



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 08:27 am BST

PDB ID : 8P16 / pdb_00008p16
EMDB ID : EMD-17346
Title : E167K RF2 on E. coli 70S release complex with UGG (Structure I)
Authors : Pundir, S.; Larsson, D.S.D.; Selmer, M.; Sanyal, S.
Deposited on : 2023-05-11
Resolution : 2.77 Å (reported)
Based on initial models : 1GQE, 7K00, 5MDV, 8B0X

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 : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
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

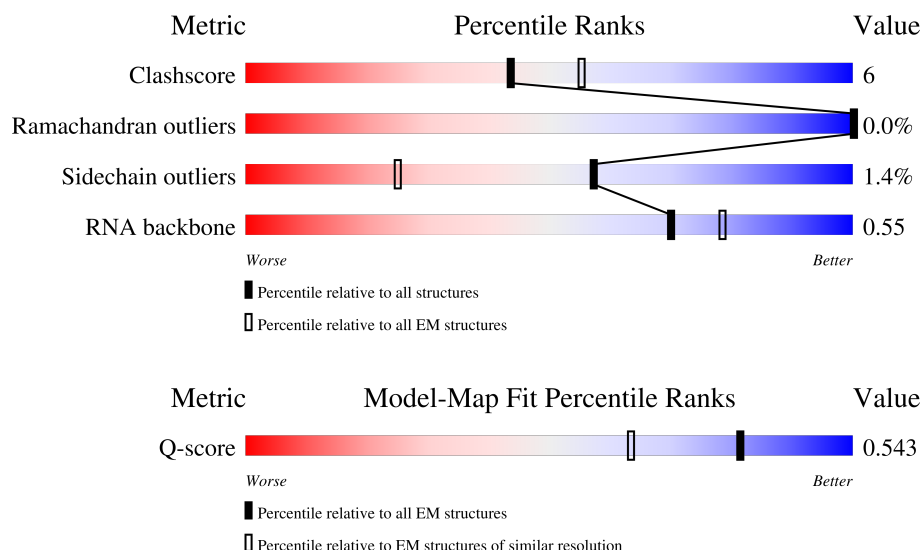
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 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.



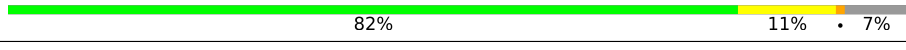
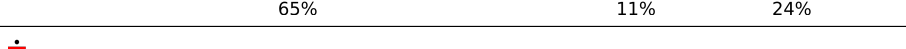
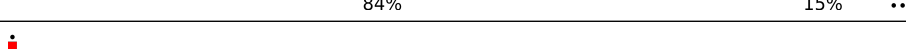
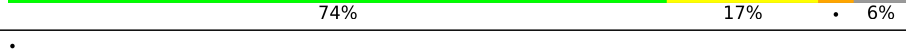
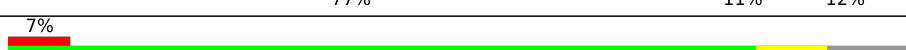
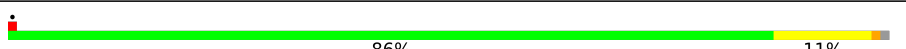
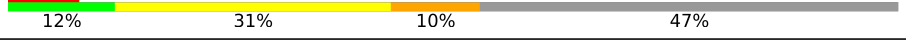
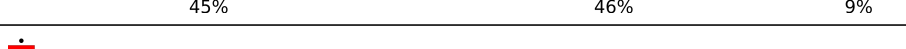
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10695 (2.27 - 3.27)

