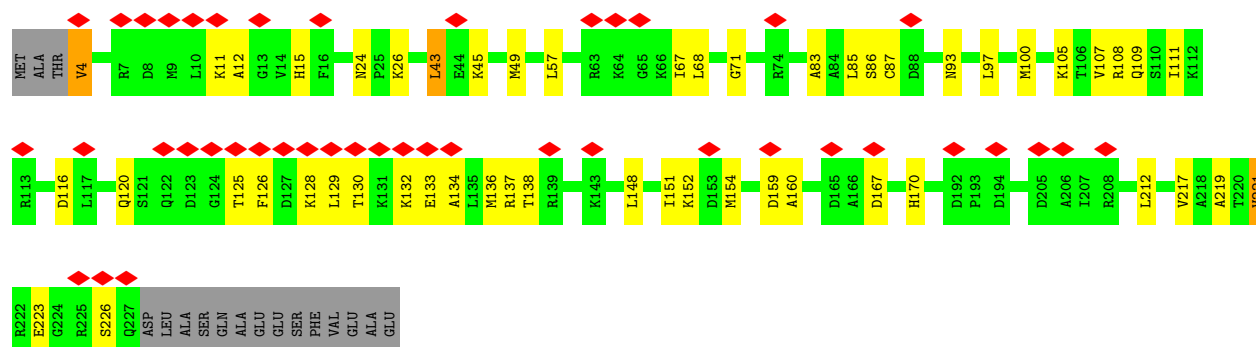


• Molecule 6: 16S rRNA



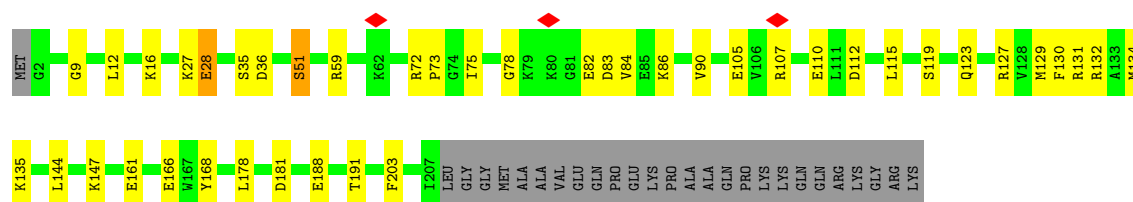
• Molecule 7: 30S ribosomal protein S2





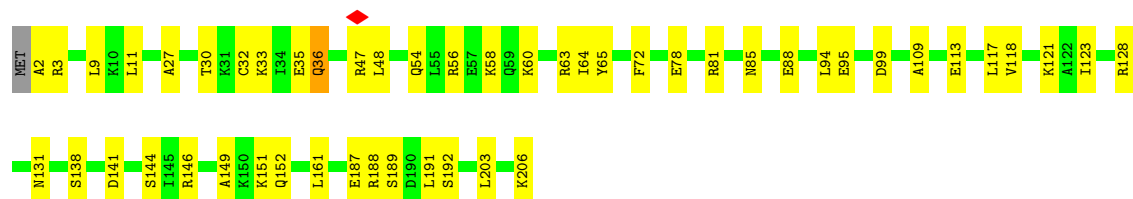
- Molecule 8: Small ribosomal subunit protein uS3

Chain C: 70% 17% 12%



- Molecule 9: Small ribosomal subunit protein uS4

Chain D: 75% 24%



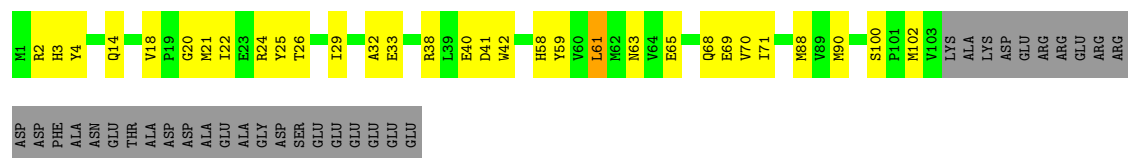
- Molecule 10: Small ribosomal subunit protein uS5

Chain E: 78% 15% 7%

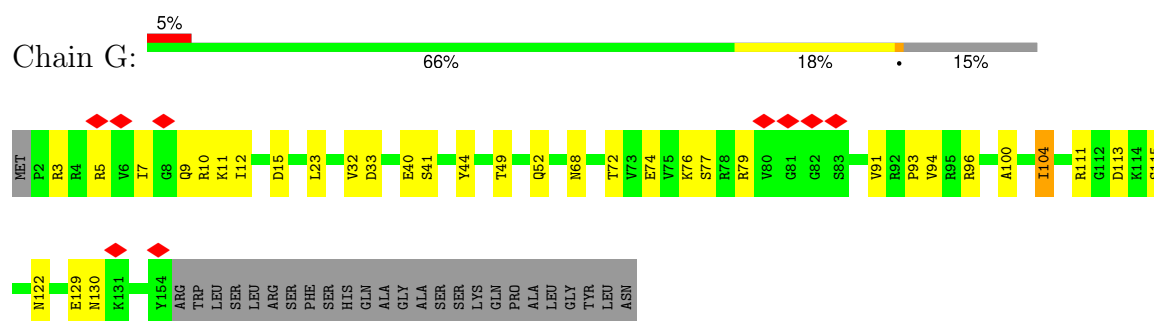


- Molecule 11: Small ribosomal subunit protein bS6

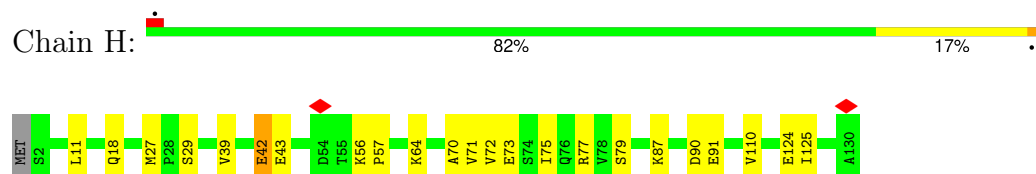
Chain F: 53% 22% 24%



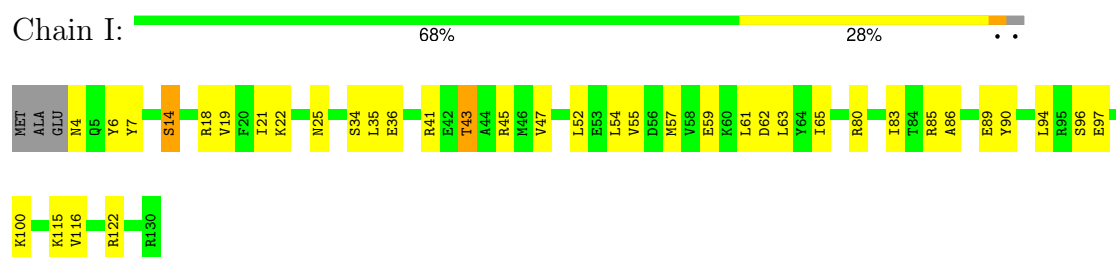
- Molecule 12: Small ribosomal subunit protein uS7



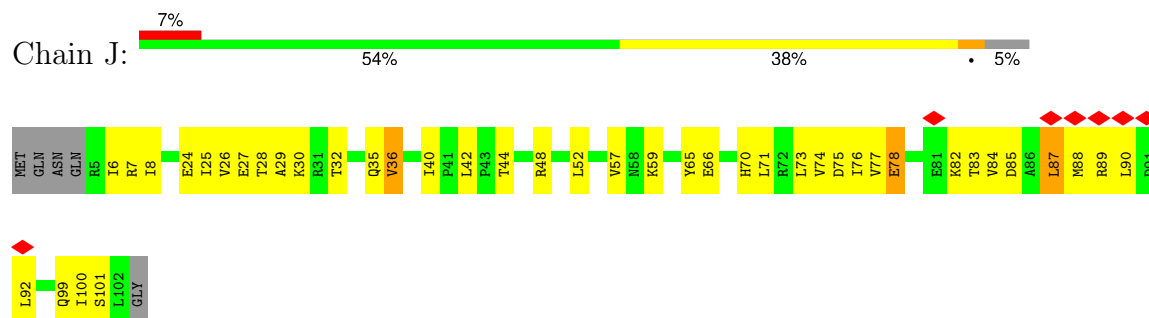
- Molecule 13: Small ribosomal subunit protein uS8



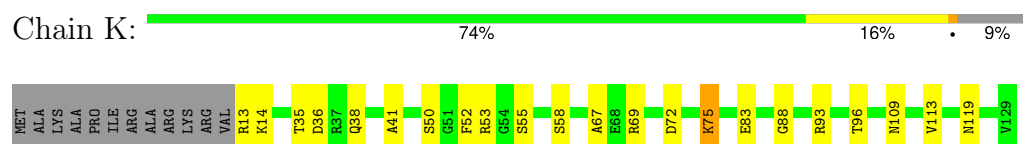
- Molecule 14: Small ribosomal subunit protein uS9



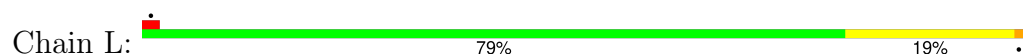
- Molecule 15: Small ribosomal subunit protein uS10

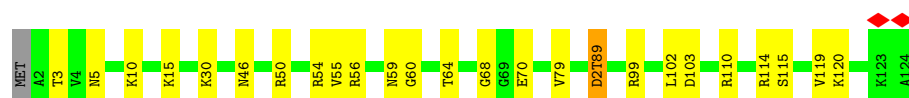


- Molecule 16: 30S ribosomal protein S11



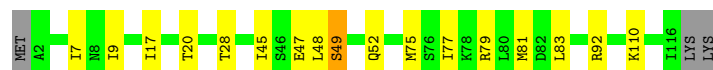
- Molecule 17: Small ribosomal subunit protein uS12





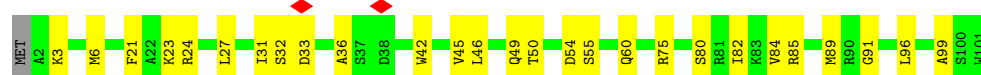
- Molecule 18: Small ribosomal subunit protein uS13

Chain M: 83% 14%



- Molecule 19: Small ribosomal subunit protein uS14

Chain N: 72% 27%



- Molecule 20: Small ribosomal subunit protein uS15

Chain O: 78% 21%



- Molecule 21: Small ribosomal subunit protein bS16

Chain P: 82% 17%



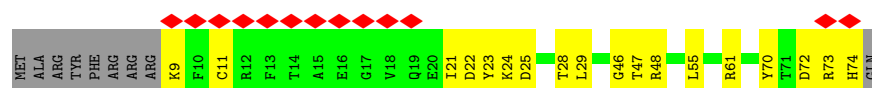
- Molecule 22: Small ribosomal subunit protein uS17

Chain Q: 71% 21% 6%

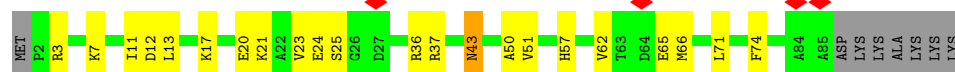


- Molecule 23: Small ribosomal subunit protein bS18

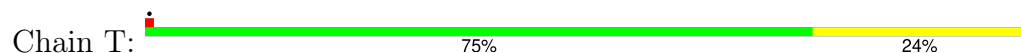
Chain R: 17% 64% 24% 12%



- Molecule 24: Small ribosomal subunit protein uS19



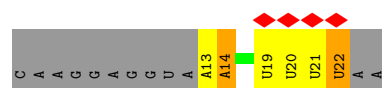
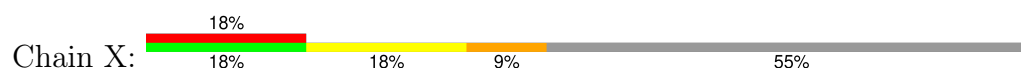
- Molecule 25: Small ribosomal subunit protein bS20



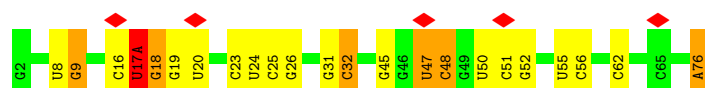
- Molecule 26: Small ribosomal subunit protein bS21



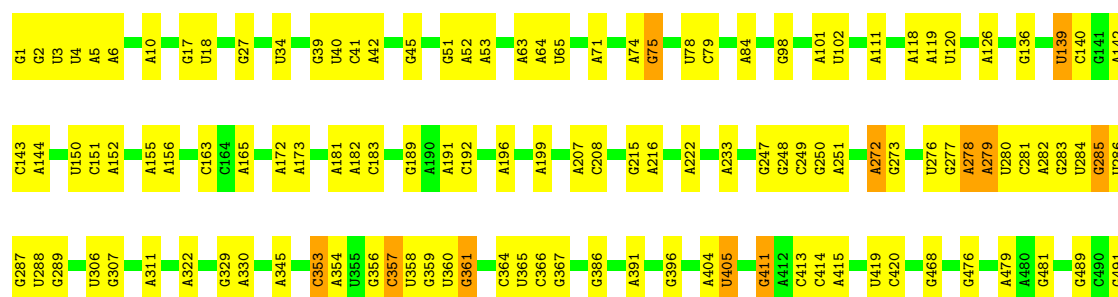
- Molecule 27: mRNA



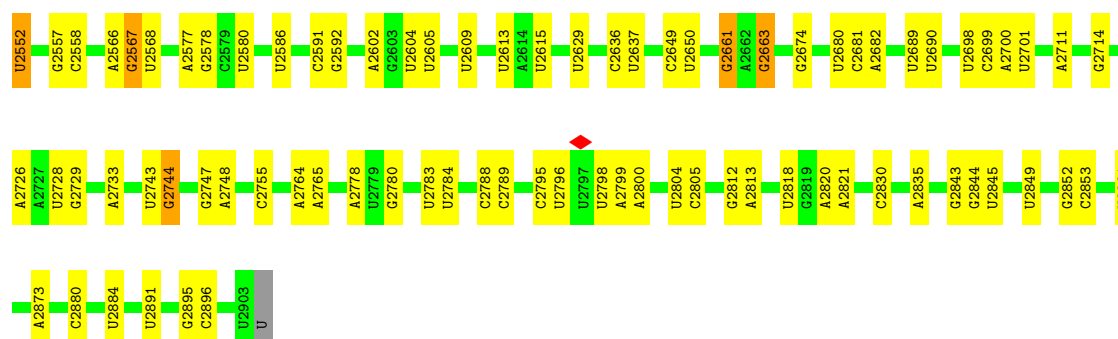
- Molecule 28: P-site tRNA



- Molecule 29: 23S rRNA



U2441	A2287	A	U	G2012	C1800	A1618	G1482	A1301	G1115	C	C898	G776	C635	U499
C2442	A2288	U	G	A2013	A1801	A1641	G1483	G1311	G1116	A	A899	A782	G636	G500
G2443	U2291	A	U	A2014	A1802	A1642	U1484	C1315	U1130	G	G907	G783	G637	A505
G2444	U2292	C	G	A2015	A1803	G1645	U1485	U1329	G1125	A	C908	G784	G638	A508
A2445	C2295	A	G	A2020	A1808	C1646	C1493	U1329	U1130	U	A909	G805	C640	C509
A2446	U2296	C	A	C2023	A1809	U1647	A1494	U1329	G1131	G	A910	G805	A644	C509
U2447	U2297	C	U	C2023	A1810	U1648	A1495	G1338	G1131	U	A911	G809	C645	C510
A2450	A2298	C	A	A2030	C1816	G1649	A1496	U1340	U1132	G	C912	G809	U646	U511
A2451	U2299	U	G	A2031	C1816	G1649	C1497	U1340	A1133	U	G914	G812	G647	G512
G2455	U2305	U	U	G2032	A1829	C1656	U1506	U1352	G1135	C	G930	U811	G650	G530
C2456	C2306	A	G	A2033	A1848	U1657	C1507	U1352	G1136	U	U931	C812	C531	C531
U2457	G2307	A	G	G2038	U1856	A1664	A1508	A1365	G1137	U	U932	U813	A532	A532
A2461	G2308	G	G	U2039	U1857	G1667	A1509	A1365	G1138	G	A933	U813	A533	G533
A2462	U2312	U	G	C2043	A1858	G1674	G1510	C1370	U1141	A	U934	U827	A555	G539
C2466	A2322	U	C	A2052	A1858	G1674	A1515	C1371	U1142	A	C935	U828	G657	G539
A2469	G2325	G	U	U2052	C1868	U1680	A1528	A1378	G1149	C	C937	U832	U658	U645
G2470	C2326	U	U	G2055	G1869	G1681	G1529	U1379	C1150	C	G938	A833	U686	U546
A2481	A2327	A	U	C2056	C1870	G1682	A1535	G1380	C1172	G	C946	G834	G697	A547
G2482	U2328	A	A	A2060	A1872	U1683	C1536	A1383	U	C	A947	U839	G698	G548
U2491	U2329	A	A	G2061	A1889	G1715	G1537	A1386	U	C	C948	C840	G549	G549
G2484	G2330	U	U	A2062	A1890	U1720	C1538	A1387	A	U	U955	U846	A563	A563
U2491	U2334	G	G	C2063	G1906	G1721	U1539	A1392	G1177	C	C961	U847	U573	U573
C2498	A2335	C	C	C2065	U1911	G1724	A1548	U1394	C1178	U	G969	C948	A574	A574
C2499	G2345	C	C	G2066	A1912	U1729	A1549	A1395	U1180	U	U970	U851	A575	A575
G2502	C2346	G	G	A2070	A1913	C1730	U1563	U1405	G1181	A	G974	U852	G577	G577
U2504	U2347	C	C	C2072	C1914	G1736	C1564	U1406	U1182	A	A983	G856	U580	U580
G2505	C2350	C	C	C2073	3TD1915	G1737	U1570	U1411	U1184	G	A996	G857	C581	C581
U2514	C2360	C	C	U2074	U1917	G1738	A1571	U1416	U1198	A	A1000	G858	A586	A586
C2515	A2381	U	U	U2075	A1928	G1738	U1578	C1417	U1199	C	A1001	G859	C587	C587
U2518	G2382	C	C	U2079	U1931	G1743	U1583	C1428	G1212	G	C1005	U870	U588	U588
U2519	U2383	C	C	U2086	A1932	A1746	U1584	G1429	A1226	U	U1012	U871	U589	U589
C2520	G2385	A	U	G2087	G1933	U1747	C1585	G1430	U1239	A	C1013	A877	U593	U593
G2523	C2395	C	G	G2093	U1946	C1748	A1586	G1432	U1240	U	G1022	A878	C594	C594
U2526	U2402	C	C	U2098	C1947	G1764	G1587	A1433	A1253	A	G1026	G879	C595	C595
G2529	A2406	C	C	U	U1955	A1773	A1597	A1434	U1254	G	G1027	G880	G596	G596
C2532	C2420	C	C	G	C1967	U1782	A1598	G1435	G1256	C	A1028	G881	G597	G597
U2537	A2425	A	C	G	A1970	G1790	U1602	G1441	G1266	C	A1029	C888	A603	A603
C2538	G2429	C	C	C	U1971	A1791	A1603	U1442	U1271	C	U1033	U754	A608	A608
A2547	U2548	U	U	U	G1972	A1794	C1605	U1443	A1272	U	U1046	C990	A614	A614
U2548	A2435	G	G	G	U1991	C1795	C1607	G1452	U1282	G	G1047	G891	U615	U615
		A	A	A	U1992	U1796	A1608	A1469	G1283		A1046	A892	A627	A627
		A	A	G	U1993	G1797	A1614	A1470	G1300		G1052	U894	A832	A832
		A	A	G									A833	A833



• Molecule 30: 5S rRNA

Chain b: 83% 15% ..



• Molecule 31: 50S ribosomal protein L2

Chain c: 92% 7% .



• Molecule 32: 50S ribosomal protein L3

Chain d: 90% 9% .



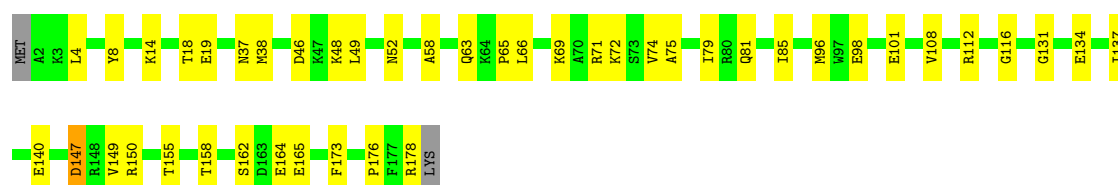
• Molecule 33: Large ribosomal subunit protein uL4

Chain e: 95% 5%




• Molecule 34: Large ribosomal subunit protein uL5

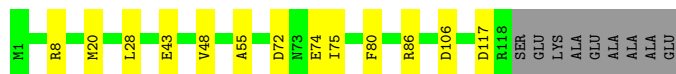
Chain f: 74% 24% ..




• Molecule 35: Large ribosomal subunit protein uL6

- Molecule 41: Large ribosomal subunit protein bL17

Chain m:  83% 10% 7%




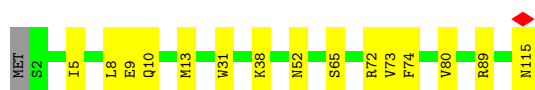
- Molecule 42: Large ribosomal subunit protein uL18

Chain n:  85% 13% ...




- Molecule 43: Large ribosomal subunit protein bL19

Chain o:  86% 13% .




- Molecule 44: 50S ribosomal protein L20

Chain p:  88% 11% .



- Molecule 45: Ribosomal protein L21

Chain q:  81% 18% .



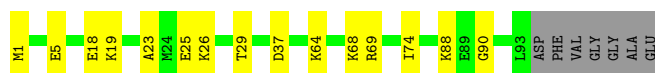
- Molecule 46: 50S ribosomal protein L22

Chain r:  92% 8%

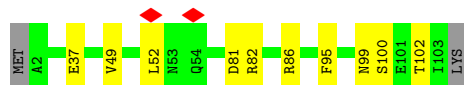
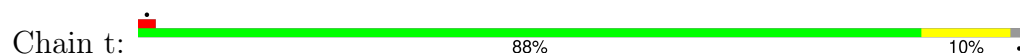


- Molecule 47: 50S ribosomal protein L23

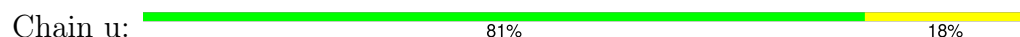
Chain s:  78% 15% 7%



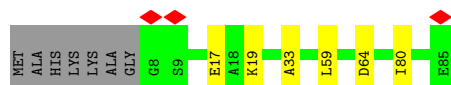
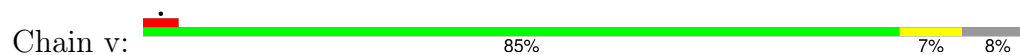
- Molecule 48: 50S ribosomal protein L24



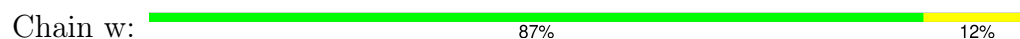
- Molecule 49: Large ribosomal subunit protein bL25



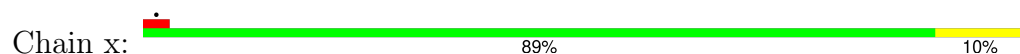
- Molecule 50: 50S ribosomal protein L27



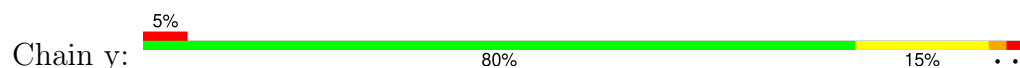
- Molecule 51: 50S ribosomal protein L28



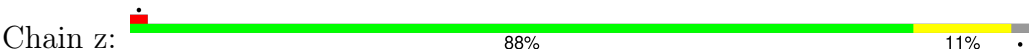
- Molecule 52: Large ribosomal subunit protein uL29



- Molecule 53: 50S ribosomal protein L30



- Molecule 54: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	628487	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.864	Depositor
Minimum map value	-0.232	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OMU, MA6, MG, 5MC, 4OC, MIY, UR3, D2T, G7M, PSU, 4SU, K, 5MU, H2U, OMC, 2MA, 6MZ, OMG, 3TD, MEQ, 1MG, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.29	0/424	0.36	0/565
2	1	0.36	0/380	0.35	0/498
3	2	0.35	0/513	0.35	0/676
4	3	0.33	0/303	0.39	0/397
5	4	0.16	0/488	0.39	0/649
6	A	0.33	0/35787	0.30	0/55816
7	B	0.20	0/1784	0.35	0/2403
8	C	0.24	0/1651	0.33	0/2225
9	D	0.24	0/1665	0.35	0/2227
10	E	0.38	0/1165	0.48	0/1568
11	F	0.26	0/858	0.42	0/1160
12	G	0.22	0/1219	0.37	0/1635
13	H	0.32	0/989	0.45	0/1326
14	I	0.31	0/1034	0.58	0/1375
15	J	0.25	0/796	0.48	0/1077
16	K	0.28	0/893	0.41	0/1205
17	L	0.27	0/960	0.33	0/1286
18	M	0.22	0/900	0.37	0/1204
19	N	0.38	0/817	0.58	0/1088
20	O	0.26	0/722	0.40	0/964
21	P	0.28	0/653	0.41	0/877
22	Q	0.26	0/650	0.37	0/871
23	R	0.26	0/553	0.39	0/742
24	S	0.40	0/685	0.48	0/922
25	T	0.26	0/676	0.40	0/895
26	U	0.20	0/597	0.34	0/792
27	X	0.52	0/235	0.60	0/363
28	Z	0.58	0/1703	0.72	1/2655 (0.0%)
29	a	0.44	0/65651	0.36	0/102413
30	b	0.32	0/2850	0.27	0/4444
31	c	0.34	0/2121	0.37	0/2852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.34	0/1576	0.34	0/2119
33	e	0.31	0/1571	0.34	0/2113
34	f	0.23	0/1434	0.40	0/1926
35	g	0.36	0/1343	0.57	0/1816
36	h	0.26	0/306	0.57	0/413
37	i	0.33	0/1152	0.33	0/1551
38	j	0.32	0/955	0.38	0/1279
39	k	0.32	0/1062	0.39	0/1413
40	l	0.37	0/1093	0.44	0/1460
41	m	0.36	0/958	0.43	0/1281
42	n	0.54	0/902	0.76	0/1209
43	o	0.33	0/929	0.33	0/1242
44	p	0.55	1/960 (0.1%)	0.54	1/1278 (0.1%)
45	q	0.34	0/829	0.44	0/1107
46	r	0.33	0/864	0.35	0/1156
47	s	0.31	0/744	0.42	0/994
48	t	0.38	0/787	0.51	0/1051
49	u	0.28	0/766	0.37	0/1025
50	v	0.33	0/593	0.33	0/785
51	w	0.35	0/635	0.43	0/848
52	x	0.26	0/502	0.35	0/667
53	y	0.79	0/453	1.04	0/605
54	z	0.32	0/450	0.35	0/599
All	All	0.38	1/150586 (0.0%)	0.37	2/225107 (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
42	n	0	1
53	y	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	p	47	TYR	C-O	7.81	1.33	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Z	17(A)	U	C2'-C3'-O3'	5.76	118.14	109.50
44	p	46	ALA	CA-C-O	-5.08	115.49	120.82