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	2	1542	
2	g	241	
3	h	233	

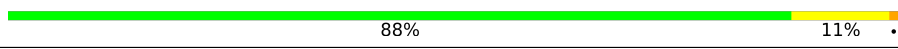
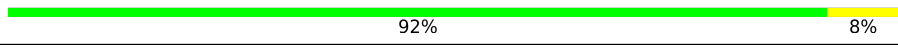
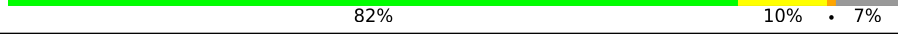
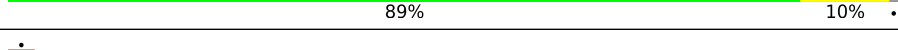
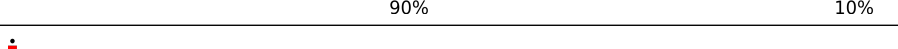
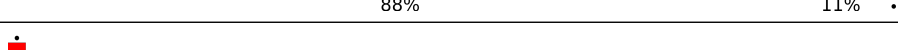
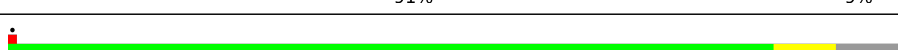
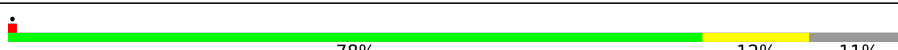
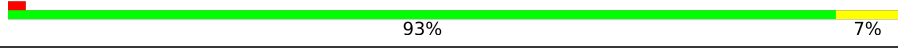
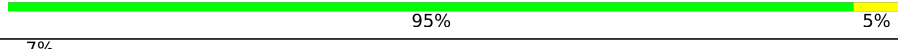
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Mol	Chain	Length	Quality of chain
4	i	206	
5	j	167	
6	k	135	
7	l	179	
8	m	130	
9	n	130	
10	o	103	
11	p	129	
12	q	124	
13	r	118	
14	s	101	
15	t	89	
16	u	82	
17	v	84	
18	w	75	
19	x	92	
20	y	87	
21	z	71	
22	4	49	
23	5	76	
24	1	2904	
25	3	120	
26	B	273	
27	C	209	
28	D	201	

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Mol	Chain	Length	Quality of chain
29	E	179	 83%16%
30	F	177	 85%14%8%
31	J	142	 88%11%
32	K	123	 92%8%
33	L	144	 89%11%
34	M	136	 75%24%
35	N	127	 82%10%7%
36	O	117	 89%10%
37	P	115	 90%10%
38	Q	118	 88%11%
39	R	103	 90%9%
40	S	110	 91%9%
41	T	100	 86%7%7%
42	U	104	 87%11%
43	V	94	 86%13%
44	W	85	 78%12%11%
45	X	78	 82%15%
46	Y	63	 87%10%
47	Z	59	 90%8%
48	b	57	 89%9%
49	c	55	 87%5%7%
50	d	46	 93%7%
51	e	65	 83%15%
52	f	38	 95%5%
53	a	70	 67%16%7%14%

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Mol	Chain	Length	Quality of chain
54	I	142	37%40%7%52%
55	6	365	35%84%14%
56	G	149	68%81%19%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 148578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1536	Total	C	N	O	P	0	0
			32966	14711	6044	10675	1536		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	h	210	Total	C	N	O	S	0	0
			1648	1043	309	292	4		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	p	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	119	IAS	ASN	variant	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4	26	Total	C	N	O	P	0	0
			562	251	104	181	26		

- Molecule 23 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

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

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	82	MS6	MET	variant	UNP P0ADY7

- Molecule 35 is a protein called 50S ribosomal protein L17.

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

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called Large ribosomal subunit protein bL31A.

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

- Molecule 54 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	I	68	Total	C	N	O	S	0	0
			484	298	89	94	3		

- Molecule 55 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	361	Total	C	N	O	S	1	0
			2863	1762	504	587	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	167	LYS	GLU	engineered mutation	UNP P07012

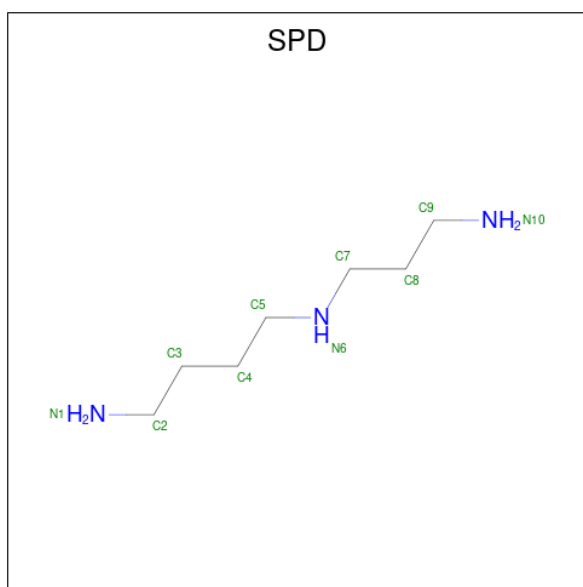
- Molecule 56 is a protein called 50S ribosomal protein L9.