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	n	94	ARG	Sidechain
53	y	11	ARG	Sidechain
53	y	31	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	2	0
2	1	377	0	418	4	0
3	2	504	0	572	6	0
4	3	302	0	340	4	0
5	4	480	0	482	8	0
6	A	32211	0	16224	273	0
7	B	1753	0	1780	30	0
8	C	1624	0	1696	28	0
9	D	1643	0	1707	33	0
10	E	1152	0	1196	19	0
11	F	839	0	833	21	0
12	G	1203	0	1254	21	0
13	H	979	0	1031	14	0
14	I	1022	0	1070	31	0
15	J	786	0	828	31	0
16	K	877	0	887	17	0
17	L	957	0	1017	17	0
18	M	891	0	952	13	0
19	N	805	0	844	25	0
20	O	714	0	734	16	0
21	P	643	0	661	12	0
22	Q	641	0	682	12	0
23	R	544	0	565	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	S	668	0	693	21	0
25	T	670	0	719	15	0
26	U	589	0	629	14	0
27	X	211	0	106	3	0
28	Z	1605	0	818	10	0
29	a	59130	0	29748	337	0
30	b	2549	0	1290	10	0
31	c	2082	0	2154	13	0
32	d	1566	0	1618	15	0
33	e	1552	0	1619	7	0
34	f	1410	0	1444	34	0
35	g	1323	0	1371	30	0
36	h	303	0	327	7	0
37	i	1129	0	1162	14	0
38	j	946	0	1023	15	0
39	k	1053	0	1129	10	0
40	l	1074	0	1157	19	0
41	m	945	0	989	8	0
42	n	892	0	923	9	0
43	o	917	0	962	12	0
44	p	947	0	1019	7	0
45	q	816	0	839	10	0
46	r	857	0	922	5	0
47	s	738	0	807	13	0
48	t	779	0	831	7	0
49	u	753	0	780	13	0
50	v	586	0	596	3	0
51	w	625	0	652	6	0
52	x	501	0	531	3	0
53	y	449	0	488	6	0
54	z	444	0	458	4	0
55	3	1	0	0	0	0
56	A	85	0	0	0	0
56	a	248	0	0	0	0
56	b	5	0	0	0	0
56	p	2	0	0	0	0
57	A	37	0	0	0	0
57	a	109	0	0	0	0
57	b	1	0	0	0	0
57	c	1	0	0	0	0
58	A	33	0	24	2	0
58	a	33	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	0	1	0	0	0	0
59	1	8	0	0	1	0
59	3	2	0	0	0	0
59	A	119	0	0	2	0
59	O	1	0	0	0	0
59	U	1	0	0	0	0
59	a	1450	0	0	5	0
59	b	10	0	0	0	0
59	c	6	0	0	0	0
59	d	3	0	0	0	0
59	e	4	0	0	0	0
59	h	1	0	0	0	0
59	i	2	0	0	0	0
59	j	1	0	0	0	0
59	k	7	0	0	0	0
59	l	1	0	0	0	0
59	m	6	0	0	0	0
59	p	5	0	0	0	0
59	q	5	0	0	1	0
59	r	2	0	0	0	0
59	s	2	0	0	0	0
59	t	1	0	0	0	0
59	u	2	0	0	0	0
59	v	2	0	0	0	0
59	w	2	0	0	0	0
59	y	1	0	0	0	0
59	z	4	0	0	0	0
All	All	141677	0	94076	1204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1204) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:76:G:H1	6:A:93:U:H3	1.23	0.86
42:n:90:VAL:HG23	42:n:117:PHE:HB3	1.60	0.83
29:a:881:G:H1	29:a:895:U:H3	1.26	0.83
15:J:66:GLU:HB2	19:N:99:ALA:HB2	1.62	0.82
6:A:1086:U:H3	6:A:1099:G:H22	1.28	0.79
20:O:26:GLU:OE2	20:O:77:ARG:HG2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:30:ASN:O	35:g:30:ASN:ND2	2.16	0.78
8:C:9:GLY:HA3	19:N:89:MET:HE3	1.67	0.77
35:g:173:GLU:OE2	35:g:173:GLU:N	2.18	0.76
34:f:165:GLU:N	34:f:165:GLU:OE2	2.20	0.75
21:P:18:GLN:HE22	21:P:35:ARG:HH11	1.35	0.75
11:F:88:MET:HE1	23:R:61:ARG:HG2	1.66	0.75
8:C:35:SER:OG	8:C:59:ARG:NH2	2.20	0.75
37:i:9:GLU:N	37:i:9:GLU:OE1	2.19	0.75
7:B:15:HIS:HB3	7:B:43:LEU:HD21	1.69	0.74
12:G:5:ARG:NH1	12:G:7:ILE:O	2.22	0.73
42:n:52:SER:N	42:n:55:GLU:OE1	2.22	0.73
49:u:69:GLU:OE2	49:u:69:GLU:N	2.22	0.73
6:A:421:U:O2	8:C:127:ARG:NH1	2.22	0.72
6:A:664:G:H22	6:A:741:G:H1	1.37	0.72
6:A:1356:G:H2'	6:A:1357:A:C8	2.25	0.72
9:D:85:ASN:HB3	9:D:88:GLU:HG2	1.72	0.72
6:A:673:A:H2'	6:A:674:G:C8	2.23	0.71
10:E:151:GLU:N	10:E:151:GLU:OE2	2.20	0.71
16:K:83:GLU:HG2	16:K:109:ASN:HB2	1.71	0.71
29:a:2052:A:H4'	32:d:148:GLN:O	1.89	0.71
12:G:79:ARG:H	12:G:79:ARG:HD3	1.53	0.71
15:J:65:TYR:HB3	19:N:96:LEU:HD11	1.72	0.71
38:j:113:MET:HA	38:j:113:MET:HE3	1.73	0.70
6:A:1126:U:OP1	15:J:7:ARG:NH2	2.24	0.70
19:N:24:ARG:NH1	19:N:55:SER:HG	1.89	0.70
29:a:547:A:H3'	29:a:548:G:C8	2.26	0.70
29:a:1802:A:H2'	29:a:1803:A:C8	2.27	0.70
49:u:35:GLU:N	49:u:35:GLU:OE2	2.25	0.70
8:C:131:ARG:NH1	8:C:168:TYR:OH	2.25	0.70
14:I:96:SER:OG	14:I:97:GLU:OE2	2.10	0.70
17:L:70:GLU:N	17:L:70:GLU:OE1	2.24	0.70
19:N:42:TRP:CD1	19:N:46:LEU:HD11	2.27	0.69
14:I:6:TYR:HB3	14:I:89:GLU:OE1	1.92	0.69
40:l:53:MET:HG3	40:l:120:ALA:HB2	1.73	0.69
5:4:35:ASP:OD1	5:4:35:ASP:N	2.26	0.69
42:n:61:GLN:OE1	42:n:61:GLN:N	2.25	0.69
6:A:717:U:O3'	16:K:119:ASN:ND2	2.25	0.69
7:B:167:ASP:O	7:B:170:HIS:ND1	2.26	0.69
7:B:129:LEU:HB3	7:B:133:GLU:HB2	1.75	0.68
49:u:55:GLU:OE2	49:u:55:GLU:N	2.21	0.68
34:f:46:ASP:HB3	34:f:49:LEU:HD12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:68:ASN:ND2	12:G:130:ASN:OD1	2.27	0.68
24:S:62:VAL:HA	24:S:66:MET:HE2	1.77	0.67
40:l:66:ARG:NH1	40:l:104:GLU:OE2	2.28	0.67
6:A:492:C:H2'	6:A:493:A:C8	2.30	0.66
6:A:993:G:O2'	6:A:994:A:N7	2.27	0.66
21:P:18:GLN:NE2	21:P:35:ARG:HD2	2.09	0.66
29:a:856:G:H2'	29:a:857:G:C8	2.30	0.66
29:a:2205:A:H61	29:a:2219:U:H3	1.41	0.66
29:a:2328:A:H2'	29:a:2329:U:C6	2.30	0.66
34:f:140:GLU:OE2	34:f:140:GLU:N	2.23	0.66
14:I:57:MET:HE1	14:I:90:TYR:HE2	1.59	0.66
41:m:74:GLU:OE1	41:m:74:GLU:N	2.22	0.66
29:a:1138:G:H21	37:i:108:MET:HE2	1.61	0.66
40:l:58:LYS:O	40:l:60:GLN:NE2	2.29	0.66
49:u:7:GLU:OE1	49:u:8:VAL:N	2.29	0.65
10:E:101:GLU:CD	10:E:101:GLU:H	2.04	0.65
37:i:98:GLU:N	37:i:98:GLU:OE1	2.27	0.65
43:o:72:ARG:HG2	43:o:74:PHE:CZ	2.31	0.65
7:B:217:VAL:O	7:B:221:VAL:HG12	1.96	0.65
36:h:17:ASP:N	36:h:17:ASP:OD1	2.30	0.65
10:E:13:GLU:OE2	10:E:68:ARG:NH1	2.29	0.65
28:Z:31:G:H3'	28:Z:32:5MC:HM53	1.79	0.65
19:N:49:GLN:NE2	24:S:12:ASP:OD1	2.30	0.65
19:N:24:ARG:NH1	19:N:55:SER:OG	2.29	0.64
19:N:42:TRP:O	19:N:46:LEU:HD12	1.97	0.64
10:E:161:VAL:HG12	10:E:165:LEU:HD23	1.78	0.64
29:a:1115:G:O2'	29:a:1116:G:O5'	2.16	0.64
8:C:110:GLU:HB2	8:C:144:LEU:HD12	1.79	0.64
29:a:191:A:H2'	29:a:192:C:C6	2.32	0.64
6:A:1530:G:O6	26:U:46:LYS:NZ	2.28	0.64
6:A:147:G:H2'	6:A:148:G:C8	2.32	0.64
29:a:358:U:H2'	29:a:359:G:H8	1.63	0.64
35:g:86:LYS:NZ	35:g:130:GLU:OE2	2.30	0.64
14:I:7:TYR:HE1	14:I:18:ARG:HB3	1.62	0.64
16:K:14:LYS:HE2	16:K:14:LYS:N	2.12	0.64
35:g:176:LYS:HE2	35:g:177:LYS:H	1.63	0.64
6:A:1441:A:H62	6:A:1461:G:H21	1.46	0.64
43:o:89:ARG:NH2	43:o:115:ASN:O	2.30	0.64
19:N:49:GLN:HE22	24:S:12:ASP:HA	1.63	0.64
16:K:35:THR:HG22	16:K:41:ALA:HA	1.79	0.63
29:a:870:U:OP1	40:l:6:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:11:LEU:HD13	9:D:63:ARG:HG2	1.79	0.63
9:D:27:ALA:HB3	9:D:30:THR:HG23	1.79	0.63
34:f:164:GLU:OE1	34:f:164:GLU:N	2.18	0.63
23:R:9:LYS:HA	23:R:46:GLY:HA3	1.80	0.63
29:a:2728:U:HO2'	29:a:2729:G:H8	1.45	0.63
9:D:47:ARG:HA	9:D:47:ARG:NH1	2.13	0.62
29:a:1138:G:N2	37:i:108:MET:HE2	2.14	0.62
10:E:115:LEU:HD13	10:E:123:VAL:HG11	1.79	0.62
11:F:22:ILE:O	11:F:26:THR:HG23	1.99	0.62
14:I:97:GLU:HA	14:I:100:LYS:NZ	2.14	0.62
14:I:6:TYR:HB2	14:I:21:ILE:HB	1.80	0.62
29:a:2305:U:H5''	34:f:131:GLY:HA3	1.82	0.62
29:a:878:A:N6	29:a:899:A:O2'	2.33	0.62
34:f:147:ASP:OD1	34:f:150:ARG:NH2	2.33	0.62
17:L:46:ASN:ND2	17:L:89:D2T:SB	2.72	0.61
6:A:946:A:H2'	6:A:947:G:C8	2.35	0.61
15:J:6:ILE:HB	15:J:76:ILE:HB	1.81	0.61
11:F:20:GLY:O	11:F:24:ARG:HG3	2.01	0.61
33:e:168:ASP:OD1	33:e:169:VAL:N	2.33	0.61
8:C:130:PHE:O	8:C:134:MET:HG3	2.00	0.61
23:R:22:ASP:OD1	23:R:24:LYS:NZ	2.33	0.61
31:c:199:GLU:OE2	31:c:199:GLU:N	2.22	0.61
40:l:77:PRO:HG2	40:l:80:VAL:HG21	1.81	0.61
41:m:86:ARG:NH2	41:m:117:ASP:OD1	2.32	0.61
19:N:24:ARG:HH11	19:N:55:SER:HG	1.43	0.61
24:S:51:VAL:HG21	24:S:71:LEU:HD22	1.82	0.61
34:f:14:LYS:O	34:f:18:THR:HG23	2.01	0.61
38:j:43:ILE:HD12	38:j:56:ASP:HB2	1.82	0.61
29:a:782:A:C2	31:c:225:MET:HG2	2.36	0.61
35:g:45:HIS:CE1	35:g:47:ASP:O	2.53	0.60
6:A:1006:G:H1	6:A:1023:U:H3	1.48	0.60
29:a:1869:G:H22	29:a:1872:A:H8	1.47	0.60
6:A:1218:C:H2'	6:A:1219:A:C8	2.37	0.60
29:a:639:U:H2'	29:a:640:C:C6	2.36	0.60
8:C:36:ASP:OD1	8:C:59:ARG:NH2	2.27	0.60
54:z:54:VAL:HG23	54:z:55:ILE:HG23	1.82	0.60
6:A:1457:G:OP1	25:T:34:LYS:NZ	2.24	0.60
8:C:73:PRO:HG3	8:C:105:GLU:HG2	1.82	0.60
32:d:18:ASP:OD1	32:d:18:ASP:N	2.33	0.60
6:A:310:G:N7	59:A:1802:HOH:O	2.31	0.60
6:A:337:G:H2'	6:A:338:A:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:48:LEU:HD21	9:D:56:ARG:HG3	1.83	0.60
18:M:7:ILE:HG22	34:f:112:ARG:HH12	1.67	0.60
22:Q:17:MET:HE3	22:Q:20:SER:OG	2.02	0.60
12:G:93:PRO:HA	12:G:96:ARG:HD3	1.83	0.59
20:O:6:GLU:CD	20:O:6:GLU:H	2.09	0.59
24:S:50:ALA:HB1	24:S:57:HIS:HB3	1.83	0.59
37:i:1:MET:HE1	45:q:13:ARG:HH21	1.66	0.59
29:a:930:G:H1'	53:y:25:LEU:HD11	1.84	0.59
51:w:41:GLU:OE2	51:w:44:LYS:NZ	2.35	0.59
26:U:51:SER:OG	26:U:55:ARG:NH2	2.34	0.59
6:A:1034:G:H2'	6:A:1035:A:C8	2.37	0.59
14:I:57:MET:HE1	14:I:90:TYR:CE2	2.37	0.59
29:a:636:G:OP1	39:k:129:LYS:HE2	2.03	0.59
6:A:458:U:H3	6:A:474:G:H1	1.51	0.59
25:T:42:GLY:HA2	25:T:86:LEU:HD21	1.85	0.59
16:K:14:LYS:HE2	16:K:14:LYS:H	1.66	0.59
29:a:1311:G:N7	59:a:3410:HOH:O	2.32	0.59
38:j:121:GLU:OE1	43:o:65:SER:OG	2.20	0.59
6:A:714:G:H2'	6:A:715:A:C8	2.38	0.58
6:A:1397:C:OP2	10:E:29:ARG:NH2	2.35	0.58
8:C:16:LYS:NZ	8:C:181:ASP:OD1	2.36	0.58
18:M:75:MET:HE3	18:M:75:MET:O	2.04	0.58
6:A:1328:C:OP1	18:M:28:THR:HG21	2.04	0.58
20:O:8:THR:O	20:O:12:VAL:HG23	2.03	0.58
29:a:812:C:O2'	44:p:13:ARG:NH2	2.36	0.58
51:w:43:GLU:OE2	51:w:45:ARG:HB2	2.04	0.58
6:A:1038:C:H2'	6:A:1039:G:H8	1.69	0.58
25:T:28:MET:O	25:T:32:ILE:HD12	2.03	0.58
29:a:288:U:H2'	29:a:289:G:C8	2.39	0.58
29:a:353:C:H2'	29:a:354:A:H8	1.68	0.58
35:g:104:ASN:ND2	35:g:114:ASP:OD1	2.37	0.58
6:A:1323:G:H2'	6:A:1324:A:C8	2.39	0.57
29:a:593:U:H2'	29:a:594:U:C6	2.38	0.57
17:L:3:THR:HG22	17:L:5:ASN:H	1.69	0.57
29:a:1469:A:H2'	29:a:1470:A:C8	2.38	0.57
35:g:2:SER:OG	35:g:3:ARG:N	2.30	0.57
35:g:19:ILE:HG13	35:g:24:ILE:HG13	1.85	0.57
37:i:96:ARG:NH1	37:i:96:ARG:HB3	2.19	0.57
28:Z:76:A:H2'	29:a:2451:A:H1'	1.86	0.57
29:a:1528:A:H2'	29:a:1529:G:O4'	2.04	0.57
6:A:1013:G:N2	6:A:1016:A:OP2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1035:A:O2'	6:A:1036:A:O5'	2.20	0.57
9:D:128:ARG:HB3	9:D:128:ARG:NH1	2.19	0.57
12:G:9:GLN:OE1	12:G:10:ARG:N	2.38	0.57
16:K:67:ALA:HB2	16:K:96:THR:HG23	1.87	0.57
29:a:849:A:H2'	29:a:850:U:C6	2.40	0.57
29:a:2591:C:H2'	29:a:2592:G:C8	2.40	0.57
9:D:109:ALA:N	9:D:113:GLU:OE1	2.28	0.57
6:A:36:C:OP1	17:L:120:LYS:NZ	2.33	0.57
6:A:1314:C:H2'	6:A:1315:U:C6	2.40	0.57
18:M:77:ILE:O	18:M:81:MET:HG3	2.05	0.57
40:l:20:LEU:HD13	49:u:81:PRO:HG2	1.86	0.57
29:a:2327:A:H2'	29:a:2328:A:C8	2.40	0.57
36:h:7:ASP:OD1	36:h:8:LYS:N	2.38	0.57
47:s:18:GLU:CD	47:s:18:GLU:H	2.12	0.57
6:A:477:C:H2'	6:A:478:A:C8	2.40	0.56
7:B:133:GLU:O	7:B:137:ARG:HD2	2.04	0.56
8:C:129:MET:SD	8:C:132:ARG:HG2	2.45	0.56
29:a:2830:C:H5''	32:d:56:LYS:HE3	1.86	0.56
6:A:1320:C:O2	24:S:36:ARG:NH2	2.38	0.56
29:a:279:A:N6	29:a:361:G:H1'	2.21	0.56
29:a:833:A:H2'	29:a:834:G:C8	2.40	0.56
40:l:111:GLU:H	40:l:111:GLU:CD	2.13	0.56
29:a:288:U:H2'	29:a:289:G:H8	1.71	0.56
38:j:34:GLY:N	38:j:37:ASP:OD2	2.38	0.56
48:t:99:ASN:O	48:t:100:SER:C	2.48	0.56
26:U:31:GLU:OE2	26:U:34:ARG:NH1	2.38	0.56
29:a:539:G:H5'	37:i:9:GLU:OE2	2.05	0.56
43:o:5:ILE:O	43:o:9:GLU:HG3	2.06	0.56
22:Q:54:GLY:N	22:Q:57:ASP:OD2	2.38	0.56
29:a:353:C:H2'	29:a:354:A:C8	2.41	0.56
6:A:1382:C:O4'	12:G:79:ARG:NH2	2.39	0.56
6:A:1477:U:H2'	6:A:1478:U:C6	2.41	0.56
14:I:94:LEU:HA	14:I:97:GLU:OE1	2.06	0.56
18:M:83:LEU:HD11	24:S:66:MET:HG2	1.86	0.56
29:a:1790:C:H2'	29:a:1791:A:C5	2.41	0.56
48:t:86:ARG:NH2	48:t:102:THR:OG1	2.39	0.56
26:U:31:GLU:OE2	26:U:35:ARG:NH1	2.39	0.56
29:a:1046:A:H3'	29:a:1047:G:H5'	1.88	0.56
6:A:1004:A:H2'	6:A:1005:A:O4'	2.06	0.56
6:A:1043:G:O2'	6:A:1044:A:O5'	2.24	0.55
15:J:8:ILE:HB	15:J:74:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Q:38:ILE:HD12	22:Q:40:ARG:HH11	1.70	0.55
6:A:1412:C:H2'	6:A:1413:A:C8	2.42	0.55
11:F:21:MET:HG2	11:F:24:ARG:NH2	2.21	0.55
29:a:1794:A:H2'	29:a:1795:C:C6	2.42	0.55
14:I:21:ILE:HG23	14:I:61:LEU:HD12	1.87	0.55
29:a:282:A:H2'	29:a:283:G:C8	2.41	0.55
6:A:1071:C:H2'	6:A:1072:G:H8	1.71	0.55
6:A:460:A:H2'	6:A:461:A:H8	1.72	0.55
23:R:11:CYS:HB3	23:R:48:ARG:HH11	1.71	0.55
50:v:33:ALA:N	50:v:64:ASP:OD1	2.39	0.55
6:A:677:U:H3	6:A:713:G:H22	1.54	0.55
29:a:851:C:H2'	29:a:852:U:C6	2.41	0.55
29:a:2071:A:H2'	29:a:2072:C:C6	2.41	0.55
6:A:1120:C:H2'	6:A:1121:U:H6	1.72	0.55
15:J:28:THR:HG21	15:J:90:LEU:HD21	1.89	0.55
19:N:46:LEU:O	19:N:50:THR:HG23	2.07	0.55
20:O:18:ASP:OD1	20:O:19:ALA:N	2.39	0.55
32:d:39:ASP:N	32:d:39:ASP:OD1	2.37	0.54
6:A:382:A:H2'	6:A:383:A:C8	2.42	0.54
7:B:71:GLY:O	7:B:93:ASN:HA	2.08	0.54
41:m:8:ARG:HD2	41:m:43:GLU:HG2	1.89	0.54
6:A:384:G:H2'	6:A:385:C:C6	2.42	0.54
6:A:451:A:H61	6:A:481:G:H5'	1.72	0.54
40:l:111:GLU:OE2	40:l:111:GLU:N	2.33	0.54
29:a:2291:U:H2'	29:a:2292:U:C6	2.43	0.54
36:h:6:LEU:HD11	36:h:37:VAL:HG13	1.90	0.54
38:j:106:GLU:OE2	38:j:106:GLU:N	2.41	0.54
52:x:10:SER:OG	52:x:13:GLU:OE2	2.21	0.54
15:J:25:ILE:HG21	15:J:74:VAL:HG11	1.90	0.54
21:P:18:GLN:HE21	21:P:35:ARG:HD2	1.71	0.54
39:k:132:ARG:O	39:k:136:GLU:HG2	2.08	0.54
6:A:437:U:OP1	9:D:151:LYS:NZ	2.40	0.54
8:C:135:LYS:HA	8:C:135:LYS:HE2	1.90	0.54
15:J:7:ARG:HD3	15:J:75:ASP:OD1	2.08	0.54
15:J:52:LEU:HD21	15:J:59:LYS:HD2	1.90	0.54
25:T:18:ARG:NH1	25:T:18:ARG:HG2	2.23	0.54
29:a:1720:U:H2'	29:a:1721:G:O4'	2.08	0.54
6:A:33:A:H2'	6:A:34:C:C6	2.43	0.54
29:a:851:C:H2'	29:a:852:U:H6	1.73	0.54
39:k:78:ARG:NH1	39:k:80:SER:OG	2.41	0.54
6:A:539:A:H2'	6:A:540:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:859:G:H2'	6:A:860:A:C8	2.43	0.54
9:D:9:LEU:HD13	9:D:32:CYS:HB3	1.89	0.54
14:I:19:VAL:HG22	14:I:65:ILE:HD12	1.89	0.54
20:O:47:LYS:HB3	20:O:47:LYS:NZ	2.23	0.54
25:T:9:LYS:O	25:T:13:GLN:HG3	2.07	0.54
29:a:357:C:H2'	29:a:358:U:C6	2.43	0.54
45:q:73:LYS:NZ	45:q:73:LYS:HB3	2.23	0.54
9:D:33:LYS:HG3	9:D:36:GLN:HB3	1.88	0.53
29:a:608:A:H2'	29:a:609:A:C8	2.44	0.53
49:u:55:GLU:H	49:u:55:GLU:CD	2.14	0.53
6:A:17:U:H2'	6:A:18:C:C6	2.43	0.53
29:a:64:A:H2'	29:a:65:U:C6	2.43	0.53
29:a:910:A:H2'	29:a:911:A:C8	2.43	0.53
29:a:1432:G:H2'	29:a:1433:A:C8	2.43	0.53
29:a:2469:A:N6	29:a:2481:G:O2'	2.41	0.53
35:g:105:LEU:HB2	35:g:113:VAL:HB	1.89	0.53
6:A:1130:A:H2'	6:A:1131:G:H8	1.72	0.53
6:A:1287:A:H2'	6:A:1288:A:C8	2.44	0.53
12:G:111:ARG:NH2	12:G:122:ASN:HB3	2.24	0.53
15:J:88:MET:O	15:J:89:ARG:NH1	2.41	0.53
7:B:45:LYS:O	7:B:49:MET:HG3	2.08	0.53
8:C:82:GLU:O	8:C:86:LYS:HG3	2.09	0.53
14:I:22:LYS:HG2	14:I:62:ASP:HB3	1.90	0.53
14:I:34:SER:OG	14:I:35:LEU:N	2.40	0.53
28:Z:23:C:H2'	28:Z:24:U:C6	2.44	0.53
29:a:272:A:H2'	29:a:273:G:C8	2.44	0.53
29:a:1746:A:H2'	29:a:1747:U:C6	2.42	0.53
29:a:1871:A:H4'	29:a:1872:A:OP1	2.09	0.53
29:a:2430:A:N3	29:a:2430:A:H2'	2.22	0.53
34:f:134:GLU:N	34:f:134:GLU:OE1	2.41	0.53
6:A:254:G:OP1	22:Q:68:SER:OG	2.27	0.53
22:Q:52:GLU:N	22:Q:52:GLU:OE1	2.42	0.53
29:a:155:A:H2'	29:a:156:A:C8	2.43	0.53
29:a:189:G:OP2	51:w:14:THR:HG21	2.08	0.53
6:A:1038:C:H2'	6:A:1039:G:C8	2.44	0.53
19:N:27:LEU:O	19:N:31:ILE:HG12	2.09	0.53
29:a:207:A:H2'	29:a:208:C:O4'	2.08	0.53
19:N:49:GLN:NE2	24:S:13:LEU:H	2.07	0.53
29:a:1141:U:H4'	29:a:1142:A:O4'	2.09	0.53
6:A:337:G:H2'	6:A:338:A:H8	1.74	0.53
6:A:459:A:H2'	6:A:460:A:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:72:PHE:HE1	9:D:94:LEU:HD11	1.73	0.53
12:G:72:THR:HG22	12:G:96:ARG:HH12	1.73	0.53
17:L:56:ARG:NH1	17:L:60:GLY:O	2.41	0.53
26:U:28:VAL:O	26:U:32:VAL:HG23	2.08	0.53
29:a:172:A:H2'	29:a:173:A:C8	2.44	0.53
6:A:475:C:H2'	6:A:476:U:H6	1.74	0.53
29:a:2799:A:O2'	29:a:2800:A:H5''	2.09	0.53
47:s:5:GLU:OE1	47:s:5:GLU:N	2.30	0.53
58:a:3005:MIY:H81	58:a:3005:MIY:H713	1.91	0.53
6:A:459:A:H2'	6:A:460:A:C8	2.44	0.52
9:D:60:LYS:O	9:D:64:ILE:HG13	2.09	0.52
10:E:149:SER:OG	10:E:151:GLU:OE2	2.27	0.52
29:a:546:U:O2'	29:a:547:A:OP1	2.25	0.52
11:F:3:HIS:NE2	11:F:65:GLU:OE2	2.43	0.52
16:K:13:ARG:HB3	16:K:14:LYS:HE2	1.90	0.52
29:a:1796:U:H2'	29:a:1797:G:H8	1.74	0.52
29:a:2483:C:N3	40:l:123:LYS:NZ	2.54	0.52
6:A:530:G:N3	27:X:22:U:H2'	2.24	0.52
6:A:1119:C:OP1	14:I:85:ARG:NH1	2.40	0.52
29:a:888:C:H2'	29:a:889:C:O4'	2.10	0.52
6:A:501:C:OP1	17:L:114:ARG:NH2	2.39	0.52
6:A:713:G:H2'	6:A:714:G:C8	2.45	0.52
29:a:1816:C:N4	31:c:35:GLU:OE2	2.37	0.52
29:a:2532:G:N2	29:a:2663:G:O2'	2.43	0.52
29:a:2547:A:H2'	29:a:2548:U:C6	2.45	0.52
47:s:68:LYS:C	47:s:69:ARG:HD2	2.35	0.52
2:1:45:SER:OG	29:a:126:A:OP1	2.21	0.52
5:4:59:ARG:NH2	5:4:63:ARG:HH12	2.08	0.52
6:A:216:U:H2'	6:A:217:C:C6	2.44	0.52
17:L:54:ARG:NH1	17:L:64:THR:OG1	2.43	0.52
29:a:1602:U:OP2	47:s:64:LYS:NZ	2.39	0.52
29:a:2788:C:H2'	29:a:2789:C:C6	2.44	0.52
32:d:40:LEU:HD23	32:d:46:ARG:HG3	1.91	0.52
45:q:78:ARG:NH2	59:q:201:HOH:O	2.43	0.52
13:H:42:GLU:N	13:H:42:GLU:OE2	2.42	0.52
23:R:21:ILE:HG21	23:R:55:LEU:HD12	1.92	0.52
29:a:580:U:H2'	29:a:581:C:C6	2.44	0.52
29:a:597:G:O2'	39:k:11:GLY:O	2.24	0.52
29:a:2312:U:H5'	34:f:85:ILE:HD11	1.92	0.52
34:f:8:TYR:HB2	34:f:173:PHE:HZ	1.74	0.52
36:h:11:ASN:O	36:h:11:ASN:ND2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:405:U:O4	9:D:2:ALA:N	2.43	0.52
13:H:64:LYS:HG3	13:H:71:VAL:HG21	1.91	0.52
24:S:43:ASN:N	24:S:43:ASN:OD1	2.42	0.52
30:b:66:A:N6	30:b:107:G:H2'	2.24	0.52
49:u:20:LEU:HD11	49:u:41:GLU:HG2	1.92	0.52
6:A:1356:G:H2'	6:A:1357:A:H8	1.72	0.52
13:H:18:GLN:NE2	13:H:70:ALA:HB1	2.25	0.52
15:J:99:GLN:OE1	15:J:99:GLN:HA	2.10	0.52
29:a:1870:C:H2'	29:a:1870:C:O2	2.10	0.52
31:c:66:ASP:OD2	31:c:102:ARG:NH1	2.42	0.52
34:f:48:LYS:O	34:f:48:LYS:HD3	2.10	0.52
36:h:34:GLY:O	36:h:36:ALA:N	2.43	0.52
6:A:674:G:H2'	6:A:675:A:H8	1.75	0.52
6:A:1120:C:H2'	6:A:1121:U:C6	2.44	0.52
11:F:4:TYR:CD2	11:F:71:ILE:HG13	2.45	0.52
29:a:1199:U:H1'	44:p:4:VAL:HG22	1.92	0.52
29:a:1889:A:H2'	29:a:1890:A:C8	2.45	0.52
29:a:2514:U:H2'	29:a:2515:C:C6	2.44	0.52
34:f:37:ASN:OD1	34:f:38:MET:N	2.43	0.52
3:2:54:ASP:HB3	39:k:57:LEU:HD22	1.90	0.52
29:a:892:A:H2'	29:a:893:C:C6	2.45	0.52
6:A:509:A:N3	6:A:543:U:O2'	2.42	0.51
6:A:1530:G:H2'	6:A:1531:A:C8	2.45	0.51
35:g:12:PRO:HD2	35:g:15:VAL:HG21	1.91	0.51
3:2:52:LYS:NZ	29:a:938:G:OP2	2.43	0.51
6:A:654:G:N7	59:A:1804:HOH:O	2.34	0.51
29:a:279:A:H61	29:a:361:G:H1'	1.76	0.51
29:a:2591:C:H2'	29:a:2592:G:H8	1.75	0.51
31:c:157:SER:O	31:c:160:THR:OG1	2.26	0.51
6:A:1124:G:H4'	15:J:40:ILE:HD11	1.91	0.51
53:y:6:LYS:HG2	53:y:37:GLU:HG2	1.91	0.51
5:4:14:ALA:HB1	5:4:34:LEU:HD11	1.93	0.51
8:C:51:SER:O	8:C:51:SER:OG	2.22	0.51
13:H:77:ARG:NH1	13:H:79:SER:O	2.44	0.51
14:I:59:GLU:N	14:I:59:GLU:OE1	2.44	0.51
29:a:1797:G:HO2'	31:c:257:THR:HG1	1.57	0.51
29:a:2243:U:H2'	29:a:2244:U:C6	2.46	0.51
6:A:1391:U:H2'	6:A:1392:G:C8	2.46	0.51
16:K:109:ASN:HD21	26:U:5:LYS:HD2	1.76	0.51
29:a:306:U:H2'	29:a:307:G:O4'	2.10	0.51
29:a:414:C:H2'	29:a:415:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:813:U:H2'	29:a:814:C:C6	2.46	0.51
15:J:77:VAL:O	15:J:78:GLU:HG2	2.10	0.51
34:f:162:SER:OG	34:f:165:GLU:OE2	2.27	0.51
6:A:524:G:H2'	6:A:525:C:C6	2.45	0.51
6:A:1010:U:H2'	6:A:1011:C:C6	2.46	0.51
29:a:644:A:H2'	29:a:645:C:O4'	2.11	0.51
29:a:652:U:OP1	29:a:654:A:N6	2.44	0.51
3:2:14:PHE:O	3:2:15:LYS:HD3	2.10	0.50
6:A:728:A:H2'	6:A:729:A:C8	2.46	0.50
6:A:1493:A:O2'	6:A:1494:G:H8	1.94	0.50
6:A:1494:G:HO2'	29:a:1912:A:HO2'	1.59	0.50
29:a:2246:G:H2'	29:a:2247:A:C8	2.45	0.50
34:f:74:VAL:HB	34:f:79:ILE:HD11	1.93	0.50
8:C:134:MET:HE2	8:C:168:TYR:CD2	2.45	0.50
29:a:272:A:H2'	29:a:273:G:H8	1.76	0.50
29:a:594:U:H2'	29:a:595:C:C6	2.47	0.50
7:B:111:ILE:HD12	7:B:152:LYS:HA	1.93	0.50
9:D:47:ARG:HA	9:D:47:ARG:HH11	1.75	0.50
12:G:79:ARG:H	12:G:79:ARG:CD	2.23	0.50
26:U:60:LEU:O	26:U:64:ASN:ND2	2.44	0.50
29:a:1266:G:O2'	29:a:2012:G:O6	2.23	0.50
29:a:2567:G:H2'	29:a:2568:U:C6	2.47	0.50
37:i:60:ASP:OD1	37:i:60:ASP:N	2.37	0.50
41:m:28:LEU:HD23	41:m:48:VAL:HG21	1.93	0.50
10:E:50:TYR:CE1	10:E:134:ILE:HD11	2.47	0.50
19:N:23:LYS:O	19:N:27:LEU:HD23	2.12	0.50
29:a:39:G:H2'	29:a:40:U:C6	2.47	0.50
29:a:577:G:O2'	29:a:1254:A:OP1	2.29	0.50
29:a:1509:A:HO2'	29:a:1510:G:H8	1.59	0.50
29:a:2328:A:H2'	29:a:2329:U:H6	1.76	0.50
6:A:1346:A:OP1	14:I:122:ARG:NH1	2.24	0.50
8:C:78:GLY:HA3	8:C:83:ASP:OD2	2.12	0.50
14:I:41:ARG:NH2	14:I:43:THR:OG1	2.44	0.50
5:4:59:ARG:NH1	6:A:1311:A:OP1	2.42	0.50
6:A:41:G:H2'	6:A:42:G:H8	1.77	0.50
6:A:1355:G:H2'	6:A:1356:G:H8	1.76	0.50
10:E:38:VAL:HG11	10:E:114:VAL:HG22	1.94	0.50
11:F:42:TRP:HB2	11:F:59:TYR:HB2	1.92	0.50
20:O:79:THR:O	20:O:83:GLU:HG3	2.12	0.50
29:a:1434:A:H2'	29:a:1435:G:C8	2.47	0.50
29:a:2537:U:H2'	29:a:2538:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:116:GLY:O	34:f:178:ARG:NH1	2.45	0.50
10:E:10:GLU:OE1	10:E:10:GLU:N	2.44	0.50
26:U:8:GLU:OE1	26:U:8:GLU:N	2.42	0.50
29:a:871:U:H2'	29:a:872:U:C6	2.46	0.50
30:b:1:U:H2'	30:b:2:G:H8	1.76	0.50
6:A:945:G:C2	6:A:946:A:C8	3.00	0.50
12:G:100:ALA:O	12:G:104:ILE:HD12	2.12	0.50
26:U:59:LYS:O	26:U:63:GLU:HG2	2.11	0.50
29:a:2273:A:H2'	29:a:2274:A:C8	2.46	0.50
5:4:25:ARG:NH1	34:f:98:GLU:OE1	2.44	0.49
6:A:1152:A:OP1	15:J:70:HIS:ND1	2.34	0.49
7:B:4:VAL:HG11	7:B:212:LEU:HD11	1.93	0.49
10:E:55:GLU:N	10:E:55:GLU:OE2	2.45	0.49
29:a:634:C:H2'	29:a:635:C:C6	2.47	0.49
29:a:1808:A:H3'	29:a:1809:A:C8	2.47	0.49
29:a:2469:A:H4'	40:l:55:ARG:CD	2.42	0.49
6:A:460:A:H2'	6:A:461:A:C8	2.48	0.49
24:S:3:ARG:HH21	24:S:7:LYS:HE3	1.77	0.49
25:T:18:ARG:HG2	25:T:18:ARG:HH11	1.75	0.49
28:Z:17(A):U:O2'	28:Z:18:G:H4'	2.12	0.49
34:f:8:TYR:HB2	34:f:173:PHE:CZ	2.46	0.49
6:A:518:C:O2'	6:A:530:G:N2	2.44	0.49
6:A:1010:U:H2'	6:A:1011:C:H6	1.77	0.49
10:E:149:SER:H	10:E:152:MET:HE2	1.78	0.49
29:a:150:U:H2'	29:a:151:C:C6	2.48	0.49
29:a:1856:U:H2'	29:a:1857:G:O4'	2.11	0.49
34:f:4:LEU:HG	34:f:101:GLU:HG3	1.94	0.49
35:g:47:ASP:OD1	35:g:48:ASN:N	2.45	0.49
35:g:60:ASP:OD1	35:g:61:GLY:N	2.38	0.49
38:j:12:ASP:OD1	38:j:14:SER:OG	2.26	0.49
44:p:86:ALA:HB2	44:p:116:ALA:HB2	1.95	0.49
47:s:69:ARG:NH2	47:s:74:ILE:HB	2.27	0.49
4:3:18:LYS:HG3	4:3:23:ILE:HD13	1.94	0.49
6:A:1162:C:H2'	6:A:1163:A:H8	1.77	0.49
46:r:95:ARG:HH11	46:r:95:ARG:HG2	1.77	0.49
6:A:35:G:N3	17:L:115:SER:OG	2.46	0.49
6:A:1039:G:H2'	6:A:1040:U:C6	2.48	0.49
29:a:947:A:H2'	29:a:948:C:C6	2.47	0.49
38:j:77:ILE:HG12	43:o:72:ARG:HD3	1.95	0.49
25:T:79:LEU:O	25:T:83:ILE:HG13	2.12	0.49
46:r:4:ILE:HG13	46:r:106:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1273:C:H2'	6:A:1274:A:O4'	2.12	0.49
6:A:1314:C:H2'	6:A:1315:U:H6	1.77	0.49
18:M:47:GLU:OE1	18:M:47:GLU:N	2.43	0.49
21:P:55:ASP:OD1	21:P:56:ARG:N	2.46	0.49
29:a:753:A:H2'	29:a:754:U:H6	1.78	0.49
29:a:848:C:H2'	29:a:849:A:C8	2.48	0.49
29:a:2014:A:H2'	29:a:2015:A:C8	2.47	0.49
6:A:501:C:H2'	6:A:502:A:C8	2.47	0.49
6:A:859:G:H2'	6:A:860:A:H8	1.78	0.49
6:A:868:C:H2'	6:A:869:G:O4'	2.13	0.49
6:A:1378:C:O2	12:G:76:LYS:NZ	2.46	0.49
29:a:155:A:H2'	29:a:156:A:H8	1.76	0.49
29:a:2038:G:H2'	29:a:2039:U:O4'	2.13	0.49
29:a:2557:G:H2'	29:a:2558:C:C6	2.48	0.49
37:i:31:GLU:HB3	37:i:142:ILE:HD13	1.95	0.49
6:A:908:A:H2'	6:A:909:A:C8	2.47	0.49
6:A:1251:A:H2'	6:A:1252:A:C8	2.46	0.49
6:A:1494:G:O2'	29:a:1912:A:O2'	2.31	0.49
29:a:1417:C:O2'	29:a:1587:G:O2'	2.28	0.49
29:a:2246:G:H2'	29:a:2247:A:H8	1.78	0.49
31:c:29:PRO:HG2	31:c:34:LEU:HD11	1.94	0.49
6:A:545:C:OP1	9:D:58:LYS:NZ	2.46	0.48
6:A:1253:G:H2'	6:A:1254:A:C8	2.47	0.48
6:A:35:G:H2'	6:A:36:C:C6	2.47	0.48
6:A:736:C:H2'	6:A:737:C:C6	2.48	0.48
6:A:1323:G:H2'	6:A:1324:A:H8	1.78	0.48
7:B:126:PHE:HA	7:B:129:LEU:HD23	1.94	0.48
15:J:85:ASP:HA	15:J:88:MET:CE	2.43	0.48
6:A:475:C:H2'	6:A:476:U:C6	2.48	0.48
25:T:49:LYS:HG2	25:T:53:GLU:OE2	2.13	0.48
29:a:632:A:H2'	29:a:633:A:C8	2.48	0.48
29:a:1664:A:H2	38:j:1:MET:HE1	1.78	0.48
29:a:2329:U:H2'	29:a:2330:G:C8	2.47	0.48
6:A:299:G:H2'	6:A:300:A:C8	2.47	0.48
6:A:1253:G:H2'	6:A:1254:A:H8	1.78	0.48
29:a:709:U:H2'	29:a:710:U:C6	2.48	0.48
29:a:1747:U:H2'	29:a:1748:C:C6	2.48	0.48
29:a:2020:A:H5'	54:z:9:THR:CG2	2.42	0.48
34:f:58:ALA:HB2	34:f:65:PRO:HD3	1.96	0.48
40:l:136:MET:HG2	49:u:77:VAL:HG12	1.94	0.48
42:n:92:PHE:HB2	42:n:117:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:464:U:O2'	6:A:466:A:N7	2.41	0.48
6:A:946:A:H2'	6:A:947:G:H8	1.77	0.48
6:A:996:A:H2'	6:A:997:U:C6	2.49	0.48
6:A:1002:G:H2'	6:A:1003:G:O4'	2.14	0.48
14:I:97:GLU:CD	14:I:97:GLU:H	2.21	0.48
18:M:92:ARG:HD3	29:a:888:C:C6	2.48	0.48
29:a:898:C:H2'	29:a:899:A:O4'	2.14	0.48
31:c:107:PRO:HD2	31:c:110:LEU:HD22	1.96	0.48
6:A:481:G:O2'	6:A:483:C:N4	2.47	0.48
29:a:1149:G:H2'	29:a:1150:C:C6	2.48	0.48
48:t:81:ASP:OD1	48:t:82:ARG:N	2.47	0.48
6:A:580:C:H2'	6:A:581:G:O4'	2.12	0.48
6:A:653:U:OP1	13:H:56:LYS:NZ	2.30	0.48
6:A:769:G:H4'	6:A:1513:A:H4'	1.94	0.48
6:A:1060:U:OP1	19:N:85:ARG:NH2	2.39	0.48
15:J:24:GLU:O	15:J:27:GLU:HG3	2.13	0.48
18:M:81:MET:HE2	29:a:888:C:O2	2.13	0.48
29:a:358:U:H2'	29:a:359:G:C8	2.47	0.48
29:a:511:U:H2'	29:a:512:G:H5'	1.96	0.48
29:a:1405:U:H2'	29:a:1406:U:C6	2.49	0.48
29:a:2064:C:H2'	29:a:2065:C:C6	2.49	0.48
29:a:2455:G:H2'	29:a:2456:C:C6	2.49	0.48
6:A:203:G:O2'	6:A:465:A:N1	2.44	0.48
6:A:1305:G:N2	6:A:1331:G:H1'	2.29	0.48
12:G:40:GLU:HG2	12:G:44:TYR:CE2	2.49	0.48
29:a:2086:U:H2'	29:a:2087:G:C8	2.49	0.48
40:l:12:MET:HE2	40:l:71:LYS:HG3	1.96	0.48
6:A:162:A:H2'	6:A:163:C:O4'	2.14	0.48
6:A:555:U:H2'	6:A:556:C:C6	2.48	0.48
6:A:1435:G:H2'	6:A:1436:U:C6	2.49	0.48
29:a:276:U:H2'	29:a:277:G:C8	2.49	0.48
29:a:278:A:OP2	29:a:361:G:N2	2.43	0.48
29:a:282:A:H2'	29:a:283:G:H8	1.79	0.48
35:g:9:VAL:HG13	35:g:50:LEU:HB2	1.95	0.48
6:A:746:A:H2'	6:A:747:A:C8	2.49	0.48
9:D:78:GLU:OE2	9:D:81:ARG:NH2	2.46	0.48
29:a:753:A:H2'	29:a:754:U:C6	2.49	0.48
29:a:2526:G:N7	59:a:3431:HOH:O	2.35	0.48
6:A:976:G:OP2	6:A:1358:U:O2'	2.32	0.47
11:F:38:ARG:NH1	11:F:61:LEU:HD21	2.29	0.47
29:a:1442:U:H2'	29:a:1443:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:59:ARG:CZ	5:4:63:ARG:HH12	2.27	0.47
6:A:674:G:H2'	6:A:675:A:C8	2.49	0.47
6:A:920:U:H2'	6:A:921:U:C6	2.49	0.47
6:A:1238:A:H2	6:A:1241:G:N3	2.13	0.47
29:a:1386:C:H2'	29:a:1387:A:C8	2.49	0.47
6:A:1014:A:C2	6:A:1219:A:H1'	2.49	0.47
6:A:1175:G:H2'	6:A:1176:A:H8	1.79	0.47
6:A:1266:G:N2	6:A:1269:A:OP2	2.41	0.47
7:B:86:SER:O	7:B:86:SER:OG	2.29	0.47
14:I:47:VAL:HG13	14:I:80:ARG:HD3	1.97	0.47
29:a:419:U:H2'	29:a:420:C:C6	2.50	0.47
40:I:42:THR:HG22	40:I:93:VAL:HG12	1.94	0.47
6:A:1040:U:H2'	6:A:1041:G:H8	1.79	0.47
6:A:1187:G:H5'	14:I:115:LYS:HE2	1.96	0.47
6:A:1359:C:OP2	19:N:75:ARG:NH1	2.44	0.47
29:a:547:A:H3'	29:a:548:G:N7	2.29	0.47
33:e:191:ASP:O	33:e:195:GLN:HG3	2.15	0.47
53:y:31:ARG:HG2	53:y:34:HIS:HB2	1.97	0.47
6:A:1004:A:O2'	6:A:1036:A:N6	2.46	0.47
6:A:1071:C:H2'	6:A:1072:G:C8	2.49	0.47
6:A:1486:G:H2'	6:A:1487:G:O4'	2.15	0.47
8:C:131:ARG:NH2	8:C:166:GLU:OE1	2.45	0.47
14:I:6:TYR:CG	14:I:90:TYR:HB2	2.50	0.47
16:K:75:LYS:HE3	16:K:75:LYS:HB3	1.83	0.47
29:a:782:A:N1	31:c:225:MET:HE2	2.28	0.47
29:a:1028:A:H2'	29:a:1029:A:C8	2.50	0.47
6:A:515:G:H2'	6:A:516:PSU:H6	1.79	0.47
58:A:1635:MIY:O1	58:A:1635:MIY:N2	2.41	0.47
15:J:26:VAL:HG12	15:J:30:LYS:HZ3	1.79	0.47
29:a:1182:G:H2'	29:a:1183:U:O4'	2.14	0.47
29:a:1641:A:H2'	29:a:1642:G:O4'	2.14	0.47
8:C:135:LYS:HE3	8:C:168:TYR:CD2	2.50	0.47
9:D:35:GLU:OE1	9:D:35:GLU:N	2.43	0.47
11:F:42:TRP:CZ2	11:F:102:MET:HG3	2.50	0.47
16:K:52:PHE:O	16:K:53:ARG:HD2	2.15	0.47
29:a:645:C:H2'	29:a:647:G:C8	2.50	0.47
29:a:721:A:H2'	29:a:722:A:C8	2.50	0.47
29:a:1028:A:N6	29:a:1125:G:H2'	2.30	0.47
29:a:1226:A:OP1	44:p:16:LYS:NZ	2.48	0.47
29:a:1645:G:H5''	29:a:1646:C:H5'	1.97	0.47
29:a:2079:U:O2'	51:w:23:ASN:OD1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:32:GLU:OE1	35:g:32:GLU:HA	2.14	0.47
41:m:20:MET:HE2	41:m:20:MET:HB3	1.81	0.47
6:A:604:G:H2'	6:A:605:U:O4'	2.15	0.47
6:A:1133:G:H2'	6:A:1134:G:O4'	2.15	0.47
19:N:80:SER:O	19:N:84:VAL:HG23	2.15	0.47
29:a:2795:C:H2'	29:a:2796:U:C6	2.50	0.47
47:s:69:ARG:HD2	47:s:69:ARG:N	2.30	0.47
6:A:933:G:O6	12:G:3:ARG:NH2	2.44	0.47
8:C:147:LYS:HB3	8:C:203:PHE:CD2	2.49	0.47
29:a:1410:G:H2'	29:a:1411:U:C6	2.49	0.47
45:q:1:MET:HE3	45:q:101:ILE:HB	1.97	0.47
54:z:55:ILE:HG13	54:z:55:ILE:O	2.14	0.47
6:A:384:G:H2'	6:A:385:C:H6	1.80	0.46
6:A:736:C:H2'	6:A:737:C:H6	1.78	0.46
6:A:900:A:H2'	6:A:901:A:C8	2.50	0.46
6:A:1250:A:H2'	6:A:1251:A:C8	2.50	0.46
9:D:187:GLU:O	9:D:191:LEU:HD22	2.15	0.46
29:a:151:C:H2'	29:a:152:A:H8	1.80	0.46
29:a:1000:A:H2'	29:a:1001:A:C8	2.49	0.46
29:a:1794:A:H2'	29:a:1795:C:H6	1.80	0.46
29:a:1796:U:H2'	29:a:1797:G:C8	2.50	0.46
34:f:108:VAL:HG11	34:f:176:PRO:HG3	1.97	0.46
40:l:70:ASP:OD1	40:l:70:ASP:N	2.45	0.46
6:A:41:G:H2'	6:A:42:G:C8	2.50	0.46
6:A:1355:G:H2'	6:A:1356:G:C8	2.49	0.46
8:C:119:SER:O	8:C:123:GLN:HG3	2.14	0.46
13:H:11:LEU:HD22	13:H:75:ILE:HD11	1.96	0.46
29:a:276:U:O2'	29:a:278:A:N7	2.47	0.46
50:v:59:LEU:HD12	50:v:80:ILE:HD12	1.97	0.46
6:A:131:A:H2'	6:A:132:C:C6	2.50	0.46
12:G:15:ASP:OD2	12:G:23:LEU:HB3	2.14	0.46
16:K:113:VAL:HG12	23:R:73:ARG:HD3	1.97	0.46
29:a:2345:G:N3	29:a:2381:A:H2'	2.30	0.46
6:A:323:U:H2'	6:A:324:G:O4'	2.16	0.46
6:A:1163:A:H2'	6:A:1164:G:C8	2.51	0.46
32:d:125:TRP:CD1	32:d:160:LYS:HB3	2.51	0.46
38:j:7:MET:SD	38:j:20:MET:HG3	2.55	0.46
41:m:72:ASP:HB3	41:m:75:ILE:HB	1.97	0.46
9:D:151:LYS:HD2	9:D:151:LYS:C	2.41	0.46
13:H:79:SER:HB3	13:H:125:ILE:O	2.15	0.46
29:a:172:A:H2'	29:a:173:A:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:376:G:H5''	21:P:5:ARG:HB2	1.98	0.46
9:D:117:LEU:HB3	9:D:123:ILE:HD11	1.97	0.46
14:I:21:ILE:HG12	14:I:86:ALA:HB1	1.98	0.46
17:L:110:ARG:HB3	17:L:119:VAL:HG21	1.97	0.46
29:a:75:G:H22	29:a:111:A:H2	1.62	0.46
29:a:139:U:N3	47:s:1:MET:HE1	2.31	0.46
29:a:811:U:H2'	39:k:21:ARG:HA	1.97	0.46
29:a:2680:U:O2'	29:a:2681:C:H5'	2.16	0.46
35:g:153:ARG:HB2	35:g:153:ARG:CZ	2.44	0.46
47:s:37:ASP:OD1	47:s:37:ASP:N	2.47	0.46
6:A:1382:C:H2'	6:A:1383:C:H6	1.81	0.46
37:i:114:LEU:HG	37:i:118:MET:HE3	1.98	0.46
6:A:918:A:H2'	6:A:919:A:C8	2.51	0.46
7:B:219:ALA:O	7:B:223:GLU:HG2	2.15	0.46
11:F:14:GLN:OE1	11:F:14:GLN:N	2.49	0.46
15:J:32:THR:HB	15:J:82:LYS:NZ	2.30	0.46
15:J:48:ARG:HG2	15:J:66:GLU:HG3	1.97	0.46
29:a:1026:G:H2'	29:a:1027:A:C8	2.51	0.46
38:j:12:ASP:CG	38:j:14:SER:HG	2.22	0.46
6:A:1169:A:H2'	6:A:1170:A:C8	2.50	0.46
6:A:1410:A:H2'	6:A:1411:C:C6	2.51	0.46
15:J:8:ILE:HG23	15:J:100:ILE:HD13	1.98	0.46
16:K:88:GLY:O	16:K:93:ARG:NH1	2.42	0.46
29:a:364:C:H2'	29:a:365:U:C6	2.51	0.46
29:a:1548:A:H2'	29:a:1549:A:C8	2.51	0.46
29:a:2074:U:H2'	29:a:2075:U:C6	2.50	0.46
29:a:2728:U:O2'	29:a:2729:G:H8	1.99	0.46
6:A:1319:A:O2'	6:A:1323:G:N7	2.44	0.46
8:C:112:ASP:OD2	8:C:115:LEU:HG	2.16	0.46
29:a:887:U:H5''	29:a:888:C:H5	1.80	0.46
29:a:1538:G:H2'	29:a:1539:U:C6	2.51	0.46
29:a:1563:U:H2'	29:a:1564:C:C6	2.51	0.46
29:a:2711:A:N7	59:a:3434:HOH:O	2.36	0.46
29:a:2812:G:H2'	29:a:2813:A:C8	2.51	0.46
29:a:2895:G:H2'	29:a:2896:C:C6	2.51	0.46
32:d:74:GLU:CD	32:d:74:GLU:H	2.24	0.46
35:g:30:ASN:HD22	35:g:30:ASN:C	2.08	0.46
45:q:31:GLU:OE1	45:q:31:GLU:N	2.49	0.46
6:A:505:G:H2'	6:A:506:G:C8	2.51	0.45
6:A:820:U:H4'	6:A:821:G:OP2	2.16	0.45
6:A:1062:U:H2'	6:A:1063:C:C6	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1428:A:H2'	6:A:1429:A:O4'	2.16	0.45
11:F:18:VAL:O	11:F:22:ILE:HG13	2.16	0.45
19:N:3:LYS:HB2	19:N:6:MET:HG2	1.98	0.45
24:S:13:LEU:HD12	24:S:13:LEU:HA	1.77	0.45
29:a:365:U:H2'	29:a:366:C:C6	2.52	0.45
29:a:1506:U:H2'	29:a:1507:C:C6	2.51	0.45
53:y:23:THR:HG23	53:y:47:MET:HG2	1.98	0.45
1:0:5:ILE:HG21	1:0:28:ARG:NH2	2.31	0.45
6:A:607:A:H2'	6:A:608:A:C8	2.50	0.45
6:A:1122:U:H2'	6:A:1123:U:C6	2.51	0.45
20:O:14:GLU:CD	20:O:84:ARG:HH12	2.24	0.45
29:a:933:A:H5'	29:a:934:U:OP2	2.17	0.45
2:1:25:LYS:NZ	59:1:102:HOH:O	2.49	0.45
6:A:1125:U:HO2'	6:A:1126:U:P	2.39	0.45
8:C:86:LYS:O	8:C:90:VAL:HG23	2.17	0.45
34:f:74:VAL:H	34:f:79:ILE:HG13	1.81	0.45
19:N:49:GLN:HE22	24:S:12:ASP:CA	2.28	0.45
25:T:20:HIS:O	25:T:24:ARG:HG2	2.15	0.45
29:a:545:U:H3'	29:a:546:U:C5'	2.46	0.45
29:a:657:U:H2'	29:a:658:U:C6	2.52	0.45
29:a:848:C:H2'	29:a:849:A:H8	1.81	0.45
29:a:1340:U:OP1	47:s:19:LYS:NZ	2.43	0.45
6:A:126:G:OP1	6:A:605:U:O2'	2.31	0.45
6:A:1163:A:H2'	6:A:1164:G:H8	1.81	0.45
7:B:132:LYS:O	7:B:136:MET:HG2	2.17	0.45
11:F:40:GLU:OE1	11:F:100:SER:HB3	2.16	0.45
17:L:30:LYS:HE2	17:L:59:ASN:HD22	1.81	0.45
22:Q:77:ARG:NH1	22:Q:79:VAL:HG22	2.32	0.45
23:R:47:THR:HG22	23:R:48:ARG:O	2.16	0.45
29:a:182:A:H2'	29:a:183:C:H6	1.81	0.45
29:a:1494:A:H2'	29:a:1495:A:C8	2.51	0.45
30:b:30:C:H2'	30:b:31:C:H5'	1.98	0.45
30:b:51:G:OP1	42:n:63:LYS:NZ	2.44	0.45
43:o:13:MET:HE2	43:o:13:MET:HB3	1.90	0.45
6:A:72:A:H2'	6:A:73:C:H5'	1.98	0.45
6:A:74:A:H2'	6:A:75:G:O4'	2.16	0.45
6:A:107:G:N7	25:T:10:ARG:NH2	2.61	0.45
6:A:294:U:OP1	6:A:610:U:O2'	2.27	0.45
6:A:718:A:H5'	16:K:119:ASN:OD1	2.17	0.45
6:A:1162:C:H2'	6:A:1163:A:C8	2.51	0.45
6:A:1371:G:OP1	14:I:14:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1464:U:H2'	6:A:1465:A:H8	1.81	0.45
12:G:74:GLU:HG2	12:G:91:VAL:HG22	1.98	0.45
23:R:72:ASP:OD1	23:R:72:ASP:N	2.40	0.45
29:a:284:U:H3	29:a:356:G:H1	1.64	0.45
29:a:639:U:H2'	29:a:640:C:H6	1.81	0.45
29:a:784:G:H5'	29:a:785:G:OP1	2.16	0.45
29:a:1378:A:O2'	29:a:1380:G:N7	2.50	0.45
29:a:1809:A:H2'	29:a:1810:A:C8	2.52	0.45
29:a:2395:C:H2'	29:a:2396:G:O4'	2.16	0.45
29:a:2700:A:H2'	29:a:2701:U:C6	2.52	0.45
30:b:42:C:C5	34:f:66:LEU:HD22	2.52	0.45
41:m:106:ASP:N	41:m:106:ASP:OD1	2.49	0.45
23:R:29:LEU:HA	23:R:29:LEU:HD23	1.81	0.45
29:a:1026:G:H2'	29:a:1027:A:H8	1.81	0.45
29:a:1115:G:O2'	29:a:1116:G:H8	2.00	0.45
34:f:4:LEU:HD23	34:f:4:LEU:HA	1.76	0.45
11:F:38:ARG:HB3	11:F:63:ASN:HB2	1.98	0.45
11:F:41:ASP:OD1	11:F:58:HIS:NE2	2.50	0.45
29:a:645:C:H2'	29:a:647:G:N7	2.31	0.45
29:a:936:A:H2'	29:a:937:C:C6	2.51	0.45
35:g:43:VAL:O	35:g:44:LYS:HG3	2.16	0.45
3:2:55:LEU:HD23	3:2:55:LEU:HA	1.72	0.45
6:A:371:A:H2'	6:A:372:C:O4'	2.17	0.45
20:O:80:GLN:HA	20:O:83:GLU:OE2	2.17	0.45
24:S:65:GLU:OE1	24:S:65:GLU:N	2.33	0.45
29:a:2251:OMG:HM23	29:a:2251:OMG:H1'	1.65	0.45
6:A:8:A:N6	9:D:206:LYS:HB2	2.32	0.45
6:A:865:A:H2'	6:A:866:C:C6	2.51	0.45
6:A:1009:U:H3	6:A:1020:G:H1	1.63	0.45
8:C:161:GLU:N	8:C:161:GLU:CD	2.75	0.45
11:F:2:ARG:NE	11:F:68:GLN:OE1	2.45	0.45
45:q:31:GLU:N	45:q:31:GLU:CD	2.75	0.45
6:A:750:C:O2	20:O:23:GLY:HA3	2.17	0.44
8:C:72:ARG:HB3	8:C:75:ILE:HG22	1.99	0.44
17:L:68:GLY:O	17:L:99:ARG:NH1	2.49	0.44
18:M:9:ILE:HD12	18:M:9:ILE:O	2.17	0.44
29:a:1667:G:O2'	29:a:1991:U:O4	2.29	0.44
29:a:2674:G:H4'	38:j:30:ARG:HD2	1.99	0.44
29:a:2780:G:OP2	37:i:120:ARG:HD3	2.16	0.44
41:m:55:ALA:HA	41:m:80:PHE:CE2	2.53	0.44
11:F:69:GLU:H	11:F:69:GLU:CD	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:79:ARG:HD3	12:G:79:ARG:N	2.27	0.44
19:N:46:LEU:HB3	24:S:13:LEU:HD13	1.99	0.44
29:a:511:U:C2'	29:a:512:G:H5'	2.47	0.44
29:a:1141:U:OP2	37:i:65:THR:OG1	2.34	0.44
29:a:2804:U:H2'	29:a:2805:C:C6	2.52	0.44
34:f:96:MET:HE2	34:f:96:MET:HB3	1.93	0.44
49:u:34:LYS:HA	49:u:34:LYS:HD3	1.63	0.44
6:A:214:C:H2'	6:A:215:C:C6	2.53	0.44
15:J:88:MET:HE2	15:J:88:MET:HB2	1.75	0.44
29:a:5:A:H2'	29:a:6:A:C8	2.52	0.44
29:a:742:A:H2'	29:a:743:A:C8	2.53	0.44
29:a:1570:A:H2'	29:a:1571:A:C8	2.52	0.44
6:A:721:G:H4'	6:A:722:G:O4'	2.18	0.44
6:A:1124:G:N2	6:A:1125:U:O4	2.36	0.44
6:A:1465:A:H2'	6:A:1466:C:C6	2.53	0.44
27:X:13:A:H2'	27:X:14:A:C8	2.53	0.44
29:a:3:U:H2'	29:a:4:U:C6	2.52	0.44
29:a:287:G:H2'	29:a:288:U:C6	2.52	0.44
29:a:596:U:H2'	29:a:597:G:C8	2.52	0.44
30:b:106:G:H2'	30:b:107:G:O4'	2.18	0.44
31:c:43:ARG:HA	31:c:48:ARG:O	2.17	0.44
35:g:72:LEU:HD13	35:g:72:LEU:HA	1.85	0.44
48:t:86:ARG:HG3	48:t:95:PHE:CD1	2.52	0.44
49:u:50:MET:HE2	49:u:50:MET:HB2	1.72	0.44
6:A:522:C:H41	17:L:50:ARG:NH2	2.15	0.44
7:B:125:THR:HA	7:B:128:LYS:NZ	2.32	0.44
29:a:2:G:H2'	29:a:3:U:C6	2.53	0.44
29:a:284:U:H2'	29:a:285:G:O4'	2.17	0.44
29:a:1338:G:O2'	29:a:1393:A:N1	2.46	0.44
32:d:74:GLU:CD	32:d:74:GLU:N	2.76	0.44
35:g:4:VAL:O	35:g:69:ARG:HD2	2.17	0.44
6:A:399:G:H2'	6:A:400:C:C6	2.53	0.44
11:F:33:GLU:OE1	11:F:33:GLU:N	2.51	0.44
19:N:33:ASP:CG	19:N:36:ALA:HB2	2.43	0.44
24:S:21:LYS:O	24:S:24:GLU:HG3	2.17	0.44
33:e:171:ASP:OD1	33:e:171:ASP:N	2.37	0.44
6:A:613:C:H2'	6:A:614:C:C6	2.53	0.44
6:A:821:G:H2'	6:A:822:U:C6	2.53	0.44
25:T:48:GLN:O	25:T:52:ASN:OD1	2.36	0.44
29:a:728:G:N7	59:a:3438:HOH:O	2.36	0.44
29:a:1441:G:H2'	29:a:1442:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:26:ILE:HG22	35:g:79:VAL:HG11	2.00	0.44
52:x:19:LEU:HD23	52:x:19:LEU:HA	1.81	0.44
6:A:161:A:H2'	6:A:162:A:C8	2.53	0.44
6:A:1004:A:C5	6:A:1026:G:H1'	2.53	0.44
6:A:1151:A:O2'	6:A:1152:A:H8	2.00	0.44
14:I:35:LEU:HB3	14:I:36:GLU:OE1	2.17	0.44
20:O:48:LYS:HA	20:O:48:LYS:HD3	1.68	0.44
22:Q:77:ARG:HG3	22:Q:77:ARG:HH11	1.82	0.44
29:a:151:C:H2'	29:a:152:A:C8	2.53	0.44
29:a:247:G:OP2	29:a:249:C:N4	2.45	0.44
29:a:1682:G:H2'	29:a:1683:U:C6	2.53	0.44
34:f:69:LYS:HE3	34:f:69:LYS:HB3	1.72	0.44
44:p:90:ILE:HG22	44:p:95:LEU:HG	2.00	0.44
45:q:46:GLU:OE1	45:q:48:LYS:NZ	2.51	0.44
47:s:23:ALA:HB1	47:s:29:THR:HB	2.00	0.44
6:A:539:A:H2'	6:A:540:G:H8	1.81	0.44
6:A:1024:G:H3'	6:A:1025:U:H6	1.83	0.44
7:B:108:ARG:HG3	7:B:109:GLN:OE1	2.18	0.44
10:E:41:ASP:OD2	10:E:45:ARG:HB2	2.18	0.44
13:H:87:LYS:HD2	13:H:91:GLU:HG3	1.99	0.44
23:R:11:CYS:HB3	23:R:48:ARG:NH1	2.33	0.44
29:a:909:A:H2'	29:a:912:C:H5	1.83	0.44
29:a:1183:U:H2'	29:a:1184:U:C6	2.53	0.44
29:a:2030:6MZ:C2	29:a:2499:C:H5''	2.48	0.44
29:a:2747:G:O6	29:a:2755:C:H5''	2.17	0.44
49:u:34:LYS:N	49:u:35:GLU:OE2	2.50	0.44
6:A:56:U:H2'	6:A:57:G:C8	2.53	0.43
6:A:751:U:H2'	6:A:752:G:O4'	2.18	0.43
6:A:1318:A:O2'	24:S:37:ARG:HD2	2.17	0.43
7:B:100:MET:HA	7:B:107:VAL:HG21	2.00	0.43
28:Z:52:G:H1	28:Z:62:C:H42	1.66	0.43
29:a:191:A:H2'	29:a:192:C:H6	1.77	0.43
29:a:1315:C:O2'	29:a:1392:A:N3	2.48	0.43
43:o:10:GLN:HA	43:o:13:MET:HG3	1.99	0.43
6:A:310:G:H5''	21:P:31:ARG:HB2	2.00	0.43
6:A:1126:U:P	15:J:7:ARG:HH22	2.41	0.43
6:A:1305:G:C2	6:A:1331:G:N3	2.86	0.43
7:B:130:THR:C	7:B:132:LYS:H	2.25	0.43
19:N:24:ARG:HD2	19:N:55:SER:OG	2.17	0.43
21:P:18:GLN:HE21	21:P:18:GLN:HB3	1.68	0.43
22:Q:5:ILE:HD12	22:Q:6:ARG:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:S:17:LYS:O	24:S:20:GLU:HG3	2.18	0.43
26:U:58:LYS:HB3	26:U:58:LYS:HE2	1.75	0.43
29:a:1022:G:O6	37:i:68:LYS:NZ	2.44	0.43
29:a:1724:G:H1	29:a:1736:U:H3	1.65	0.43
29:a:2586:U:O4	58:a:3005:MIY:HN72	2.17	0.43
29:a:2804:U:H2'	29:a:2805:C:H6	1.83	0.43
29:a:2845:U:H5''	43:o:52:ASN:O	2.18	0.43
31:c:35:GLU:HG3	31:c:64:ILE:HD11	2.00	0.43
35:g:60:ASP:O	35:g:62:TRP:N	2.49	0.43
52:x:12:GLU:O	52:x:16:THR:HG22	2.19	0.43
6:A:429:U:H3'	9:D:9:LEU:HD12	2.00	0.43
6:A:1315:U:H2'	6:A:1316:G:O4'	2.18	0.43
12:G:32:VAL:HG23	12:G:33:ASP:HB2	2.00	0.43
29:a:52:A:H2'	29:a:53:A:C8	2.52	0.43
29:a:361:G:H8	29:a:361:G:OP2	2.00	0.43
29:a:2443:C:H2'	29:a:2444:G:H8	1.83	0.43
45:q:29:THR:O	45:q:29:THR:OG1	2.25	0.43
6:A:662:U:H2'	6:A:663:A:C8	2.54	0.43
29:a:78:U:H2'	29:a:79:C:C6	2.54	0.43
29:a:391:A:H1'	29:a:411:G:O4'	2.18	0.43
29:a:2502:G:H5''	29:a:2503:2MA:H5''	2.00	0.43
39:k:132:ARG:HG3	39:k:142:ILE:HD13	2.01	0.43
6:A:246:A:C2	6:A:282:A:C5	3.06	0.43
6:A:1305:G:H22	6:A:1331:G:H1'	1.83	0.43
8:C:107:ARG:HB2	8:C:107:ARG:HH11	1.84	0.43
29:a:548:G:H2'	29:a:549:G:O4'	2.17	0.43
29:a:2743:U:H2'	29:a:2744:G:O4'	2.18	0.43
34:f:49:LEU:HA	34:f:52:ASN:OD1	2.18	0.43
48:t:37:GLU:OE2	48:t:37:GLU:HA	2.19	0.43
15:J:6:ILE:HD13	15:J:6:ILE:HA	1.84	0.43
15:J:32:THR:HB	15:J:82:LYS:HZ1	1.83	0.43
29:a:143:C:H2'	29:a:144:A:C8	2.53	0.43
29:a:588:U:H2'	29:a:589:U:C6	2.54	0.43
35:g:98:VAL:HG23	35:g:125:CYS:SG	2.58	0.43
40:l:53:MET:HE1	40:l:103:TYR:CD1	2.53	0.43
6:A:1157:A:C2	6:A:1181:G:C4	3.07	0.43
13:H:43:GLU:OE1	13:H:43:GLU:HA	2.19	0.43
21:P:56:ARG:HD2	21:P:56:ARG:HA	1.68	0.43
29:a:286:U:H2'	29:a:287:G:C8	2.54	0.43
31:c:78:VAL:HG21	31:c:110:LEU:HD21	2.00	0.43
38:j:114:LYS:NZ	38:j:118:LEU:HD21	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:k:85:VAL:HG21	39:k:90:VAL:HG22	2.00	0.43
42:n:63:LYS:HG3	42:n:64:TYR:N	2.34	0.43
51:w:3:ARG:O	51:w:12:PRO:HD3	2.19	0.43
6:A:160:A:H2'	6:A:161:A:O4'	2.18	0.43
6:A:864:A:H2'	6:A:865:A:C8	2.54	0.43
7:B:24:ASN:OD1	7:B:26:LYS:HG3	2.18	0.43
20:O:35:GLN:HA	20:O:35:GLN:OE1	2.18	0.43
43:o:31:TRP:CE3	43:o:38:LYS:HE3	2.53	0.43
1:O:54:ILE:HD12	1:O:54:ILE:HA	1.86	0.43
6:A:636:U:H2'	6:A:637:C:H6	1.84	0.43
20:O:17:ARG:HH11	20:O:18:ASP:HB2	1.83	0.43
29:a:280:U:H3	29:a:360:U:H3	1.65	0.43
29:a:414:C:H2'	29:a:415:A:H8	1.82	0.43
29:a:1429:G:H2'	29:a:1430:G:H8	1.84	0.43
29:a:1597:A:H5''	29:a:1598:A:H5'	2.01	0.43
29:a:1715:G:O2'	29:a:1743:G:O6	2.26	0.43
37:i:70:THR:OG1	37:i:71:ASP:OD1	2.35	0.43
39:k:108:ALA:HB3	39:k:125:LEU:HD22	2.01	0.43
2:1:3:ARG:HA	2:1:3:ARG:HD3	1.82	0.43
6:A:33:A:H2'	6:A:34:C:H6	1.83	0.43
6:A:592:G:H2'	6:A:593:U:C6	2.54	0.43
6:A:1228:C:H2'	6:A:1229:A:H8	1.84	0.43
13:H:29:SER:HB3	13:H:57:PRO:HB2	2.01	0.43
29:a:404:A:H1'	29:a:405:U:OP2	2.19	0.43
29:a:596:U:H2'	29:a:597:G:H8	1.84	0.43
29:a:881:G:N2	29:a:895:U:O2	2.42	0.43
29:a:1198:U:H2'	29:a:1199:U:C6	2.54	0.43
29:a:1656:C:H2'	29:a:1657:U:H6	1.83	0.43
29:a:2461:A:H2'	29:a:2462:C:C6	2.53	0.43
35:g:42:GLU:OE2	35:g:42:GLU:HA	2.19	0.43
42:n:92:PHE:HB2	42:n:117:PHE:HD1	1.84	0.43
44:p:76:TYR:CZ	44:p:80:ILE:HG13	2.54	0.43
9:D:188:ARG:HD2	9:D:188:ARG:HA	1.67	0.42
15:J:82:LYS:HA	15:J:85:ASP:OD1	2.19	0.42
20:O:14:GLU:OE1	20:O:84:ARG:NH2	2.47	0.42
29:a:322:A:OP2	33:e:163:ASN:HB2	2.19	0.42
29:a:413:C:H2'	29:a:414:C:C6	2.54	0.42
29:a:580:U:H2'	29:a:581:C:H6	1.84	0.42
29:a:594:U:H2'	29:a:595:C:H6	1.82	0.42
29:a:839:U:H2'	29:a:840:C:C6	2.54	0.42
29:a:1614:A:C2	46:r:93:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:19:ILE:HG12	35:g:43:VAL:HG11	2.00	0.42
36:h:41:LYS:HD3	36:h:41:LYS:HA	1.90	0.42
40:l:57:VAL:HG11	40:l:105:MET:SD	2.59	0.42
42:n:60:GLU:HB2	42:n:61:GLN:OE1	2.18	0.42
42:n:88:LYS:O	42:n:89:ASP:HB2	2.19	0.42
45:q:37:GLU:HB2	45:q:53:PHE:CD1	2.54	0.42
46:r:74:ILE:HD12	46:r:105:VAL:HG22	2.01	0.42
6:A:405:U:OP2	9:D:3:ARG:NH1	2.51	0.42
9:D:121:LYS:HG3	9:D:131:ASN:HB3	2.01	0.42
11:F:90:MET:HE1	23:R:23:TYR:OH	2.19	0.42
13:H:79:SER:OG	13:H:124:GLU:OE2	2.30	0.42
16:K:36:ASP:OD1	16:K:38:GLN:N	2.48	0.42
25:T:44:LYS:HD2	25:T:87:ALA:HA	2.00	0.42
29:a:1:G:H2'	29:a:2:G:H8	1.85	0.42
29:a:1932:A:H2'	29:a:1933:G:O4'	2.19	0.42
29:a:2065:C:H2'	29:a:2066:C:C6	2.54	0.42
38:j:76:VAL:HG13	43:o:73:VAL:HB	2.01	0.42
6:A:1003:G:N2	6:A:1005:A:H5'	2.33	0.42
6:A:1040:U:C2	6:A:1041:G:N7	2.88	0.42
6:A:1319:A:C8	6:A:1323:G:C6	3.07	0.42
9:D:65:TYR:OH	9:D:95:GLU:OE2	2.24	0.42
9:D:118:VAL:HA	9:D:123:ILE:HD13	2.01	0.42
11:F:32:ALA:CB	11:F:70:VAL:HG21	2.49	0.42
29:a:476:G:N1	29:a:479:A:OP2	2.43	0.42
29:a:1773:A:H5''	59:a:4227:HOH:O	2.19	0.42
29:a:2649:C:H2'	29:a:2650:U:H6	1.83	0.42
32:d:56:LYS:O	32:d:60:VAL:HG23	2.19	0.42
35:g:116:GLN:HA	35:g:116:GLN:NE2	2.34	0.42
6:A:148:G:O2'	6:A:1446:A:N3	2.45	0.42
6:A:779:C:H2'	6:A:780:A:O4'	2.19	0.42
6:A:911:U:H2'	6:A:912:C:C6	2.55	0.42
6:A:1504:G:H4'	6:A:1505:G:C4	2.55	0.42
58:A:1635:MIY:O5	58:A:1635:MIY:O6	2.38	0.42
7:B:85:LEU:HD23	7:B:85:LEU:HA	1.86	0.42
15:J:29:ALA:O	15:J:32:THR:OG1	2.26	0.42
15:J:42:LEU:HB2	15:J:71:LEU:HD23	2.00	0.42
23:R:70:TYR:HB2	23:R:74:HIS:NE2	2.34	0.42
28:Z:25:C:H2'	28:Z:26:G:O4'	2.19	0.42
29:a:250:G:H2'	29:a:251:A:C8	2.54	0.42
29:a:645:C:O2'	29:a:646:U:H5'	2.19	0.42
29:a:969:G:H2'	29:a:970:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1495:A:H2'	29:a:1496:A:C8	2.54	0.42
29:a:1509:A:O2'	29:a:1510:G:H8	2.02	0.42
29:a:1735:A:H2'	29:a:1736:U:C6	2.54	0.42
29:a:2443:C:H2'	29:a:2444:G:C8	2.54	0.42
29:a:2552:OMU:H6	29:a:2552:OMU:O5'	2.18	0.42
30:b:1:U:H2'	30:b:2:G:C8	2.55	0.42
35:g:23:VAL:C	35:g:24:ILE:HD12	2.45	0.42
4:3:4:ARG:HB2	29:a:2466:C:OP1	2.19	0.42
6:A:512:U:H2'	6:A:513:C:C6	2.54	0.42
6:A:635:A:H2'	6:A:636:U:C6	2.55	0.42
6:A:693:G:C8	27:X:13:A:H1'	2.54	0.42
6:A:1007:U:O2'	6:A:1008:U:H5'	2.18	0.42
6:A:1513:A:H2'	6:A:1514:G:C8	2.55	0.42
10:E:32:SER:OG	10:E:33:PHE:N	2.52	0.42
10:E:37:THR:HG21	10:E:64:MET:HE2	2.01	0.42
20:O:6:GLU:CD	20:O:6:GLU:N	2.76	0.42
21:P:18:GLN:NE2	21:P:35:ARG:HH11	2.10	0.42
29:a:139:U:C4	47:s:1:MET:HE1	2.54	0.42
29:a:739:A:H1'	29:a:740:C:H5	1.84	0.42
29:a:1410:G:H2'	29:a:1411:U:H6	1.83	0.42
29:a:2636:C:H2'	29:a:2637:U:C6	2.55	0.42
6:A:985:C:H2'	6:A:986:U:C6	2.55	0.42
7:B:67:ILE:HD12	7:B:160:ALA:HB3	2.01	0.42
7:B:159:ASP:OD1	7:B:159:ASP:N	2.52	0.42
15:J:40:ILE:HB	15:J:73:LEU:HB3	2.02	0.42
16:K:50:SER:OG	16:K:69:ARG:HD3	2.20	0.42
17:L:79:VAL:O	17:L:103:ASP:HB2	2.19	0.42
18:M:110:LYS:HB3	18:M:110:LYS:HE3	1.90	0.42
23:R:25:ASP:CG	23:R:28:THR:HG22	2.45	0.42
29:a:832:U:H2'	29:a:833:A:C8	2.55	0.42
29:a:1370:C:H2'	29:a:1371:G:O4'	2.20	0.42
29:a:2228:G:H2'	29:a:2229:U:C6	2.55	0.42
33:e:149:ILE:HB	33:e:188:MET:HG2	2.01	0.42
6:A:6:G:O2'	6:A:7:A:H8	2.03	0.42
6:A:215:C:H2'	6:A:216:U:C6	2.55	0.42
6:A:1073:U:O2'	7:B:105:LYS:HE3	2.20	0.42
6:A:1328:C:H2'	6:A:1329:A:O4'	2.20	0.42
29:a:17:G:H2'	29:a:18:U:C6	2.54	0.42
32:d:48:ILE:HG23	32:d:84:LEU:HD11	2.02	0.42
32:d:105:LYS:HA	32:d:105:LYS:HD3	1.62	0.42
36:h:34:GLY:C	36:h:36:ALA:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:z:28:LEU:HD12	54:z:37:LYS:HD3	2.02	0.42
6:A:321:A:H2'	6:A:322:C:C6	2.54	0.42
6:A:857:C:H2'	6:A:858:G:O4'	2.20	0.42
6:A:1011:C:H2'	6:A:1012:A:H8	1.85	0.42
6:A:1218:C:H2'	6:A:1219:A:H8	1.82	0.42
6:A:1318:A:H1'	24:S:37:ARG:HH11	1.84	0.42
7:B:83:ALA:O	7:B:87:CYS:HB2	2.18	0.42
7:B:116:ASP:O	7:B:120:GLN:HG3	2.19	0.42
7:B:151:ILE:HB	7:B:154:MET:HE2	2.00	0.42
29:a:723:C:H2'	29:a:724:U:O4'	2.20	0.42
29:a:1179:G:H2'	29:a:1180:U:C6	2.55	0.42
30:b:2:G:H2'	30:b:3:C:H6	1.85	0.42
46:r:95:ARG:HG2	46:r:95:ARG:NH1	2.34	0.42
47:s:69:ARG:HH21	47:s:74:ILE:HB	1.85	0.42
4:3:1:MET:HE2	4:3:1:MET:HB2	1.90	0.42
6:A:216:U:H2'	6:A:217:C:H6	1.85	0.42
6:A:500:G:H2'	6:A:501:C:C6	2.54	0.42
6:A:718:A:C5'	16:K:119:ASN:HD21	2.33	0.42
6:A:978:A:C4	6:A:1319:A:C2	3.08	0.42
7:B:134:ALA:O	7:B:138:THR:OG1	2.35	0.42
29:a:1946:U:H2'	29:a:1947:C:C6	2.55	0.42
6:A:401:C:O2'	6:A:621:A:N3	2.48	0.42
6:A:763:G:H2'	6:A:764:C:C6	2.55	0.42
6:A:1011:C:H2'	6:A:1012:A:C8	2.54	0.42
6:A:1463:U:H2'	6:A:1464:U:C6	2.55	0.42
12:G:72:THR:HG22	12:G:96:ARG:NH1	2.35	0.42
13:H:27:MET:HB3	13:H:27:MET:HE2	1.83	0.42
14:I:35:LEU:HG	14:I:45:ARG:HG2	2.00	0.42
21:P:23:ASP:C	21:P:23:ASP:OD1	2.62	0.42
29:a:84:A:N1	29:a:98:G:O2'	2.45	0.42
29:a:2484:G:OP1	40:l:44:ARG:NH1	2.50	0.42
29:a:2783:U:H2'	29:a:2784:U:C6	2.55	0.42
35:g:24:ILE:HG21	35:g:72:LEU:HD11	2.00	0.42
6:A:404:G:N7	9:D:2:ALA:HB3	2.34	0.41
6:A:1103:C:H5''	7:B:97:LEU:HD22	2.01	0.41
6:A:1491:G:H2'	6:A:1492:A:C8	2.54	0.41
9:D:36:GLN:HE21	9:D:36:GLN:HB2	1.72	0.41
12:G:113:ASP:OD1	12:G:113:ASP:N	2.53	0.41
17:L:102:LEU:H	17:L:102:LEU:HG	1.65	0.41
24:S:62:VAL:HA	24:S:66:MET:CE	2.49	0.41
29:a:1868:C:H2'	29:a:1869:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2298:A:H2'	29:a:2299:U:O4'	2.20	0.41
29:a:2537:U:H2'	29:a:2538:C:H6	1.85	0.41
3:2:34:THR:OG1	29:a:2420:C:OP1	2.29	0.41
7:B:11:LYS:HE3	7:B:12:ALA:N	2.35	0.41
8:C:27:LYS:HD3	8:C:27:LYS:HA	1.81	0.41
16:K:53:ARG:HD2	16:K:53:ARG:HA	1.72	0.41
26:U:60:LEU:HD13	26:U:60:LEU:HA	1.94	0.41
29:a:279:A:H2'	29:a:280:U:O4'	2.20	0.41
29:a:1680:U:H2'	29:a:1681:G:O4'	2.21	0.41
29:a:2843:G:H2'	29:a:2844:G:O4'	2.20	0.41
34:f:72:LYS:HA	34:f:81:GLN:OE1	2.21	0.41
6:A:150:U:H2'	6:A:151:A:H8	1.85	0.41
6:A:171:A:H2'	6:A:172:A:C8	2.55	0.41
6:A:636:U:H2'	6:A:637:C:C6	2.56	0.41
6:A:1014:A:H2	6:A:1219:A:H1'	1.85	0.41
6:A:1107:C:C4	6:A:1108:G:C8	3.08	0.41
10:E:101:GLU:CD	10:E:101:GLU:N	2.76	0.41
15:J:83:THR:O	15:J:87:LEU:HD22	2.19	0.41
20:O:3:LEU:HD23	20:O:3:LEU:HA	1.88	0.41
21:P:4:ILE:HG12	21:P:21:VAL:HG22	2.02	0.41
24:S:66:MET:HB3	24:S:74:PHE:CZ	2.55	0.41
26:U:63:GLU:OE1	26:U:66:ARG:NH2	2.52	0.41
29:a:1585:C:H2'	29:a:1586:A:O4'	2.20	0.41
29:a:2291:U:OP1	29:a:2380:C:O2'	2.33	0.41
29:a:2298:A:OP1	34:f:71:ARG:NH1	2.44	0.41
50:v:17:GLU:O	50:v:19:LYS:NZ	2.53	0.41
6:A:407:U:H2'	6:A:408:A:H8	1.85	0.41
6:A:505:G:H2'	6:A:506:G:H8	1.86	0.41
6:A:1521:C:H2'	6:A:1522:U:C6	2.56	0.41
11:F:90:MET:HE3	11:F:90:MET:HB2	1.63	0.41
25:T:36:TYR:CE2	25:T:79:LEU:HD21	2.56	0.41
29:a:143:C:H2'	29:a:144:A:H8	1.85	0.41
29:a:2193:G:H2'	29:a:2194:U:C6	2.56	0.41
39:k:132:ARG:NH2	39:k:144:GLU:OE2	2.53	0.41
28:Z:56:C:O2'	34:f:75:ALA:N	2.54	0.41
29:a:697:G:H2'	29:a:698:C:C6	2.56	0.41
29:a:857:G:H2'	29:a:858:G:O4'	2.21	0.41
29:a:1239:G:H2'	29:a:1240:U:O4'	2.20	0.41
29:a:1928:A:H2'	29:a:1929:G:O4'	2.21	0.41
29:a:2698:U:H2'	29:a:2699:C:C6	2.55	0.41
38:j:58:LEU:HD11	38:j:86:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:27:ALA:O	3:2:28:ASN:HB2	2.21	0.41
6:A:559:A:H4'	6:A:560:A:H3'	2.03	0.41
6:A:676:A:H2'	6:A:677:U:H6	1.86	0.41
6:A:1516:2MG:N2	6:A:1519:MA6:OP2	2.52	0.41
26:U:39:GLU:HG3	26:U:43:THR:HB	2.03	0.41
29:a:833:A:H2'	29:a:834:G:H8	1.83	0.41
29:a:2661:G:H8	29:a:2661:G:OP2	2.04	0.41
31:c:82:GLU:OE1	31:c:103:TYR:OH	2.32	0.41
34:f:19:GLU:C	34:f:19:GLU:OE2	2.63	0.41
38:j:15:GLY:HA2	38:j:47:ILE:HG12	2.03	0.41
45:q:65:ALA:HB3	45:q:95:ASP:HB2	2.03	0.41
49:u:26:PHE:HE2	49:u:89:ILE:HG13	1.85	0.41
6:A:181:A:N6	6:A:195:A:C8	2.89	0.41
6:A:412:A:O2'	6:A:413:G:H4'	2.20	0.41
6:A:501:C:H2'	6:A:502:A:H8	1.84	0.41
6:A:1367:C:H5''	14:I:116:VAL:HG22	2.01	0.41
12:G:49:THR:O	12:G:52:GLN:HG3	2.20	0.41
17:L:15:LYS:H	17:L:15:LYS:HG2	1.62	0.41
28:Z:47:U:H5'	28:Z:48:C:H5'	2.03	0.41
29:a:1115:G:HO2'	29:a:1116:G:P	2.43	0.41
29:a:1484:U:H2'	29:a:1485:U:H6	1.85	0.41
29:a:1604:C:H2'	29:a:1605:C:H6	1.85	0.41
29:a:2191:A:H2'	29:a:2192:U:C6	2.55	0.41
35:g:7:ALA:HA	35:g:8:PRO:HD3	1.89	0.41
48:t:99:ASN:OD1	48:t:99:ASN:N	2.53	0.41
49:u:20:LEU:HD23	49:u:20:LEU:HA	1.95	0.41
6:A:236:A:H2'	6:A:237:G:C8	2.56	0.41
9:D:149:ALA:O	9:D:152:GLN:HG3	2.20	0.41
10:E:149:SER:N	10:E:152:MET:HE2	2.35	0.41
10:E:163:GLU:OE1	10:E:163:GLU:N	2.53	0.41
14:I:25:ASN:OD1	14:I:25:ASN:N	2.53	0.41
14:I:97:GLU:HA	14:I:100:LYS:HZ1	1.85	0.41
15:J:35:GLN:OE1	15:J:36:VAL:N	2.53	0.41
29:a:880:G:C2	29:a:898:C:C2	3.09	0.41
29:a:1047:G:N2	29:a:1110:G:O2'	2.53	0.41
29:a:2469:A:H4'	40:l:55:ARG:HD3	2.01	0.41
29:a:2523:G:O2'	29:a:2764:A:O2'	2.38	0.41
32:d:19:GLY:HA3	43:o:80:VAL:HG23	2.02	0.41
5:4:63:ARG:HG3	5:4:64:PHE:N	2.36	0.41
6:A:67:C:H2'	6:A:68:G:C8	2.55	0.41
6:A:253:A:O2'	22:Q:17:MET:SD	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:259:G:OP1	25:T:36:TYR:OH	2.36	0.41
6:A:696:A:H2'	6:A:697:U:H6	1.85	0.41
6:A:737:C:H2'	6:A:738:C:H6	1.86	0.41
6:A:1101:A:H4'	6:A:1102:A:O5'	2.21	0.41
6:A:1291:U:H2'	6:A:1292:G:H8	1.86	0.41
9:D:138:SER:HG	9:D:141:ASP:CG	2.29	0.41
14:I:96:SER:O	14:I:100:LYS:HE3	2.21	0.41
17:L:3:THR:HG22	17:L:5:ASN:N	2.35	0.41
18:M:17:ILE:O	18:M:20:THR:OG1	2.29	0.41
18:M:49:SER:N	18:M:52:GLN:OE1	2.40	0.41
18:M:79:ARG:HH12	24:S:65:GLU:HB3	1.85	0.41
21:P:6:LEU:HB3	21:P:17:TYR:HB3	2.03	0.41
22:Q:60:GLU:OE1	22:Q:77:ARG:NE	2.54	0.41
29:a:27:G:N2	29:a:512:G:H1'	2.36	0.41
29:a:2233:U:H2'	29:a:2234:G:C8	2.55	0.41
43:o:8:LEU:HD23	43:o:8:LEU:HA	1.88	0.41
53:y:3:LYS:O	53:y:4:THR:HG22	2.21	0.41
53:y:3:LYS:HB3	53:y:40:ASP:HB3	2.03	0.41
5:4:4:ASP:OD1	5:4:4:ASP:C	2.64	0.41
6:A:218:U:H2'	6:A:219:U:O4'	2.21	0.41
7:B:57:LEU:HD13	7:B:217:VAL:HG13	2.02	0.41
13:H:18:GLN:NE2	13:H:72:VAL:H	2.19	0.41
15:J:92:LEU:HD23	15:J:92:LEU:HA	1.89	0.41
25:T:79:LEU:HD23	25:T:79:LEU:HA	1.83	0.41
29:a:499:U:H2'	29:a:500:G:O4'	2.21	0.41
29:a:586:A:N1	29:a:809:G:O2'	2.48	0.41
29:a:2295:C:O2'	29:a:2296:U:H5'	2.21	0.41
35:g:104:ASN:HA	35:g:113:VAL:O	2.21	0.41
44:p:91:ASP:OD1	44:p:91:ASP:C	2.64	0.41
2:1:39:ARG:NH2	29:a:468:G:N7	2.60	0.40
6:A:486:U:H2'	6:A:487:A:H8	1.86	0.40
6:A:715:A:H2'	6:A:716:A:C8	2.55	0.40
6:A:908:A:H2'	6:A:909:A:H8	1.85	0.40
6:A:1526:G:N7	26:U:40:LYS:NZ	2.69	0.40
9:D:99:ASP:OD1	9:D:99:ASP:N	2.52	0.40
10:E:45:ARG:HH11	10:E:45:ARG:HG3	1.86	0.40
12:G:11:LYS:HZ2	12:G:12:ILE:C	2.28	0.40
17:L:10:LYS:HB3	17:L:10:LYS:HE3	1.85	0.40
28:Z:50:U:H2'	28:Z:51:C:C6	2.57	0.40
29:a:64:A:H2'	29:a:65:U:H6	1.86	0.40
29:a:880:G:H2'	29:a:881:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1484:U:H2'	29:a:1485:U:C6	2.55	0.40
29:a:1496:A:H2'	29:a:1498:C:C5	2.56	0.40
33:e:1:MET:HE3	33:e:1:MET:HB3	1.84	0.40
35:g:73:ASN:C	35:g:73:ASN:OD1	2.64	0.40
7:B:68:LEU:HD22	7:B:154:MET:HE1	2.04	0.40
9:D:54:GLN:HB3	9:D:203:LEU:HB2	2.03	0.40
14:I:52:LEU:HD11	14:I:63:LEU:HD21	2.03	0.40
22:Q:9:GLN:OE1	22:Q:79:VAL:HG21	2.21	0.40
22:Q:59:VAL:HB	22:Q:75:LEU:HD21	2.02	0.40
28:Z:9:G:N3	28:Z:45:G:H2'	2.36	0.40
29:a:2577:A:H5''	29:a:2578:G:H5'	2.02	0.40
30:b:42:C:O2'	34:f:63:GLN:HG2	2.22	0.40
30:b:42:C:C6	34:f:66:LEU:HB2	2.56	0.40
47:s:88:LYS:O	47:s:90:GLY:N	2.54	0.40
6:A:224:U:H2'	6:A:225:C:C6	2.56	0.40
6:A:1039:G:H2'	6:A:1040:U:H6	1.85	0.40
8:C:75:ILE:HD12	8:C:75:ILE:HA	1.88	0.40
14:I:19:VAL:HG11	14:I:83:ILE:HA	2.02	0.40
19:N:82:ILE:H	19:N:82:ILE:HG13	1.62	0.40
29:a:150:U:H2'	29:a:151:C:H6	1.85	0.40
29:a:909:A:H2'	29:a:912:C:C5	2.56	0.40
29:a:1394:U:H2'	29:a:1395:A:O4'	2.22	0.40
40:l:56:ALA:HB2	40:l:119:LEU:HD12	2.03	0.40
48:t:49:VAL:HG13	48:t:52:LEU:O	2.21	0.40
51:w:56:MET:HE2	51:w:56:MET:HB3	1.77	0.40
6:A:471:U:H2'	6:A:472:U:C6	2.57	0.40
8:C:12:LEU:HD11	19:N:91:GLY:HA2	2.03	0.40
11:F:25:TYR:O	11:F:29:ILE:HG12	2.22	0.40
13:H:39:VAL:HG21	13:H:110:VAL:HG12	2.04	0.40
19:N:21:PHE:C	19:N:21:PHE:CD1	2.99	0.40
29:a:754:U:H2'	29:a:755:U:C6	2.56	0.40
29:a:2305:U:H2'	29:a:2306:C:C6	2.56	0.40
32:d:178:VAL:N	32:d:188:LEU:O	2.50	0.40
33:e:127:GLU:H	33:e:127:GLU:CD	2.29	0.40
34:f:37:ASN:OD1	34:f:37:ASN:C	2.65	0.40
4:3:16:ILE:HD13	4:3:25:VAL:HG22	2.04	0.40
6:A:71:A:C6	6:A:72:A:N7	2.89	0.40
6:A:1024:G:H3'	6:A:1025:U:C6	2.56	0.40
6:A:1530:G:H2'	6:A:1531:A:H8	1.85	0.40
8:C:28:GLU:OE1	8:C:28:GLU:N	2.53	0.40
14:I:6:TYR:HD2	14:I:21:ILE:HG22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:67:LEU:HA	20:O:67:LEU:HD23	1.90	0.40
29:a:40:U:H2'	29:a:41:C:C6	2.56	0.40
29:a:356:G:C6	29:a:357:C:C4	3.10	0.40
29:a:548:G:H2'	29:a:549:G:C8	2.57	0.40
29:a:760:G:H2'	29:a:761:A:O4'	2.22	0.40
29:a:1282:U:H2'	29:a:1283:G:O4'	2.21	0.40
29:a:2852:G:H2'	29:a:2853:C:O4'	2.22	0.40
32:d:38:LYS:O	32:d:46:ARG:HA	2.22	0.40
32:d:110:THR:CG2	32:d:202:ILE:HB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	54 (96%)	2 (4%)	0	100	100
7	B	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
8	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
9	D	203/206 (98%)	202 (100%)	1 (0%)	0	100	100
10	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
11	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
12	G	151/179 (84%)	140 (93%)	11 (7%)	0	100	100
13	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
14	I	125/130 (96%)	118 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	11
16	K	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
17	L	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
18	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
19	N	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
20	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
21	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
22	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
23	R	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
24	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
25	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	U	68/71 (96%)	68 (100%)	0	0	100	100
31	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
32	d	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
33	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
34	f	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
35	g	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
36	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
37	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
38	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
39	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
40	l	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
41	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
42	n	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	14	14
43	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
44	p	115/118 (98%)	115 (100%)	0	0	100	100
45	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
46	r	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
47	s	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
48	t	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
49	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
51	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
52	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
53	y	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	6	4
54	z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
All	All	5485/5913 (93%)	5292 (96%)	190 (4%)	3 (0%)	49	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	n	89	ASP
15	J	57	VAL
53	y	4	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	37 (97%)	1 (3%)	40	55
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	32 (94%)	2 (6%)	18	22
5	4	55/62 (89%)	52 (94%)	3 (6%)	19	24
7	B	186/199 (94%)	181 (97%)	5 (3%)	39	53
8	C	170/190 (90%)	164 (96%)	6 (4%)	32	43
9	D	172/173 (99%)	166 (96%)	6 (4%)	32	43
10	E	119/126 (94%)	116 (98%)	3 (2%)	42	56
11	F	90/116 (78%)	89 (99%)	1 (1%)	65	79
12	G	126/147 (86%)	120 (95%)	6 (5%)	23	30
13	H	104/105 (99%)	101 (97%)	3 (3%)	37	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	I	105/107 (98%)	100 (95%)	5 (5%)	23	30
15	J	86/90 (96%)	80 (93%)	6 (7%)	14	16
16	K	90/99 (91%)	86 (96%)	4 (4%)	25	34
17	L	102/103 (99%)	101 (99%)	1 (1%)	68	81
18	M	93/96 (97%)	90 (97%)	3 (3%)	34	47
19	N	83/84 (99%)	79 (95%)	4 (5%)	23	30
20	O	76/77 (99%)	76 (100%)	0	100	100
21	P	65/65 (100%)	62 (95%)	3 (5%)	24	32
22	Q	73/78 (94%)	69 (94%)	4 (6%)	19	24
23	R	57/65 (88%)	57 (100%)	0	100	100
24	S	72/79 (91%)	68 (94%)	4 (6%)	19	24
25	T	65/66 (98%)	64 (98%)	1 (2%)	57	73
26	U	60/61 (98%)	57 (95%)	3 (5%)	22	28
31	c	216/218 (99%)	214 (99%)	2 (1%)	70	84
32	d	163/163 (100%)	159 (98%)	4 (2%)	42	56
33	e	165/165 (100%)	164 (99%)	1 (1%)	78	89
34	f	148/150 (99%)	143 (97%)	5 (3%)	32	44
35	g	137/138 (99%)	128 (93%)	9 (7%)	15	18
36	h	32/114 (28%)	30 (94%)	2 (6%)	16	19
37	i	116/116 (100%)	111 (96%)	5 (4%)	26	35
38	j	104/104 (100%)	103 (99%)	1 (1%)	68	81
39	k	103/103 (100%)	102 (99%)	1 (1%)	68	81
40	l	109/109 (100%)	105 (96%)	4 (4%)	30	41
41	m	98/103 (95%)	98 (100%)	0	100	100
42	n	86/87 (99%)	79 (92%)	7 (8%)	11	12
43	o	99/100 (99%)	99 (100%)	0	100	100
44	p	89/90 (99%)	88 (99%)	1 (1%)	65	79
45	q	84/84 (100%)	76 (90%)	8 (10%)	8	8
46	r	93/93 (100%)	90 (97%)	3 (3%)	34	47
47	s	80/84 (95%)	78 (98%)	2 (2%)	42	56
48	t	83/85 (98%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	u	78/78 (100%)	72 (92%)	6 (8%)	12	13
50	v	58/63 (92%)	58 (100%)	0	100	100
51	w	67/68 (98%)	67 (100%)	0	100	100
52	x	54/55 (98%)	53 (98%)	1 (2%)	50	66
53	y	48/49 (98%)	47 (98%)	1 (2%)	47	63
54	z	47/48 (98%)	46 (98%)	1 (2%)	47	63
All	All	4575/4828 (95%)	4437 (97%)	138 (3%)	37	49

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	29	GLN
4	3	6	SER
4	3	16	ILE
5	4	13	THR
5	4	34	LEU
5	4	35	ASP
7	B	4	VAL
7	B	43	LEU
7	B	148	LEU
7	B	221	VAL
7	B	226	SER
8	C	28	GLU
8	C	51	SER
8	C	84	VAL
8	C	178	LEU
8	C	188	GLU
8	C	191	THR
9	D	36	GLN
9	D	144	SER
9	D	146	ARG
9	D	161	LEU
9	D	189	SER
9	D	192	SER
10	E	38	VAL
10	E	86	LYS
10	E	160	SER
11	F	61	LEU
12	G	41	SER
12	G	77	SER

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Mol	Chain	Res	Type
12	G	94	VAL
12	G	104	ILE
12	G	115	SER
12	G	129	GLU
13	H	42	GLU
13	H	73	GLU
13	H	90	ASP
14	I	4	ASN
14	I	14	SER
14	I	43	THR
14	I	54	LEU
14	I	55	VAL
15	J	36	VAL
15	J	44	THR
15	J	78	GLU
15	J	84	VAL
15	J	87	LEU
15	J	101	SER
16	K	55	SER
16	K	58	SER
16	K	72	ASP
16	K	75	LYS
17	L	55	VAL
18	M	45	ILE
18	M	48	LEU
18	M	49	SER
19	N	32	SER
19	N	45	VAL
19	N	54	ASP
19	N	60	GLN
21	P	12	LYS
21	P	54	LEU
21	P	78	VAL
22	Q	9	GLN
22	Q	13	VAL
22	Q	42	THR
22	Q	74	THR
24	S	11	ILE
24	S	23	VAL
24	S	25	SER
24	S	43	ASN
25	T	3	ASN

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Mol	Chain	Res	Type
26	U	3	VAL
26	U	53	VAL
26	U	68	THR
31	c	10	SER
31	c	110	LEU
32	d	18	ASP
32	d	92	VAL
32	d	97	SER
32	d	202	ILE
33	e	6	LYS
34	f	137	ILE
34	f	147	ASP
34	f	149	VAL
34	f	155	THR
34	f	158	THR
35	g	9	VAL
35	g	15	VAL
35	g	19	ILE
35	g	34	THR
35	g	43	VAL
35	g	48	ASN
35	g	84	THR
35	g	90	VAL
35	g	128	GLN
36	h	11	ASN
36	h	17	ASP
37	i	1	MET
37	i	5	THR
37	i	17	VAL
37	i	70	THR
37	i	141	ASP
38	j	76	VAL
39	k	112	LEU
40	l	90	GLU
40	l	126	ILE
40	l	133	LYS
40	l	135	VAL
42	n	45	SER
42	n	48	LEU
42	n	83	LEU
42	n	89	ASP
42	n	90	VAL

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Mol	Chain	Res	Type
42	n	98	GLN
42	n	112	GLU
44	p	89	GLU
45	q	6	GLN
45	q	20	VAL
45	q	29	THR
45	q	33	VAL
45	q	45	GLU
45	q	62	GLU
45	q	64	VAL
45	q	96	VAL
46	r	70	LYS
46	r	108	SER
46	r	109	ASP
47	s	25	GLU
47	s	26	LYS
49	u	8	VAL
49	u	10	LYS
49	u	25	LYS
49	u	62	THR
49	u	65	VAL
49	u	73	LYS
52	x	4	LYS
53	y	4	THR
54	z	46	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	35	GLN
7	B	18	HIS
7	B	39	HIS
8	C	139	GLN
8	C	190	HIS
10	E	12	GLN
10	E	89	HIS
10	E	132	ASN
11	F	63	ASN
11	F	94	HIS
12	G	68	ASN
13	H	4	GLN
13	H	18	GLN

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Mol	Chain	Res	Type
14	I	4	ASN
17	L	6	GLN
19	N	43	ASN
19	N	49	GLN
19	N	66	GLN
21	P	18	GLN
21	P	59	HIS
22	Q	45	HIS
24	S	69	HIS
25	T	61	GLN
31	c	25	HIS
31	c	134	ASN
31	c	143	ASN
32	d	94	GLN
33	e	136	GLN
33	e	165	HIS
34	f	27	GLN
34	f	63	GLN
35	g	45	HIS
37	i	80	HIS
37	i	86	GLN
41	m	9	GLN
42	n	29	HIS
42	n	98	GLN
44	p	20	GLN
44	p	72	ASN
45	q	6	GLN
47	s	91	GLN
48	t	74	ASN
49	u	24	ASN
50	v	46	HIS
53	y	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	9/22 (40%)	5 (55%)	0
28	Z	74/75 (98%)	8 (10%)	3 (4%)
29	a	2749/2904 (94%)	267 (9%)	0
30	b	118/120 (98%)	10 (8%)	0
6	A	1495/1542 (96%)	159 (10%)	2 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4445/4663 (95%)	449 (10%)	5 (0%)

All (449) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	6	G
6	A	9	G
6	A	13	U
6	A	22	G
6	A	32	A
6	A	39	G
6	A	47	C
6	A	48	C
6	A	50	A
6	A	51	A
6	A	72	A
6	A	73	C
6	A	74	A
6	A	77	A
6	A	96	U
6	A	120	A
6	A	121	U
6	A	130	A
6	A	131	A
6	A	141	G
6	A	149	A
6	A	173	U
6	A	182	A
6	A	183	C
6	A	197	A
6	A	240	G
6	A	245	U
6	A	247	G
6	A	251	G
6	A	266	G
6	A	267	C
6	A	289	G
6	A	321	A
6	A	328	C
6	A	347	G
6	A	352	C

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Mol	Chain	Res	Type
6	A	354	G
6	A	367	U
6	A	372	C
6	A	384	G
6	A	397	A
6	A	406	G
6	A	412	A
6	A	413	G
6	A	414	A
6	A	421	U
6	A	422	C
6	A	424	G
6	A	429	U
6	A	434	U
6	A	453	G
6	A	458	U
6	A	467	U
6	A	468	A
6	A	478	A
6	A	481	G
6	A	484	G
6	A	486	U
6	A	511	C
6	A	518	C
6	A	521	G
6	A	527	G7M
6	A	531	U
6	A	532	A
6	A	547	A
6	A	564	C
6	A	572	A
6	A	573	A
6	A	576	C
6	A	577	G
6	A	596	A
6	A	608	A
6	A	633	G
6	A	650	G
6	A	653	U
6	A	665	A
6	A	703	G
6	A	718	A

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Mol	Chain	Res	Type
6	A	723	U
6	A	724	G
6	A	747	A
6	A	748	G
6	A	755	G
6	A	777	A
6	A	793	U
6	A	794	A
6	A	815	A
6	A	817	C
6	A	890	G
6	A	902	G
6	A	914	A
6	A	926	G
6	A	934	C
6	A	935	A
6	A	960	U
6	A	969	A
6	A	971	G
6	A	975	A
6	A	976	G
6	A	977	A
6	A	993	G
6	A	996	A
6	A	1003	G
6	A	1004	A
6	A	1008	U
6	A	1020	G
6	A	1023	U
6	A	1025	U
6	A	1035	A
6	A	1036	A
6	A	1037	C
6	A	1044	A
6	A	1065	U
6	A	1085	U
6	A	1088	G
6	A	1094	G
6	A	1095	U
6	A	1101	A
6	A	1132	C
6	A	1134	G

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Mol	Chain	Res	Type
6	A	1137	C
6	A	1139	G
6	A	1159	U
6	A	1160	G
6	A	1184	G
6	A	1196	A
6	A	1197	A
6	A	1213	A
6	A	1227	A
6	A	1238	A
6	A	1258	G
6	A	1280	A
6	A	1286	U
6	A	1287	A
6	A	1300	G
6	A	1302	C
6	A	1305	G
6	A	1317	C
6	A	1320	C
6	A	1346	A
6	A	1353	G
6	A	1363	A
6	A	1378	C
6	A	1379	G
6	A	1398	A
6	A	1419	G
6	A	1422	G
6	A	1441	A
6	A	1446	A
6	A	1451	U
6	A	1487	G
6	A	1493	A
6	A	1497	G
6	A	1503	A
6	A	1506	U
6	A	1517	G
6	A	1529	G
6	A	1530	G
27	X	14	A
27	X	19	U
27	X	20	U
27	X	21	U

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Mol	Chain	Res	Type
27	X	22	U
28	Z	9	G
28	Z	16	C
28	Z	17(A)	U
28	Z	18	G
28	Z	20	U
28	Z	47	U
28	Z	48	C
28	Z	76	A
29	a	10	A
29	a	34	U
29	a	42	A
29	a	45	G
29	a	51	G
29	a	63	A
29	a	71	A
29	a	74	A
29	a	75	G
29	a	101	A
29	a	102	U
29	a	118	A
29	a	119	A
29	a	120	U
29	a	136	G
29	a	139	U
29	a	140	C
29	a	142	A
29	a	163	C
29	a	165	A
29	a	181	A
29	a	196	A
29	a	199	A
29	a	215	G
29	a	216	A
29	a	222	A
29	a	233	A
29	a	248	G
29	a	272	A
29	a	278	A
29	a	279	A
29	a	281	C
29	a	285	G

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Mol	Chain	Res	Type
29	a	311	A
29	a	329	G
29	a	330	A
29	a	345	A
29	a	353	C
29	a	357	C
29	a	361	G
29	a	367	G
29	a	386	G
29	a	396	G
29	a	405	U
29	a	411	G
29	a	481	G
29	a	489	G
29	a	491	G
29	a	505	A
29	a	508	A
29	a	509	C
29	a	530	G
29	a	532	A
29	a	533	G
29	a	545	U
29	a	546	U
29	a	547	A
29	a	548	G
29	a	563	A
29	a	573	U
29	a	575	A
29	a	603	A
29	a	614	A
29	a	615	U
29	a	627	A
29	a	637	A
29	a	645	C
29	a	646	U
29	a	647	G
29	a	654	A
29	a	655	A
29	a	686	U
29	a	711	G
29	a	717	C
29	a	730	A

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Mol	Chain	Res	Type
29	a	740	C
29	a	747	5MU
29	a	764	A
29	a	775	G
29	a	776	G
29	a	782	A
29	a	784	G
29	a	785	G
29	a	805	G
29	a	812	C
29	a	827	U
29	a	828	U
29	a	846	U
29	a	847	U
29	a	859	G
29	a	877	A
29	a	888	C
29	a	890	C
29	a	891	G
29	a	893	C
29	a	895	U
29	a	896	A
29	a	897	C
29	a	899	A
29	a	907	G
29	a	910	A
29	a	914	G
29	a	931	U
29	a	946	C
29	a	961	C
29	a	974	G
29	a	983	A
29	a	996	A
29	a	1005	C
29	a	1012	U
29	a	1013	C
29	a	1033	U
29	a	1047	G
29	a	1108	U
29	a	1111	A
29	a	1112	G
29	a	1116	G

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Mol	Chain	Res	Type
29	a	1130	U
29	a	1132	U
29	a	1133	A
29	a	1135	C
29	a	1136	G
29	a	1142	A
29	a	1212	G
29	a	1253	A
29	a	1256	G
29	a	1271	G
29	a	1272	A
29	a	1300	G
29	a	1301	A
29	a	1329	U
29	a	1352	U
29	a	1365	A
29	a	1379	U
29	a	1383	A
29	a	1395	A
29	a	1416	G
29	a	1428	C
29	a	1434	A
29	a	1452	G
29	a	1482	G
29	a	1493	C
29	a	1508	A
29	a	1509	A
29	a	1510	G
29	a	1515	A
29	a	1535	A
29	a	1536	C
29	a	1537	G
29	a	1569	A
29	a	1578	U
29	a	1583	A
29	a	1584	U
29	a	1585	C
29	a	1607	C
29	a	1608	A
29	a	1647	U
29	a	1648	U
29	a	1649	G

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Mol	Chain	Res	Type
29	a	1674	G
29	a	1715	G
29	a	1729	U
29	a	1730	C
29	a	1738	G
29	a	1764	C
29	a	1773	A
29	a	1782	U
29	a	1800	C
29	a	1801	A
29	a	1808	A
29	a	1816	C
29	a	1829	A
29	a	1848	A
29	a	1858	A
29	a	1870	C
29	a	1872	A
29	a	1906	G
29	a	1913	A
29	a	1914	C
29	a	1929	G
29	a	1930	G
29	a	1955	U
29	a	1967	C
29	a	1970	A
29	a	1971	U
29	a	1972	G
29	a	1991	U
29	a	1993	U
29	a	2023	C
29	a	2030	6MZ
29	a	2031	A
29	a	2033	A
29	a	2043	C
29	a	2055	C
29	a	2056	G
29	a	2060	A
29	a	2061	G
29	a	2062	A
29	a	2069	G7M
29	a	2093	G
29	a	2198	A

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Mol	Chain	Res	Type
29	a	2204	G
29	a	2211	A
29	a	2225	A
29	a	2238	G
29	a	2239	G
29	a	2279	G
29	a	2283	C
29	a	2287	A
29	a	2288	A
29	a	2305	U
29	a	2308	G
29	a	2322	A
29	a	2325	G
29	a	2333	A
29	a	2335	A
29	a	2347	C
29	a	2350	C
29	a	2383	G
29	a	2385	C
29	a	2402	U
29	a	2406	A
29	a	2425	A
29	a	2429	G
29	a	2430	A
29	a	2435	A
29	a	2441	U
29	a	2445	2MG
29	a	2448	A
29	a	2470	G
29	a	2491	U
29	a	2502	G
29	a	2505	G
29	a	2518	A
29	a	2520	C
29	a	2529	G
29	a	2547	A
29	a	2566	A
29	a	2567	G
29	a	2602	A
29	a	2609	U
29	a	2613	U
29	a	2615	U

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Mol	Chain	Res	Type
29	a	2629	U
29	a	2661	G
29	a	2663	G
29	a	2682	A
29	a	2689	U
29	a	2690	U
29	a	2714	G
29	a	2726	A
29	a	2733	A
29	a	2744	G
29	a	2748	A
29	a	2765	A
29	a	2778	A
29	a	2798	U
29	a	2818	U
29	a	2820	A
29	a	2821	A
29	a	2835	A
29	a	2849	U
29	a	2861	U
29	a	2873	A
29	a	2880	C
29	a	2884	U
29	a	2891	U
30	b	16	G
30	b	35	C
30	b	42	C
30	b	45	A
30	b	56	G
30	b	67	G
30	b	89	U
30	b	90	C
30	b	99	A
30	b	109	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	182	A
6	A	1035	A
28	Z	17(A)	U
28	Z	19	G

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Mol	Chain	Res	Type
28	Z	48	C

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

41 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
29	PSU	a	955	29	18,21,22	1.04	1 (5%)	21,30,33	1.93	4 (19%)
29	5MU	a	747	29	19,22,23	0.65	0	27,32,35	0.59	0
6	MA6	A	1518	6	23,26,27	1.69	6 (26%)	33,38,41	4.25	14 (42%)
29	5MC	a	1962	29,57	19,22,23	0.79	0	26,32,35	0.59	0
29	PSU	a	746	29,56	18,21,22	1.09	2 (11%)	21,30,33	1.85	3 (14%)
32	MEQ	d	150	32	8,9,10	0.94	0	5,10,12	0.72	0
29	6MZ	a	2030	29	22,25,26	2.27	8 (36%)	29,36,39	2.66	14 (48%)
6	5MC	A	967	6	19,22,23	0.69	0	26,32,35	0.64	0
29	2MG	a	1835	29	23,26,27	0.66	0	33,38,41	0.47	0
29	G7M	a	2069	29,57	23,26,27	0.70	1 (4%)	34,39,42	0.62	1 (2%)
6	PSU	A	516	6,56	18,21,22	1.07	3 (16%)	21,30,33	1.90	5 (23%)
28	5MC	Z	32	28	19,22,23	0.77	1 (5%)	26,32,35	0.50	0
28	5MU	Z	54	28	19,22,23	0.25	0	27,32,35	0.35	0
29	OMC	a	2498	29,56	19,22,23	0.76	1 (5%)	25,31,34	0.67	0
29	2MA	a	2503	29,56,57	22,25,26	1.70	6 (27%)	32,37,40	3.44	12 (37%)
28	PSU	Z	55	28	18,21,22	0.92	1 (5%)	21,30,33	0.75	1 (4%)
29	3TD	a	1915	29	19,22,23	4.12	7 (36%)	23,32,35	1.83	3 (13%)
29	6MZ	a	1618	29	22,25,26	2.30	7 (31%)	29,36,39	2.47	9 (31%)
29	PSU	a	2504	29,57	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
6	5MC	A	1407	6	19,22,23	0.82	1 (5%)	26,32,35	0.61	0
17	D2T	L	89	17	8,9,10	1.80	2 (25%)	6,11,13	1.56	1 (16%)
29	PSU	a	2580	29	18,21,22	1.10	3 (16%)	21,30,33	2.04	5 (23%)
6	2MG	A	1207	6,57	23,26,27	0.51	0	33,38,41	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	2MG	A	966	6	23,26,27	0.57	0	33,38,41	0.51	0
29	PSU	a	2604	29	18,21,22	1.08	2 (11%)	21,30,33	2.03	4 (19%)
29	2MG	a	2445	29	23,26,27	0.75	0	33,38,41	0.52	0
29	PSU	a	1917	29	18,21,22	1.01	1 (5%)	21,30,33	1.95	4 (19%)
6	UR3	A	1498	6	19,22,23	2.61	8 (42%)	26,32,35	1.67	3 (11%)
6	2MG	A	1516	6	23,26,27	0.59	0	33,38,41	0.59	0
28	4SU	Z	8	28	18,21,22	3.81	8 (44%)	25,30,33	2.41	5 (20%)
29	PSU	a	1911	29	18,21,22	1.08	1 (5%)	21,30,33	2.07	5 (23%)
29	1MG	a	745	29	23,26,27	2.76	8 (34%)	33,39,42	1.76	8 (24%)
29	PSU	a	2605	29	18,21,22	1.10	2 (11%)	21,30,33	2.09	5 (23%)
29	5MU	a	1939	29,57	19,22,23	0.71	0	27,32,35	0.53	0
29	PSU	a	2457	29	18,21,22	1.15	3 (16%)	21,30,33	2.22	6 (28%)
29	OMG	a	2251	29,28,57	23,26,27	0.64	0	32,38,41	0.50	0
6	G7M	A	527	6,57	23,26,27	2.59	8 (34%)	34,39,42	2.40	11 (32%)
29	OMU	a	2552	29,57	19,22,23	2.82	6 (31%)	25,31,34	1.97	5 (20%)
6	MA6	A	1519	6	23,26,27	1.66	6 (26%)	33,38,41	4.39	14 (42%)
6	4OC	A	1402	6	20,23,24	3.12	8 (40%)	25,32,35	0.94	2 (8%)
29	H2U	a	2449	29	18,21,22	0.65	0	19,30,33	0.98	1 (5%)

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
29	PSU	a	955	29	-	0/7/25/26	0/2/2/2
29	5MU	a	747	29	-	1/7/25/26	0/2/2/2
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
29	5MC	a	1962	29,57	-	2/7/25/26	0/2/2/2
29	PSU	a	746	29,56	-	2/7/25/26	0/2/2/2
32	MEQ	d	150	32	-	4/8/9/11	-
29	6MZ	a	2030	29	-	2/9/27/28	0/3/3/3
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
29	2MG	a	1835	29	-	0/9/27/28	0/3/3/3
29	G7M	a	2069	29,57	-	0/7/25/26	0/3/3/3
6	PSU	A	516	6,56	-	0/7/25/26	0/2/2/2
28	5MC	Z	32	28	-	0/7/25/26	0/2/2/2
28	5MU	Z	54	28	-	0/7/25/26	0/2/2/2
29	OMC	a	2498	29,56	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	2MA	a	2503	29,56,57	-	2/7/25/26	0/3/3/3
28	PSU	Z	55	28	-	0/7/25/26	0/2/2/2
29	3TD	a	1915	29	-	0/7/25/26	0/2/2/2
29	6MZ	a	1618	29	-	0/9/27/28	0/3/3/3
29	PSU	a	2504	29,57	-	2/7/25/26	0/2/2/2
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
17	D2T	L	89	17	-	5/7/12/14	-
29	PSU	a	2580	29	-	0/7/25/26	0/2/2/2
6	2MG	A	1207	6,57	-	0/9/27/28	0/3/3/3
6	2MG	A	966	6	-	0/9/27/28	0/3/3/3
29	PSU	a	2604	29	-	0/7/25/26	0/2/2/2
29	2MG	a	2445	29	-	2/9/27/28	0/3/3/3
29	PSU	a	1917	29	-	0/7/25/26	0/2/2/2
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
6	2MG	A	1516	6	-	0/9/27/28	0/3/3/3
28	4SU	Z	8	28	-	0/7/25/26	0/2/2/2
29	PSU	a	1911	29	-	0/7/25/26	0/2/2/2
29	1MG	a	745	29	-	0/7/25/26	0/3/3/3
29	PSU	a	2605	29	-	0/7/25/26	0/2/2/2
29	5MU	a	1939	29,57	-	0/7/25/26	0/2/2/2
29	PSU	a	2457	29	-	0/7/25/26	0/2/2/2
29	OMG	a	2251	29,28,57	-	1/9/27/28	0/3/3/3
6	G7M	A	527	6,57	-	3/7/25/26	0/3/3/3
29	OMU	a	2552	29,57	-	0/9/27/28	0/2/2/2
6	MA6	A	1519	6	-	2/11/29/30	0/3/3/3
6	4OC	A	1402	6	-	0/9/29/30	0/2/2/2
29	H2U	a	2449	29	-	0/7/38/39	0/2/2/2

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	1915	3TD	C6-C5	12.83	1.49	1.35
29	a	1915	3TD	C2-N1	9.18	1.48	1.37
28	Z	8	4SU	C4-N3	8.42	1.46	1.37
29	a	1618	6MZ	C6-N6	7.81	1.43	1.34
29	a	745	1MG	C2-N3	7.22	1.45	1.33
6	A	1402	4OC	C4-N3	7.03	1.44	1.32
28	Z	8	4SU	C2-N3	6.97	1.50	1.38
29	a	2030	6MZ	C6-N6	6.91	1.42	1.34
6	A	1498	UR3	C2-N1	6.76	1.47	1.38
29	a	2552	OMU	C2-N1	6.55	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	2552	OMU	C2-N3	6.52	1.49	1.38
28	Z	8	4SU	C2-N1	6.44	1.48	1.38
6	A	1402	4OC	C6-C5	6.29	1.49	1.35
6	A	527	G7M	C4-N3	6.15	1.48	1.34
29	a	745	1MG	C4-N3	6.06	1.48	1.34
29	a	745	1MG	C2-N2	5.82	1.44	1.34
6	A	1402	4OC	C2-N3	5.78	1.47	1.36
29	a	2552	OMU	C6-C5	5.72	1.48	1.35
6	A	1498	UR3	C6-C5	5.67	1.48	1.35
28	Z	8	4SU	C6-C5	5.57	1.48	1.35
6	A	527	G7M	C5-N7	-5.45	1.32	1.39
28	Z	8	4SU	C4-S4	-5.42	1.59	1.68
29	a	1915	3TD	C6-N1	5.42	1.45	1.36
6	A	527	G7M	C2-N3	4.88	1.45	1.33
29	a	1915	3TD	C2-N3	4.75	1.48	1.38
6	A	1402	4OC	C4-N4	4.74	1.45	1.36
28	Z	8	4SU	C5-C4	4.73	1.48	1.42
6	A	1498	UR3	C2-N3	4.54	1.47	1.39
6	A	527	G7M	C2-N2	4.53	1.44	1.34
29	a	2503	2MA	C6-N6	4.19	1.44	1.34
6	A	1519	MA6	C6-N6	4.05	1.48	1.36
29	a	2030	6MZ	C5-N7	-3.90	1.32	1.39
6	A	1518	MA6	C6-N6	3.88	1.47	1.36
6	A	1402	4OC	C2-N1	3.87	1.48	1.40
29	a	2503	2MA	C5-C4	-3.84	1.32	1.39
29	a	1618	6MZ	C5-N7	-3.76	1.32	1.39
6	A	1402	4OC	C5-C4	3.72	1.49	1.41
29	a	2552	OMU	C4-N3	3.69	1.44	1.38
29	a	2030	6MZ	C5-C4	-3.62	1.32	1.39
6	A	1518	MA6	C5-C4	-3.60	1.32	1.39
28	Z	55	PSU	C6-C5	3.52	1.39	1.35
17	L	89	D2T	CB-CA	-3.50	1.53	1.54
6	A	527	G7M	C5-C6	3.50	1.53	1.43
6	A	1519	MA6	C5-C4	-3.44	1.33	1.39
29	a	745	1MG	C5-N7	-3.43	1.32	1.39
29	a	745	1MG	C2-N1	3.37	1.43	1.37
6	A	1519	MA6	C5-N7	-3.30	1.33	1.39
6	A	1518	MA6	C5-N7	-3.30	1.33	1.39
29	a	1618	6MZ	C5-C4	-3.23	1.33	1.39
29	a	1911	PSU	C6-C5	3.18	1.38	1.35
29	a	2030	6MZ	C6-N1	-3.16	1.30	1.35
6	A	1402	4OC	O2-C2	-3.15	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	516	PSU	C6-C5	3.08	1.38	1.35
29	a	2503	2MA	C5-N7	-3.07	1.33	1.39
28	Z	32	5MC	C5-C4	-3.05	1.41	1.44
29	a	2504	PSU	C6-C5	3.03	1.38	1.35
28	Z	8	4SU	C6-N1	3.02	1.45	1.38
6	A	1402	4OC	C6-N1	3.01	1.45	1.38
29	a	2604	PSU	C6-C5	3.00	1.38	1.35
6	A	527	G7M	O6-C6	-2.95	1.18	1.23
29	a	2605	PSU	C6-C5	2.95	1.38	1.35
29	a	746	PSU	C6-C5	2.94	1.38	1.35
29	a	2457	PSU	C6-C5	2.93	1.38	1.35
29	a	1917	PSU	C6-C5	2.84	1.38	1.35
29	a	2580	PSU	C6-C5	2.81	1.38	1.35
6	A	1518	MA6	C8-N9	-2.81	1.32	1.37
29	a	955	PSU	C6-C5	2.80	1.38	1.35
28	Z	8	4SU	O2-C2	-2.78	1.18	1.23
29	a	2503	2MA	C8-N9	-2.73	1.32	1.37
6	A	1498	UR3	C6-N1	2.73	1.44	1.38
29	a	1618	6MZ	C8-N9	-2.70	1.33	1.37
29	a	745	1MG	O6-C6	-2.65	1.17	1.23
29	a	745	1MG	C5-C6	2.64	1.52	1.45
29	a	1618	6MZ	C6-N1	-2.61	1.30	1.35
29	a	2030	6MZ	C8-N9	-2.61	1.33	1.37
29	a	1915	3TD	O2-C2	-2.60	1.18	1.23
6	A	1498	UR3	O4-C4	-2.58	1.18	1.23
29	a	745	1MG	C4-N9	-2.58	1.31	1.38
6	A	1519	MA6	C8-N9	-2.57	1.33	1.37
6	A	527	G7M	C2-N1	2.56	1.43	1.37
29	a	2030	6MZ	C9-N6	-2.56	1.40	1.45
6	A	1498	UR3	O2-C2	-2.49	1.17	1.22
6	A	527	G7M	C4-N9	-2.43	1.31	1.38
29	a	2030	6MZ	C4-N9	-2.39	1.32	1.37
29	a	1618	6MZ	C5-C6	-2.38	1.36	1.41
6	A	1518	MA6	C6-N1	-2.37	1.30	1.34
29	a	2552	OMU	O4-C4	-2.37	1.19	1.24
29	a	2030	6MZ	C5-C6	-2.37	1.36	1.41
6	A	1518	MA6	C2-N1	2.37	1.38	1.33
6	A	1519	MA6	C2-N1	2.36	1.38	1.33
29	a	2069	G7M	C8-N7	2.33	1.37	1.33
29	a	1618	6MZ	C9-N6	-2.28	1.41	1.45
29	a	2503	2MA	C6-N1	-2.24	1.32	1.35
6	A	1498	UR3	C4-N3	2.24	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	2580	PSU	O4'-C1'	-2.23	1.40	1.43
29	a	1915	3TD	O4-C4	-2.21	1.18	1.23
29	a	1915	3TD	C4-N3	2.21	1.45	1.40
29	a	2552	OMU	C6-N1	2.19	1.43	1.38
29	a	2457	PSU	C4-C5	-2.18	1.38	1.44
29	a	746	PSU	C4-C5	-2.17	1.38	1.44
29	a	2605	PSU	C4-C5	-2.16	1.38	1.44
29	a	2580	PSU	C4-C5	-2.13	1.38	1.44
17	L	89	D2T	CB1-SB	-2.11	1.75	1.79
29	a	2498	OMC	C4-N3	-2.11	1.30	1.34
6	A	516	PSU	O4'-C1'	-2.10	1.40	1.43
29	a	2503	2MA	C4-N9	-2.09	1.33	1.37
6	A	1519	MA6	C6-N1	-2.07	1.30	1.34
6	A	1407	5MC	C4-N3	-2.07	1.30	1.34
6	A	516	PSU	C4-C5	-2.06	1.38	1.44
6	A	1498	UR3	C5-C4	2.04	1.49	1.43
29	a	2604	PSU	C4-C5	-2.03	1.38	1.44
29	a	2457	PSU	O4'-C1'	-2.01	1.41	1.43

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1519	MA6	N1-C6-N6	-16.07	97.28	116.86
6	A	1518	MA6	N1-C6-N6	-15.49	97.99	116.86
6	A	1519	MA6	C5-C6-N6	11.18	143.03	125.33
6	A	1518	MA6	C5-C6-N6	10.62	142.14	125.33
29	a	2503	2MA	CM2-C2-N3	10.10	132.25	117.13
29	a	2503	2MA	N6-C6-N1	-9.44	104.29	117.03
28	Z	8	4SU	C4-N3-C2	-8.25	119.40	127.31
29	a	2503	2MA	C5-C4-N3	-6.84	119.97	127.18
6	A	1518	MA6	C4-N9-C1'	-6.63	111.13	126.63
6	A	1519	MA6	C4-N9-C1'	-6.62	111.15	126.63
6	A	527	G7M	C1'-N9-C4	6.34	145.22	126.49
29	a	2552	OMU	C4-N3-C2	-6.21	118.90	126.61
29	a	2503	2MA	CM2-C2-N1	-6.05	108.07	117.13
6	A	1519	MA6	C1'-N9-C8	6.03	140.47	127.09
6	A	527	G7M	C1'-N9-C8	-5.98	106.55	126.74
6	A	1498	UR3	C4-N3-C2	-5.92	119.81	124.58
29	a	2030	6MZ	N1-C2-N3	-5.89	119.66	128.58
6	A	1518	MA6	C1'-N9-C8	5.87	140.13	127.09
29	a	1915	3TD	N1-C2-N3	5.85	120.38	116.13
29	a	2457	PSU	N1-C2-N3	5.78	121.26	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	1618	6MZ	C5-C4-N3	-5.76	118.78	126.72
29	a	1618	6MZ	N1-C2-N3	-5.73	119.91	128.58
29	a	2030	6MZ	C9-N6-C6	-5.70	117.56	122.85
28	Z	8	4SU	C5-C4-N3	5.68	120.03	114.75
6	A	1519	MA6	N1-C2-N3	-5.62	120.07	128.58
6	A	1519	MA6	C5-C4-N3	-5.59	119.02	126.72
29	a	2605	PSU	C4-N3-C2	-5.36	118.98	126.37
6	A	1518	MA6	C5-C4-N3	-5.35	119.35	126.72
29	a	2457	PSU	C4-N3-C2	-5.34	119.02	126.37
29	a	2604	PSU	N1-C2-N3	5.25	120.71	115.17
6	A	1518	MA6	N1-C2-N3	-5.23	120.67	128.58
29	a	1911	PSU	N1-C2-N3	5.22	120.67	115.17
29	a	2605	PSU	N1-C2-N3	5.22	120.67	115.17
29	a	1911	PSU	C4-N3-C2	-5.19	119.22	126.37
29	a	2604	PSU	C4-N3-C2	-5.18	119.24	126.37
6	A	1518	MA6	C4-C5-C6	5.17	121.26	115.91
29	a	746	PSU	C4-N3-C2	-5.12	119.32	126.37
6	A	1519	MA6	C4-C5-C6	5.09	121.17	115.91
29	a	2580	PSU	N1-C2-N3	5.04	120.49	115.17
29	a	2030	6MZ	C5-C4-N3	-5.01	119.82	126.72
29	a	955	PSU	N1-C2-N3	5.00	120.44	115.17
29	a	2504	PSU	N1-C2-N3	4.99	120.44	115.17
29	a	1917	PSU	C4-N3-C2	-4.93	119.58	126.37
29	a	1917	PSU	N1-C2-N3	4.91	120.35	115.17
29	a	955	PSU	C4-N3-C2	-4.90	119.63	126.37
29	a	745	1MG	C5-C4-N3	-4.89	120.60	128.39
29	a	2580	PSU	C4-N3-C2	-4.76	119.81	126.37
29	a	2030	6MZ	N9-C8-N7	-4.72	107.24	113.94
29	a	2503	2MA	C5-C6-N6	4.71	134.95	123.29
29	a	2504	PSU	C4-N3-C2	-4.66	119.95	126.37
6	A	516	PSU	C4-N3-C2	-4.64	119.97	126.37
6	A	516	PSU	N1-C2-N3	4.55	119.97	115.17
29	a	746	PSU	N1-C2-N3	4.55	119.96	115.17
29	a	2503	2MA	N9-C8-N7	-4.42	107.66	113.94
29	a	1618	6MZ	C4-C5-C6	4.33	120.38	116.78
6	A	1518	MA6	N9-C8-N7	-4.28	107.86	113.94
28	Z	8	4SU	C5-C4-S4	-4.28	119.42	124.31
6	A	527	G7M	C2-N3-C4	4.22	119.57	112.30
29	a	1915	3TD	C4-N3-C2	-4.21	120.16	124.61
6	A	1519	MA6	N9-C8-N7	-4.13	108.07	113.94
29	a	2552	OMU	N3-C2-N1	4.10	120.23	114.89
29	a	1618	6MZ	N9-C8-N7	-4.07	108.17	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	2552	OMU	C5-C4-N3	4.04	120.45	114.80
6	A	1518	MA6	N3-C4-N9	4.03	134.03	127.17
6	A	1519	MA6	N3-C4-N9	4.03	134.02	127.17
6	A	527	G7M	CN7-N7-C5	4.01	131.79	126.80
6	A	527	G7M	C5-C6-N1	3.95	120.01	111.84
29	a	2503	2MA	N3-C4-N9	3.91	131.96	126.99
6	A	1498	UR3	C5-C4-N3	3.80	120.04	115.04
29	a	1618	6MZ	N3-C4-N9	3.77	133.58	127.17
28	Z	8	4SU	N3-C2-N1	3.76	119.79	114.89
6	A	527	G7M	C5-C4-N3	-3.73	121.11	128.15
29	a	1618	6MZ	C2-N3-C4	3.68	120.82	111.83
29	a	2030	6MZ	C2-N3-C4	3.56	120.53	111.83
6	A	1519	MA6	C2-N3-C4	3.52	120.42	111.83
29	a	745	1MG	C2-N3-C4	3.50	119.85	111.98
29	a	2580	PSU	O2-C2-N1	-3.46	119.22	122.79
6	A	527	G7M	O6-C6-C5	-3.46	120.29	128.01
29	a	2503	2MA	N3-C2-N1	-3.45	119.68	125.77
29	a	2030	6MZ	C4-N9-C1'	-3.41	118.66	126.63
29	a	2030	6MZ	C5-N7-C8	3.39	108.77	103.45
29	a	745	1MG	N9-C8-N7	-3.37	107.15	113.40
29	a	1618	6MZ	C9-N6-C6	-3.35	119.74	122.85
6	A	1518	MA6	C2-N3-C4	3.20	119.65	111.83
29	a	2449	H2U	C5-C4-N3	-3.19	113.29	116.69
6	A	1519	MA6	C2-N1-C6	3.19	119.63	111.83
6	A	527	G7M	CN7-N7-C8	-3.19	119.96	124.79
6	A	527	G7M	C2-N1-C6	-3.08	119.52	125.11
29	a	2552	OMU	O4-C4-C5	-3.03	119.93	125.16
29	a	1618	6MZ	C5-N7-C8	3.03	108.21	103.45
29	a	745	1MG	N9-C4-N3	3.02	132.00	125.95
6	A	1518	MA6	C2-N1-C6	3.01	119.19	111.83
29	a	2457	PSU	C6-C5-C4	2.97	120.18	118.17
29	a	2030	6MZ	C4-C5-C6	2.95	119.23	116.78
29	a	2503	2MA	C5-N7-C8	2.93	108.05	103.45
29	a	2580	PSU	C6-N1-C2	-2.91	119.99	122.69
29	a	2504	PSU	C6-N1-C2	-2.90	120.00	122.69
29	a	1911	PSU	O2-C2-N1	-2.88	119.82	122.79
29	a	1917	PSU	O2-C2-N1	-2.86	119.83	122.79
29	a	2030	6MZ	C1'-N9-C8	2.86	133.45	127.09
6	A	1518	MA6	C4-N9-C8	2.86	108.74	105.74
6	A	516	PSU	O2-C2-N1	-2.83	119.87	122.79
29	a	955	PSU	O2-C2-N1	-2.82	119.88	122.79
29	a	745	1MG	C5-C6-N1	2.76	120.12	115.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	746	PSU	O2-C2-N1	-2.71	119.99	122.79
29	a	2030	6MZ	C5-C6-N1	2.71	121.06	118.15
6	A	1519	MA6	C5-N7-C8	2.70	107.69	103.45
6	A	1518	MA6	C5-N7-C8	2.70	107.69	103.45
29	a	2457	PSU	C6-N1-C2	-2.67	120.21	122.69
29	a	2030	6MZ	C4-C5-N7	-2.65	107.55	110.58
29	a	2552	OMU	O2-C2-N1	-2.64	119.36	122.80
29	a	2030	6MZ	N3-C4-N9	2.63	131.64	127.17
29	a	955	PSU	C6-N1-C2	-2.56	120.31	122.69
29	a	1915	3TD	C6-C5-C4	2.56	119.91	118.19
29	a	1618	6MZ	C5-C6-N1	2.56	120.89	118.15
29	a	2605	PSU	O2-C2-N1	-2.54	120.17	122.79
29	a	745	1MG	N2-C2-N1	2.54	120.83	118.79
29	a	2457	PSU	O2-C2-N1	-2.54	120.17	122.79
29	a	2504	PSU	O2-C2-N1	-2.53	120.18	122.79
29	a	2604	PSU	C6-N1-C2	-2.51	120.36	122.69
29	a	2030	6MZ	C5-C4-N9	2.51	108.54	105.81
6	A	516	PSU	O4'-C1'-C2'	2.50	108.60	105.15
29	a	2580	PSU	O4'-C1'-C2'	2.48	108.59	105.15
6	A	1519	MA6	C4-N9-C8	2.46	108.32	105.74
29	a	2605	PSU	C6-C5-C4	2.45	119.83	118.17
6	A	516	PSU	C6-N1-C2	-2.45	120.42	122.69
29	a	1911	PSU	C6-C5-C4	2.43	119.82	118.17
29	a	1917	PSU	C6-N1-C2	-2.42	120.44	122.69
29	a	1911	PSU	C6-N1-C2	-2.41	120.46	122.69
6	A	1518	MA6	C6-C5-N7	-2.37	129.65	133.43
29	a	2604	PSU	O2-C2-N1	-2.36	120.35	122.79
29	a	2503	2MA	C4-N9-C8	2.35	108.20	105.74
29	a	745	1MG	C8-N7-C5	2.28	108.33	104.26
29	a	2503	2MA	C4-C5-N7	-2.25	108.01	110.58
6	A	1519	MA6	C6-C5-N7	-2.23	129.88	133.43
6	A	1402	4OC	CM4-N4-C4	-2.20	118.16	122.45
28	Z	55	PSU	C2'-C3'-C4'	-2.17	98.41	102.61
6	A	527	G7M	N9-C4-N3	2.14	130.24	125.95
29	a	2069	G7M	N9-C8-N7	-2.13	107.32	112.48
28	Z	8	4SU	O2-C2-N1	-2.12	120.03	122.80
29	a	2457	PSU	O4'-C1'-C2'	2.12	108.09	105.15
6	A	527	G7M	N9-C8-N7	-2.10	107.39	112.48
29	a	2503	2MA	C5-C4-N9	2.07	108.07	105.81
29	a	2030	6MZ	C4-N9-C8	2.05	107.89	105.74
6	A	1402	4OC	C6-C5-C4	2.04	119.46	117.00
29	a	2605	PSU	C5-C6-N1	-2.03	119.32	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	745	1MG	C1'-N9-C4	-2.03	120.49	126.49
17	L	89	D2T	O-C-CA	-2.00	119.62	124.77
6	A	1498	UR3	C1'-N1-C2	2.00	120.32	117.04

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	O-C-CA-CB
17	L	89	D2T	CA-CB-CG-OD1
17	L	89	D2T	CA-CB-CG-OD2
32	d	150	MEQ	C-CA-CB-CG
32	d	150	MEQ	O-C-CA-CB
29	a	2251	OMG	C1'-C2'-O2'-CM2
6	A	527	G7M	C3'-C4'-C5'-O5'
29	a	2445	2MG	C3'-C4'-C5'-O5'
32	d	150	MEQ	NE2-CD-CG-CB
32	d	150	MEQ	OE1-CD-CG-CB
29	a	2030	6MZ	O4'-C4'-C5'-O5'
29	a	2030	6MZ	C3'-C4'-C5'-O5'
29	a	2504	PSU	O4'-C4'-C5'-O5'
6	A	527	G7M	O4'-C4'-C5'-O5'
29	a	2445	2MG	O4'-C4'-C5'-O5'
6	A	1519	MA6	O4'-C4'-C5'-O5'
17	L	89	D2T	CG-CB-SB-CB1
29	a	2503	2MA	O4'-C4'-C5'-O5'
6	A	527	G7M	C4'-C5'-O5'-P
17	L	89	D2T	SB-CB-CG-OD2
29	a	2504	PSU	C3'-C4'-C5'-O5'
29	a	746	PSU	O4'-C1'-C5-C6
29	a	746	PSU	C2'-C1'-C5-C6
6	A	1519	MA6	C3'-C4'-C5'-O5'
29	a	2503	2MA	C4'-C5'-O5'-P
29	a	1962	5MC	C2'-C1'-N1-C6
29	a	1962	5MC	O4'-C1'-N1-C6
29	a	747	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	2030	6MZ	1	0
6	A	516	PSU	1	0
28	Z	32	5MC	1	0
29	a	2503	2MA	1	0
17	L	89	D2T	1	0
6	A	1516	2MG	1	0
29	a	2251	OMG	1	0
29	a	2552	OMU	1	0
6	A	1519	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 491 ligands modelled in this entry, 489 are monoatomic - leaving 2 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	$\# Z > 2$
58	MIY	A	1635	56	36,36,36	1.50	8 (22%)	42,58,58	1.88	10 (23%)
58	MIY	a	3005	-	36,36,36	1.36	4 (11%)	42,58,58	1.89	11 (26%)

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
58	MIY	A	1635	56	-	1/12/70/70	0/4/4/4
58	MIY	a	3005	-	-	7/12/70/70	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	a	3005	MIY	C18-C5	3.98	1.56	1.53
58	A	1635	MIY	C18-C1	-3.66	1.50	1.55
58	A	1635	MIY	C7-C16	-3.38	1.48	1.51
58	a	3005	MIY	C7-C16	-3.17	1.48	1.51
58	A	1635	MIY	O7-C18	-3.08	1.37	1.42
58	A	1635	MIY	C18-C17	-2.80	1.49	1.52
58	A	1635	MIY	C2-C3	-2.57	1.34	1.40
58	a	3005	MIY	C71-N7	2.44	1.51	1.45
58	a	3005	MIY	C2-C3	-2.16	1.35	1.40
58	A	1635	MIY	C16-C17	-2.11	1.33	1.36
58	A	1635	MIY	C5-C4	2.04	1.56	1.54
58	A	1635	MIY	C14-C13	-2.02	1.38	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	A	1635	MIY	C21-C2-C1	-5.66	114.27	120.97
58	a	3005	MIY	C21-C2-C1	-5.33	114.67	120.97
58	a	3005	MIY	C11-C10-N7	-4.21	115.86	121.65
58	A	1635	MIY	C11-C12-C13	-4.16	116.34	120.50
58	A	1635	MIY	C11-C10-N7	-3.93	116.23	121.65
58	a	3005	MIY	C11-C12-C13	-3.93	116.57	120.50
58	a	3005	MIY	O6-C17-C16	-3.09	117.53	123.52
58	a	3005	MIY	C18-C17-C16	3.09	126.20	123.06
58	A	1635	MIY	O6-C17-C16	-3.07	117.56	123.52
58	a	3005	MIY	C19-N1-C4	3.06	121.06	114.10
58	A	1635	MIY	C19-N1-C4	2.96	120.84	114.10
58	A	1635	MIY	C18-C17-C16	2.54	125.64	123.06
58	a	3005	MIY	O7-C18-C17	-2.49	106.16	110.14
58	A	1635	MIY	C12-C13-C14	2.45	123.27	120.15
58	A	1635	MIY	C71-N7-CN7	2.41	123.93	116.18
58	A	1635	MIY	O6-C17-C18	2.36	116.79	113.37
58	a	3005	MIY	C9-C10-N7	2.27	121.58	118.87
58	a	3005	MIY	C12-C13-C14	2.24	123.01	120.15
58	A	1635	MIY	C9-C8-C7	-2.22	110.19	113.12
58	a	3005	MIY	C71-N7-C10	2.17	121.90	115.16
58	a	3005	MIY	O6-C17-C18	2.00	116.27	113.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	a	3005	MIY	C1-C2-C21-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	a	3005	MIY	C3-C2-C21-O8
58	a	3005	MIY	C1-C2-C21-N2
58	a	3005	MIY	C3-C2-C21-N2
58	a	3005	MIY	C3-C4-N1-C20
58	A	1635	MIY	C1-C2-C21-N2
58	a	3005	MIY	C3-C4-N1-C19
58	a	3005	MIY	C9-C10-N7-CN7

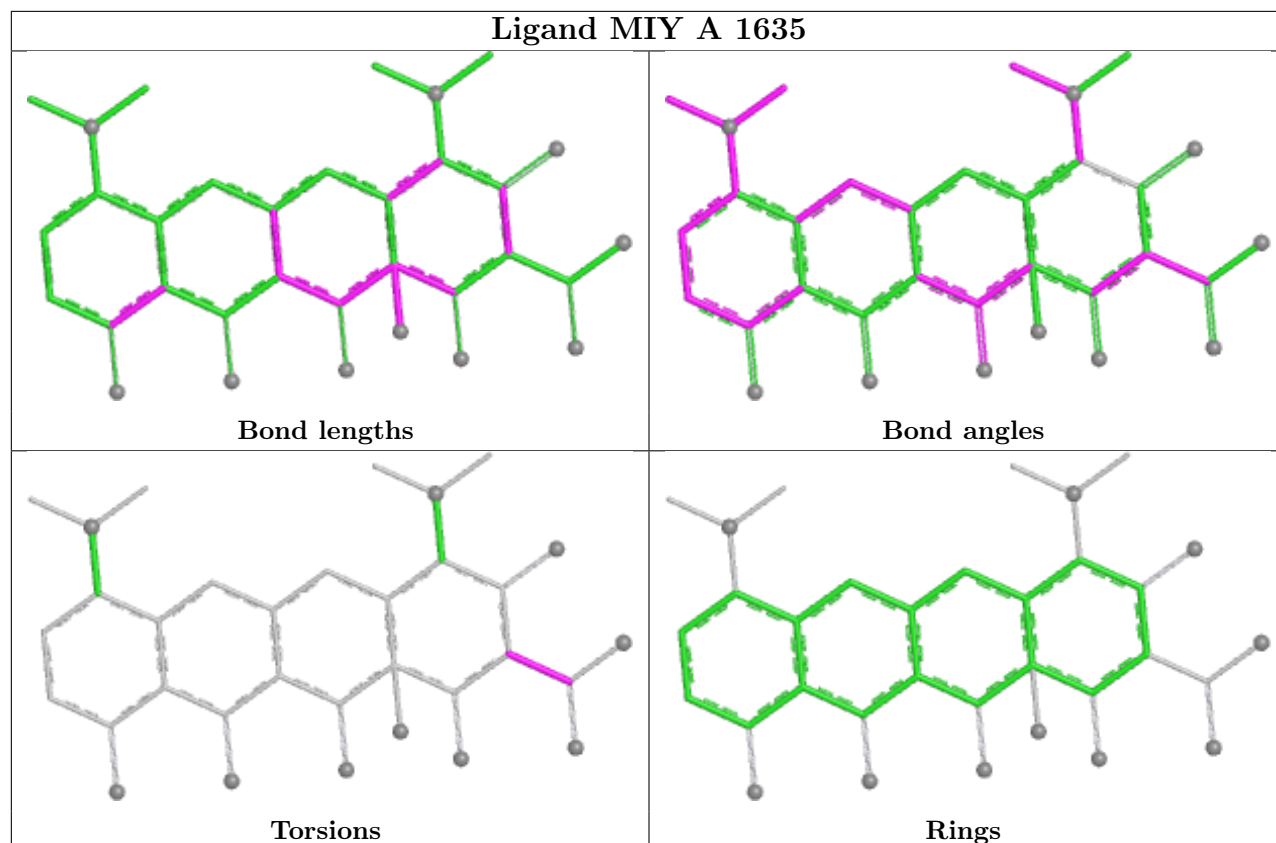
There are no ring outliers.

2 monomers are involved in 4 short contacts:

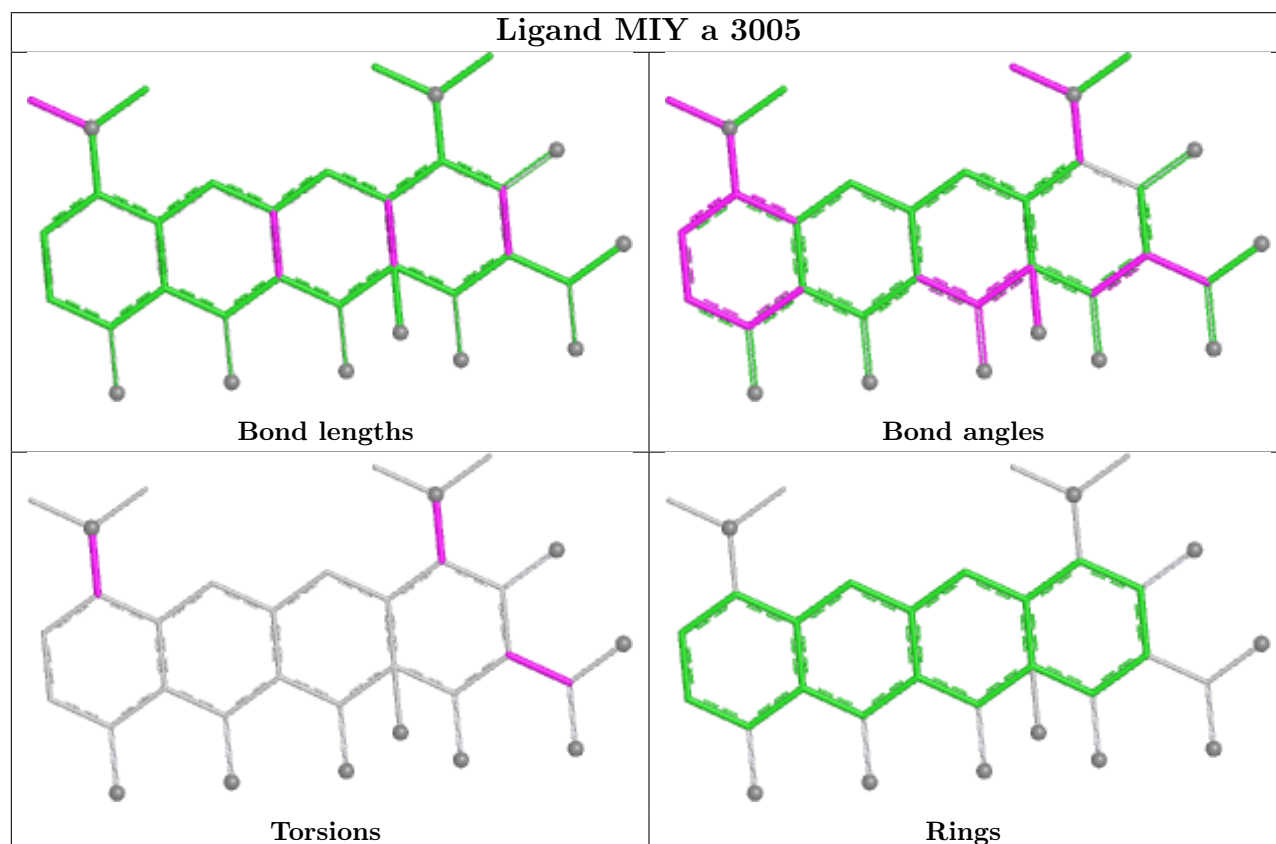
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	A	1635	MIY	2	0
58	a	3005	MIY	2	0

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

Ligand MIY A 1635



Ligand MIY a 3005



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

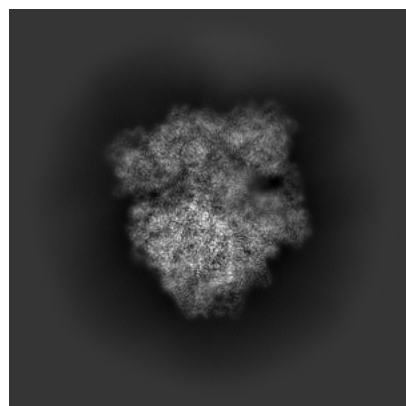
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71669. These allow visual inspection of the internal detail of the map and identification of artifacts.

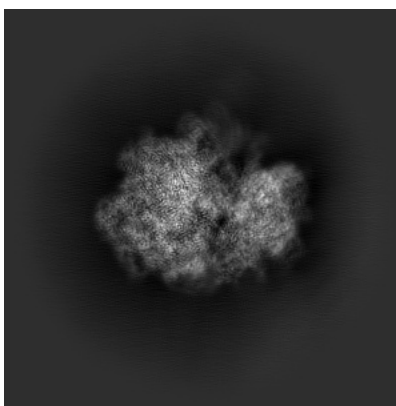
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

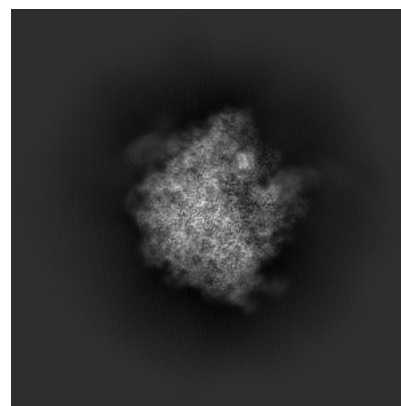
6.1.1 Primary map



X

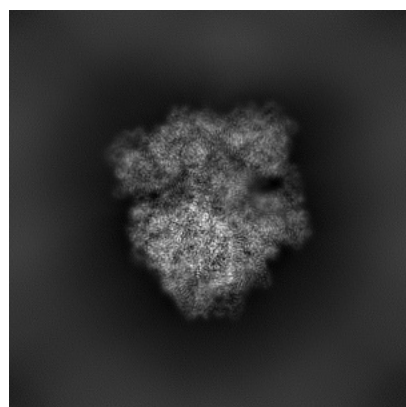


Y

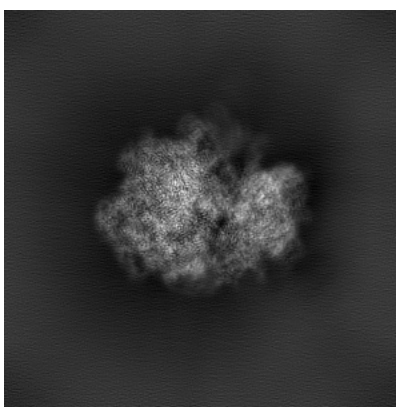


Z

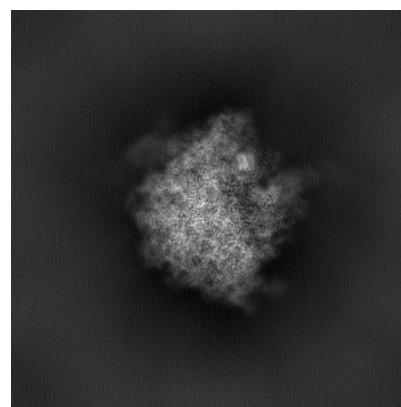
6.1.2 Raw map



X



Y

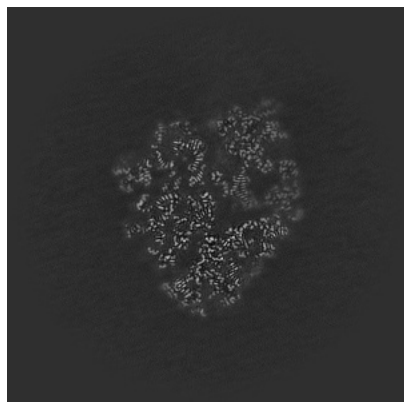


Z

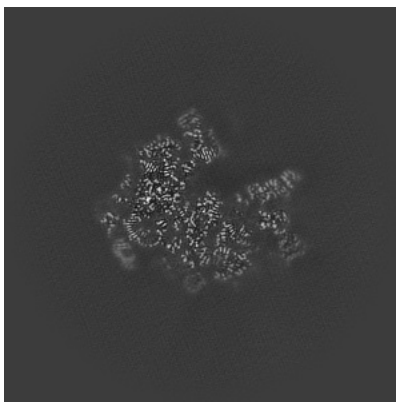
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

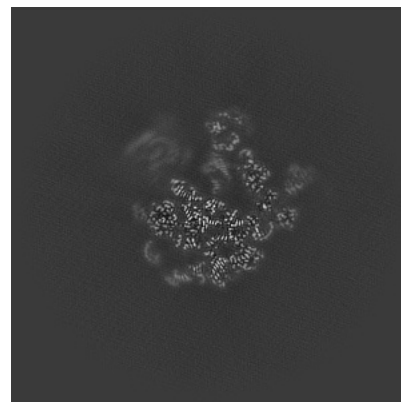
6.2.1 Primary map



X Index: 220

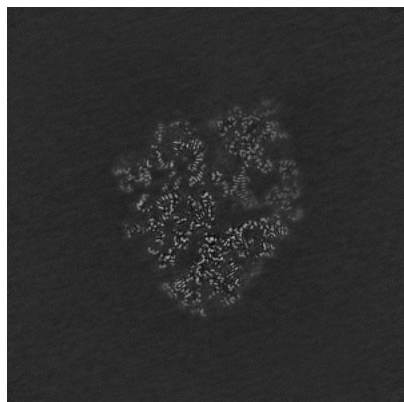


Y Index: 220

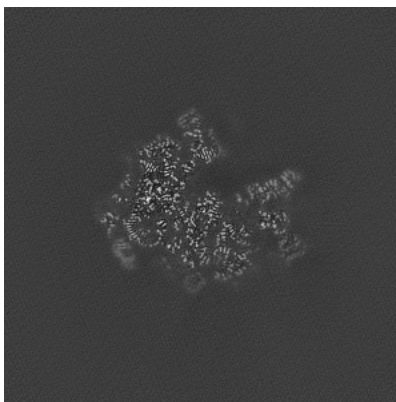


Z Index: 220

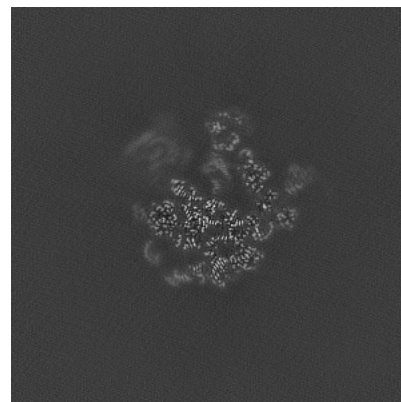
6.2.2 Raw map



X Index: 220



Y Index: 220

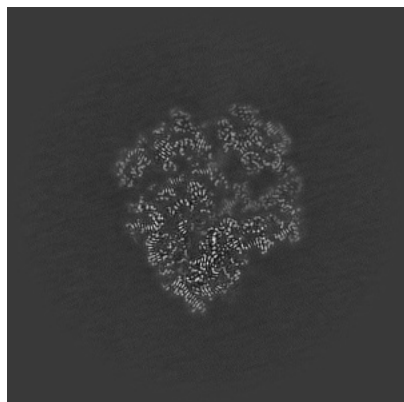


Z Index: 220

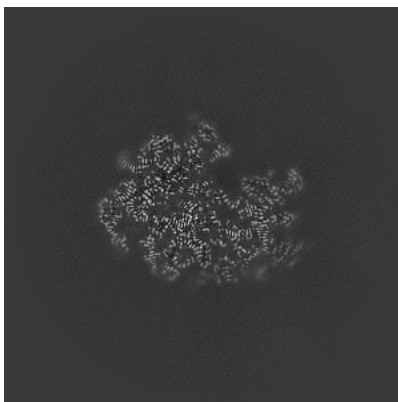
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

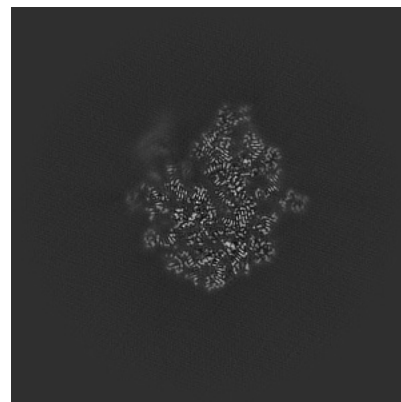
6.3.1 Primary map



X Index: 227

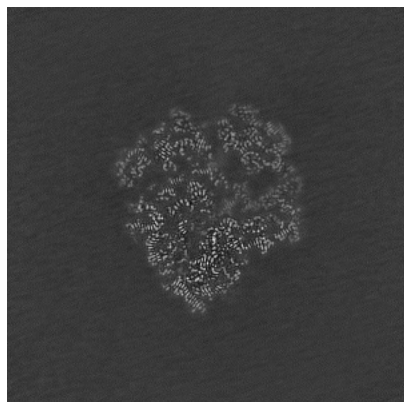


Y Index: 210

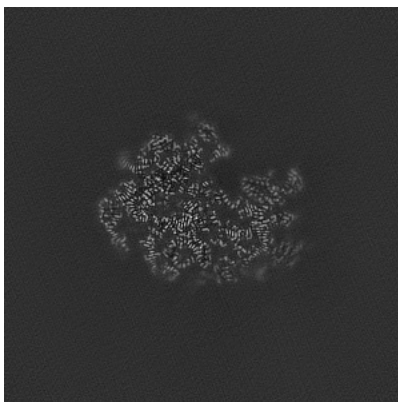


Z Index: 199

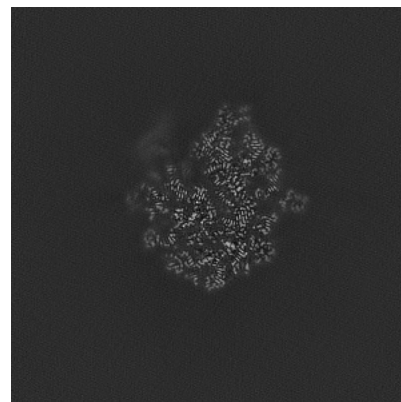
6.3.2 Raw map



X Index: 227



Y Index: 210

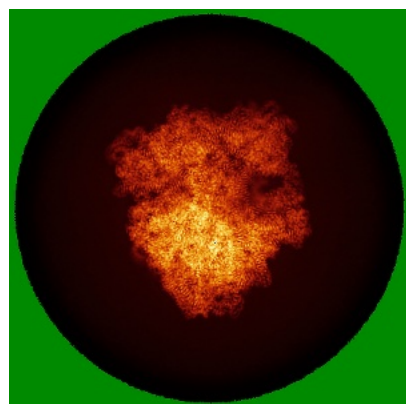


Z Index: 199

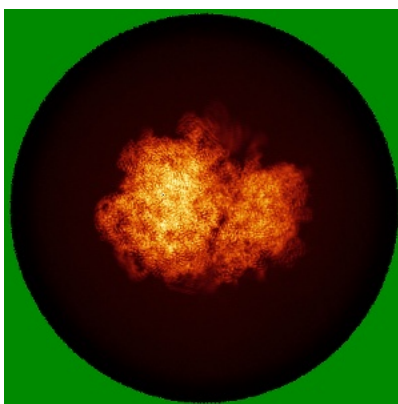
The images above show the largest variance slices of the map in three orthogonal directions.

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

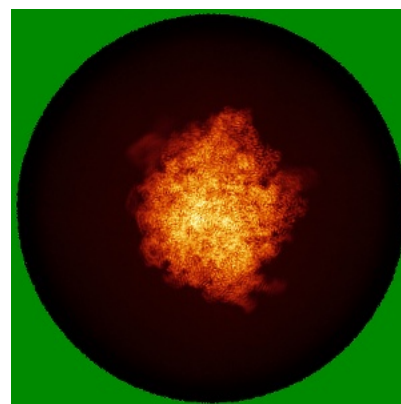
6.4.1 Primary map



X

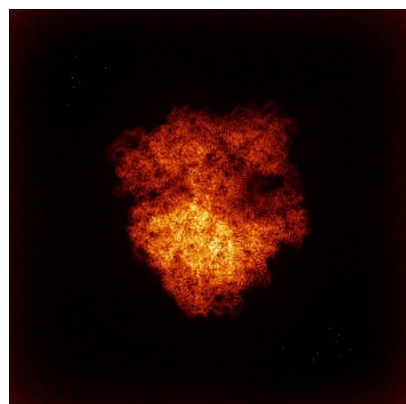


Y

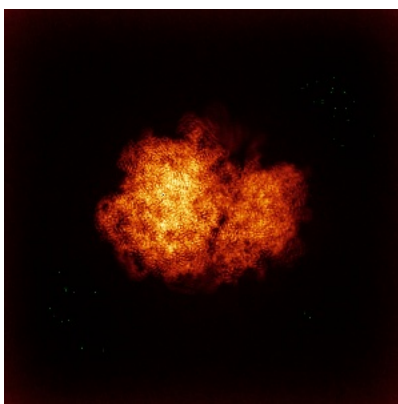


Z

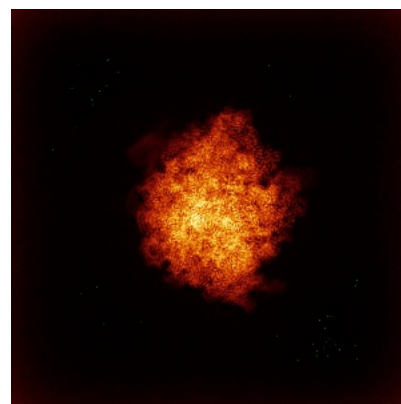
6.4.2 Raw map



X



Y

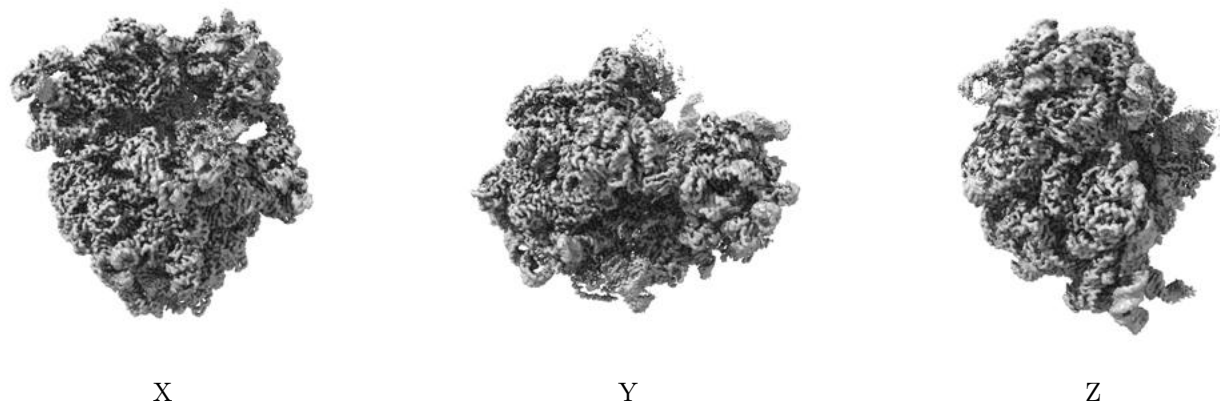


Z

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

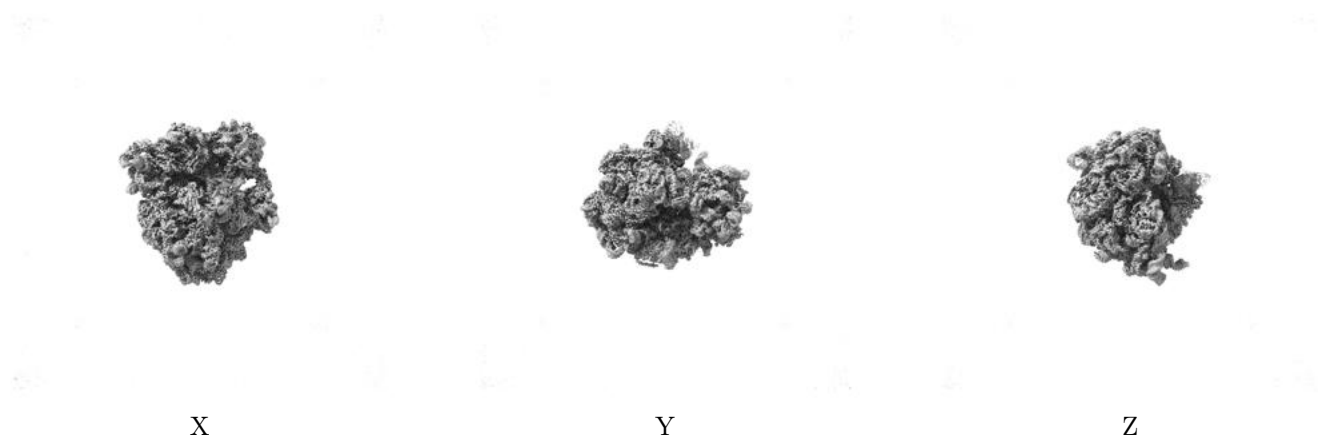
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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



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.

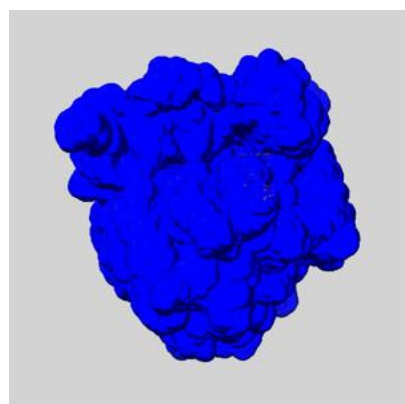
6.6 Mask visualisation [i](#)

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

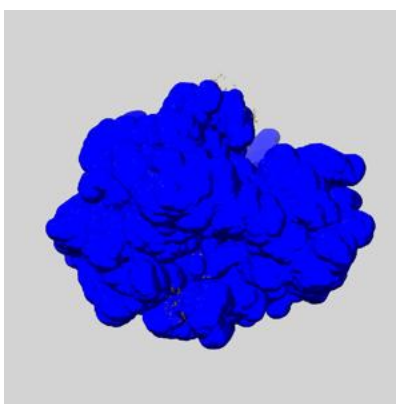
A mask typically either:

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

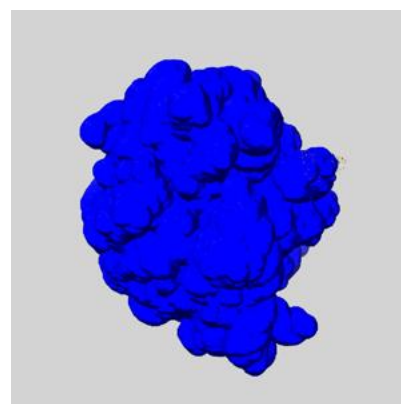
6.6.1 emd_71669_msk_1.map [i](#)



X



Y

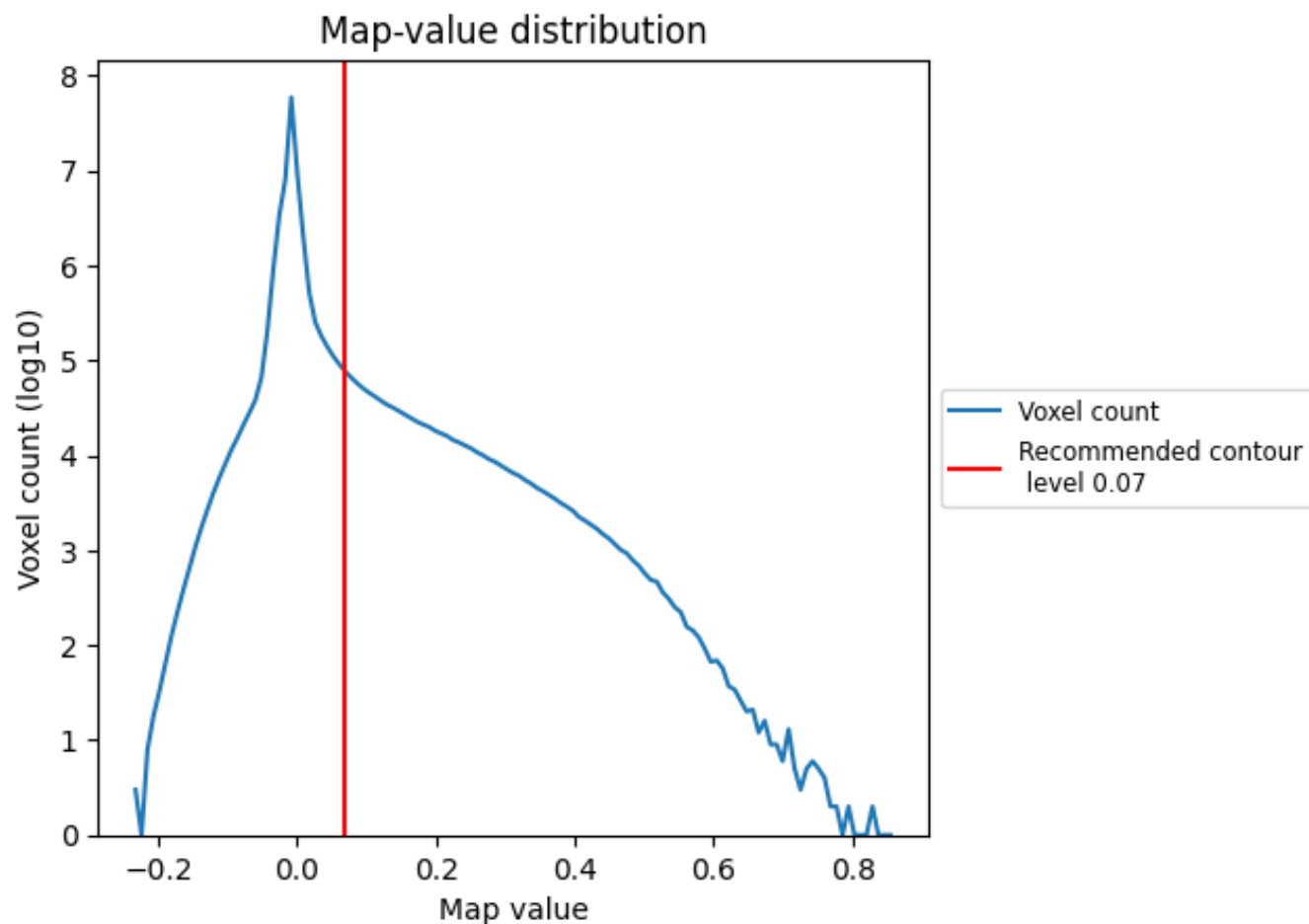


Z

7 Map analysis [i](#)

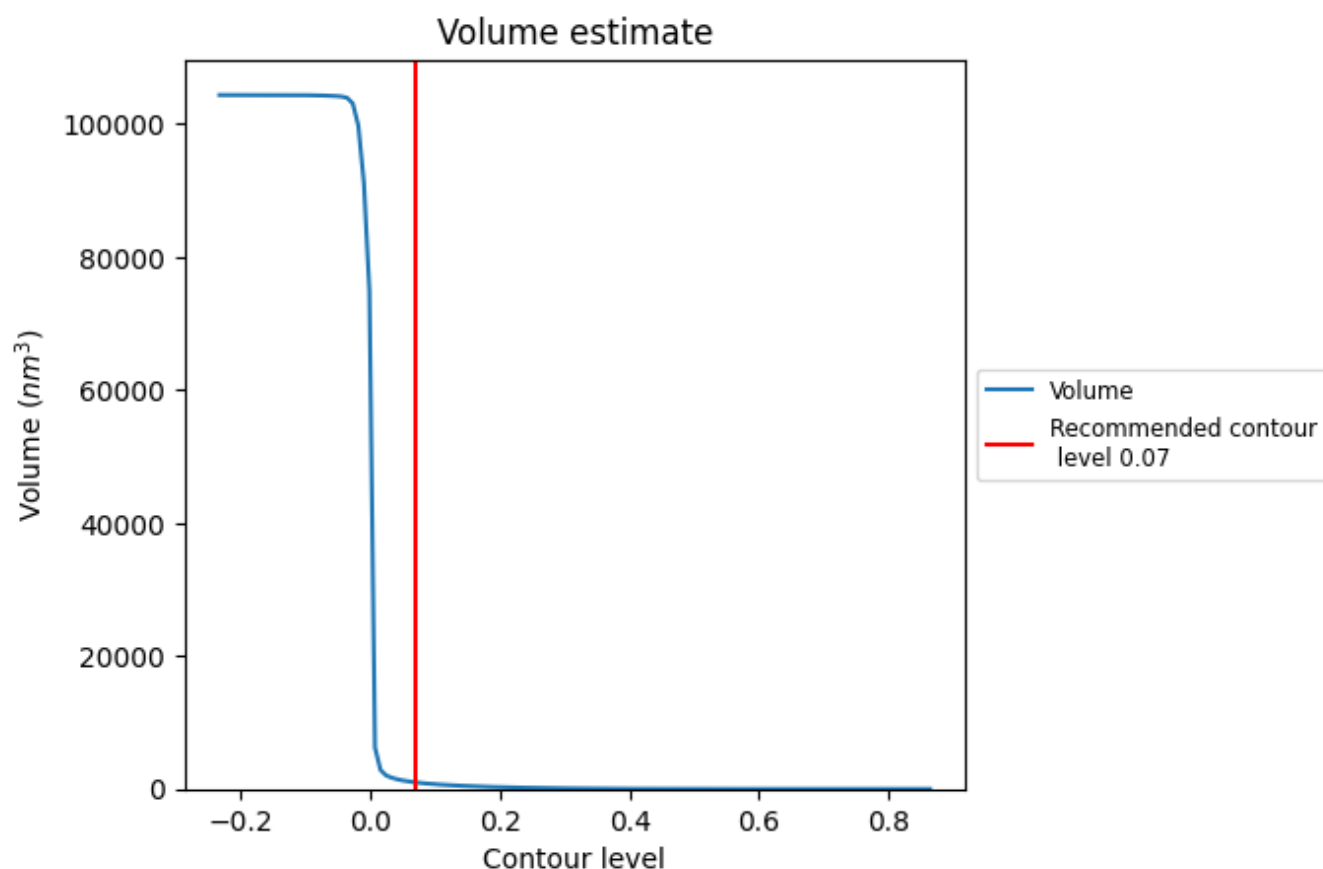
This section contains the results of statistical analysis of the map.

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.

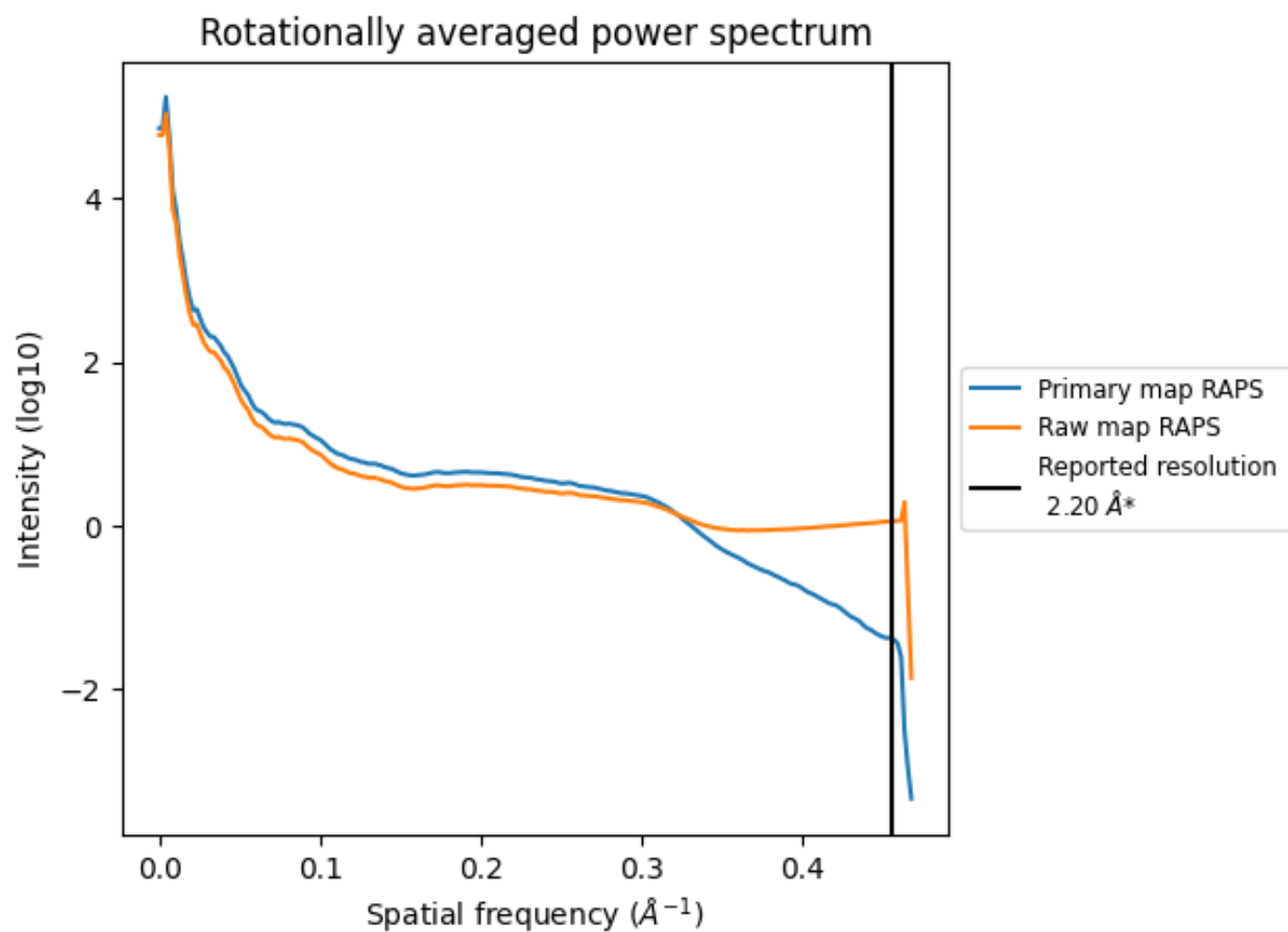
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 989 nm^3 ; this corresponds to an approximate mass of 893 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 ⓘ

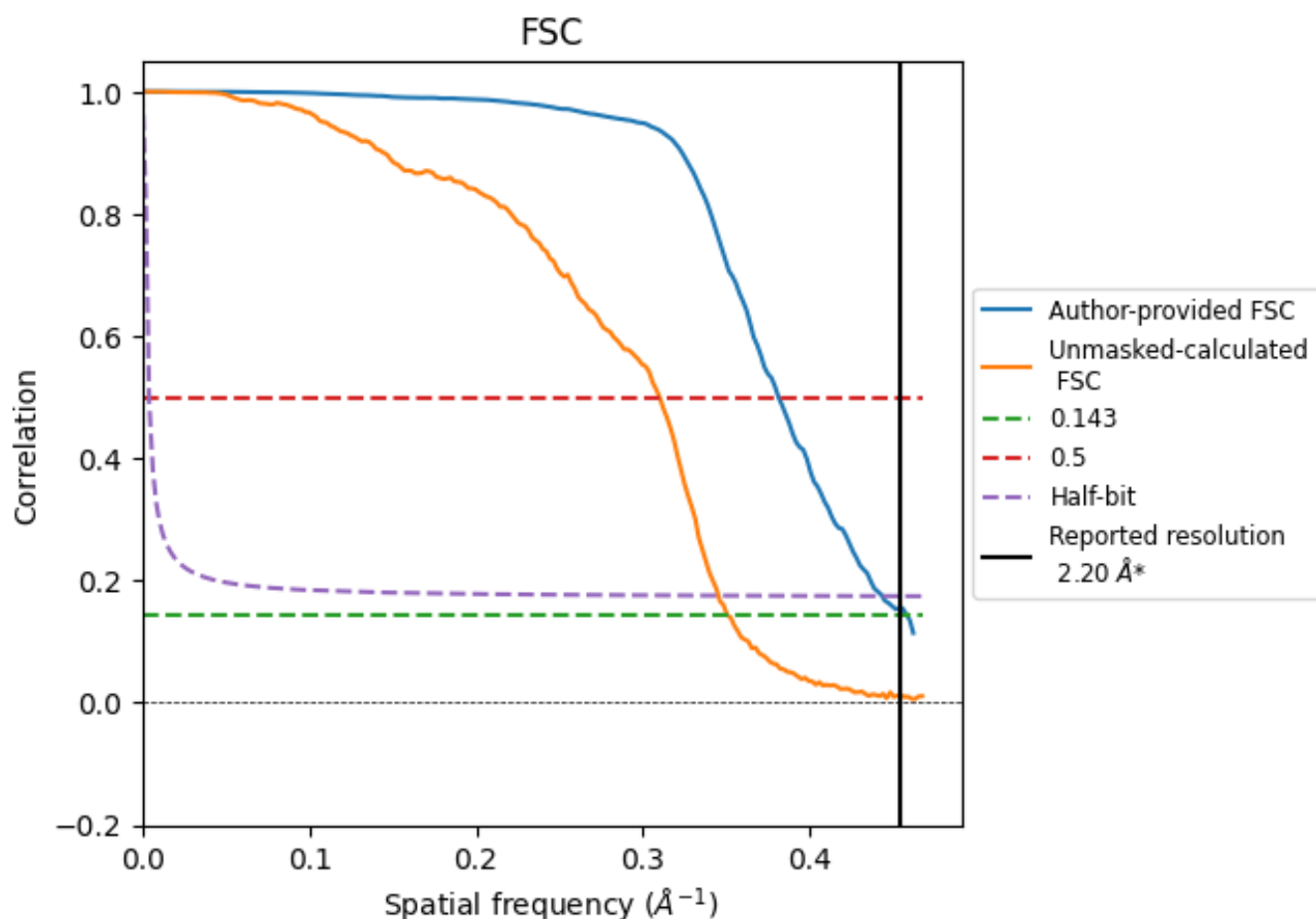


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

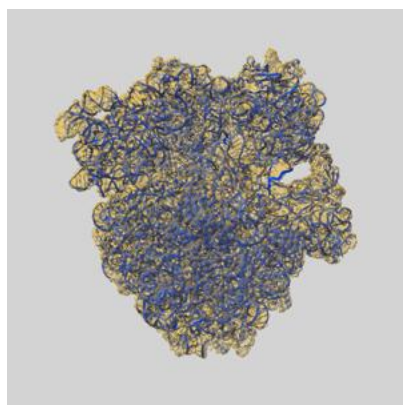
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.18	2.62	2.26
Unmasked-calculated*	2.85	3.23	2.90

*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 2.85 differs from the reported value 2.2 by more than 10 %

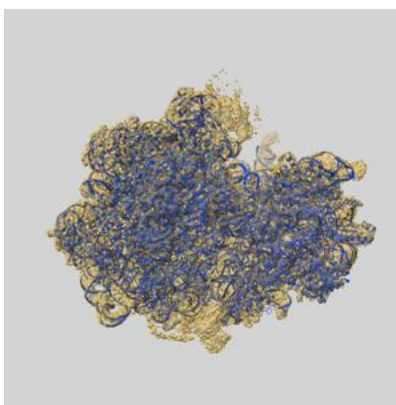
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71669 and PDB model 9PIJ. Per-residue inclusion information can be found in section 3 on page 17.

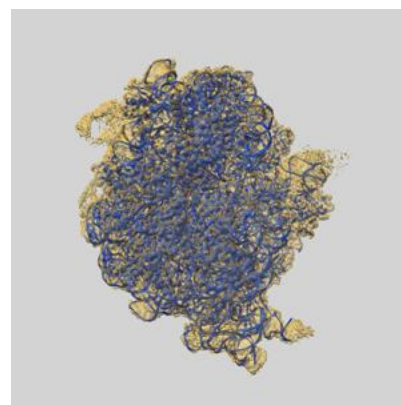
9.1 Map-model overlay [i](#)



X



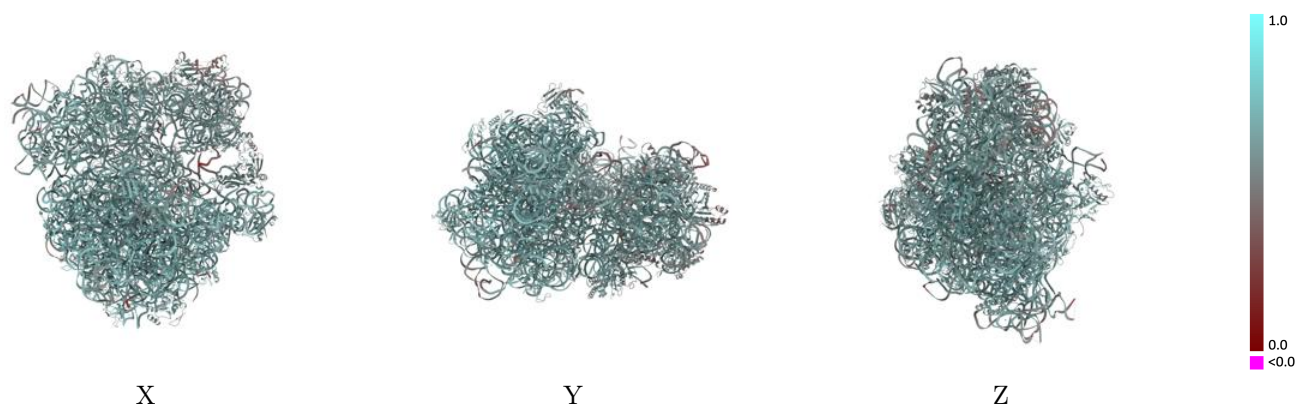
Y



Z

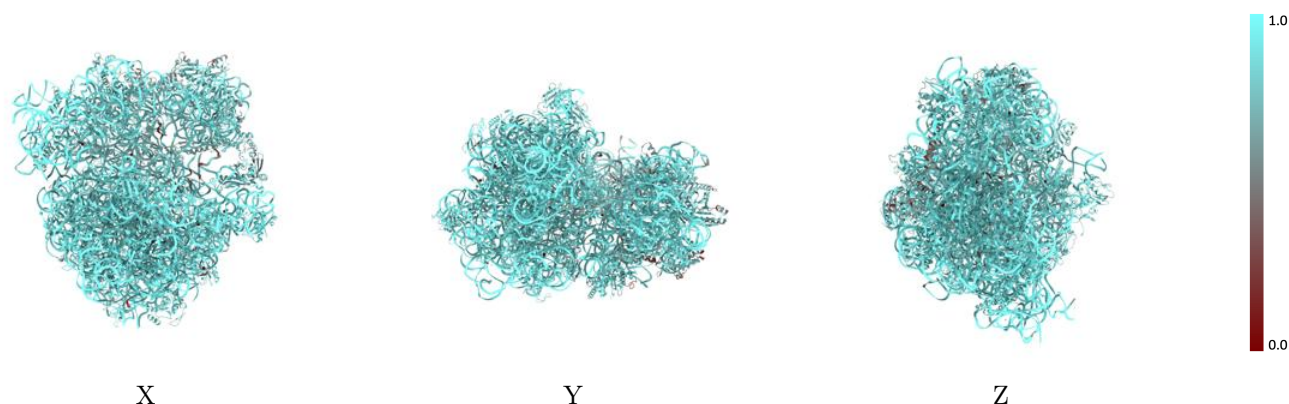
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



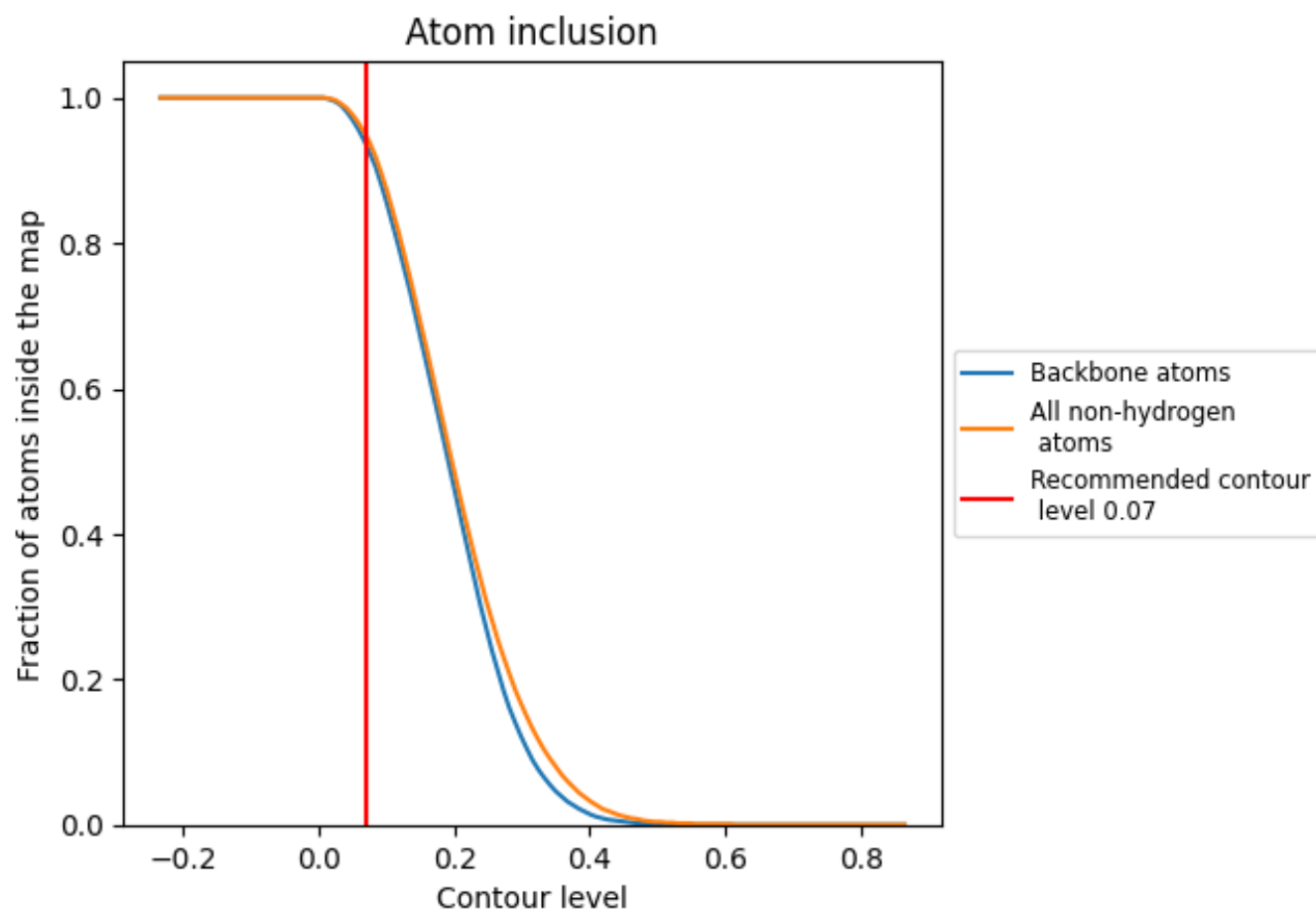
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.6310
0	 0.9000	 0.6430
1	 0.9660	 0.6850
2	 0.9700	 0.6800
3	 0.9390	 0.6540
4	 0.5750	 0.5310
A	 0.9830	 0.6190
B	 0.6130	 0.5450
C	 0.8580	 0.5910
D	 0.8660	 0.5960
E	 0.9170	 0.6310
F	 0.8580	 0.5810
G	 0.7770	 0.5510
H	 0.9150	 0.6280
I	 0.8590	 0.5710
J	 0.7740	 0.5370
K	 0.9040	 0.6110
L	 0.9020	 0.6310
M	 0.8370	 0.5720
N	 0.8750	 0.5820
O	 0.9120	 0.6070
P	 0.9190	 0.6200
Q	 0.8800	 0.5990
R	 0.7360	 0.5510
S	 0.8250	 0.5580
T	 0.8950	 0.6050
U	 0.7000	 0.5460
X	 0.6020	 0.4330
Z	 0.8140	 0.5700
a	 0.9850	 0.6510
b	 0.9830	 0.6180
c	 0.9570	 0.6730
d	 0.9460	 0.6610
e	 0.9200	 0.6370
f	 0.8460	 0.5680



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Chain	Atom inclusion	Q-score
g	 0.8540	 0.5650
h	 0.8470	 0.5880
i	 0.9460	 0.6600
j	 0.9330	 0.6580
k	 0.9440	 0.6580
l	 0.9290	 0.6530
m	 0.9710	 0.6680
n	 0.9200	 0.6050
o	 0.9190	 0.6510
p	 0.9740	 0.6750
q	 0.9370	 0.6450
r	 0.9290	 0.6550
s	 0.9130	 0.6220
t	 0.9090	 0.6160
u	 0.9000	 0.6180
v	 0.9180	 0.6610
w	 0.9380	 0.6530
x	 0.8850	 0.6010
y	 0.9150	 0.6370
z	 0.9370	 0.6650