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	2	95	Total	Mg	0
			95	95	
57	s	1	Total	Mg	0
			1	1	
57	5	2	Total	Mg	0
			2	2	
57	1	223	Total	Mg	0
			223	223	
57	3	5	Total	Mg	0
			5	5	
57	B	1	Total	Mg	0
			1	1	
57	C	1	Total	Mg	0
			1	1	
57	Q	1	Total	Mg	0
			1	1	
57	b	1	Total	Mg	0
			1	1	

- Molecule 58 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).

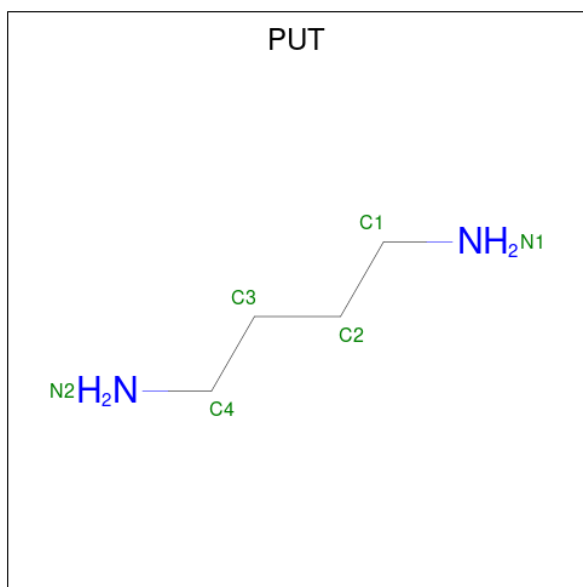


Mol	Chain	Residues	Atoms			AltConf
58	2	1	Total	C	N	0
			10	7	3	
58	2	1	Total	C	N	0
			10	7	3	
58	1	1	Total	C	N	0
			10	7	3	
58	1	1	Total	C	N	0
			10	7	3	
58	1	1	Total	C	N	0
			10	7	3	
58	1	1	Total	C	N	0
			10	7	3	
58	1	1	Total	C	N	0
			10	7	3	
58	1	1	Total	C	N	0
			10	7	3	
58	1	1	Total	C	N	0
			10	7	3	
58	1	1	Total	C	N	0
			10	7	3	

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
59	2	35	Total	K	0
			35	35	
59	1	93	Total	K	0
			93	93	

- Molecule 60 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



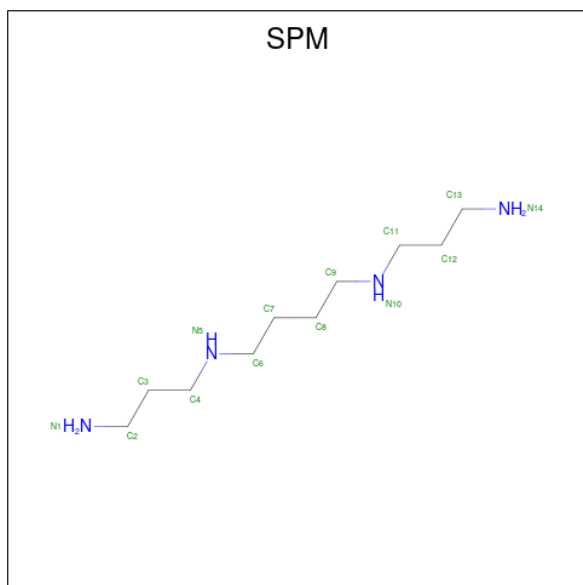
Mol	Chain	Residues	Atoms			AltConf
60	2	1	Total	C	N	0
			6	4	2	
60	2	1	Total	C	N	0
			6	4	2	
60	1	1	Total	C	N	0
			6	4	2	
60	1	1	Total	C	N	0
			6	4	2	
60	1	1	Total	C	N	0
			6	4	2	
60	1	1	Total	C	N	0
			6	4	2	
60	1	1	Total	C	N	0
			6	4	2	
60	1	1	Total	C	N	0
			6	4	2	

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Mol	Chain	Residues	Atoms			AltConf
60	1	1	Total	C	N	0
			6	4	2	
60	1	1	Total	C	N	0
			6	4	2	
60	1	1	Total	C	N	0
			6	4	2	

- Molecule 61 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
61	1	1	Total	C	N	0
			14	10	4	

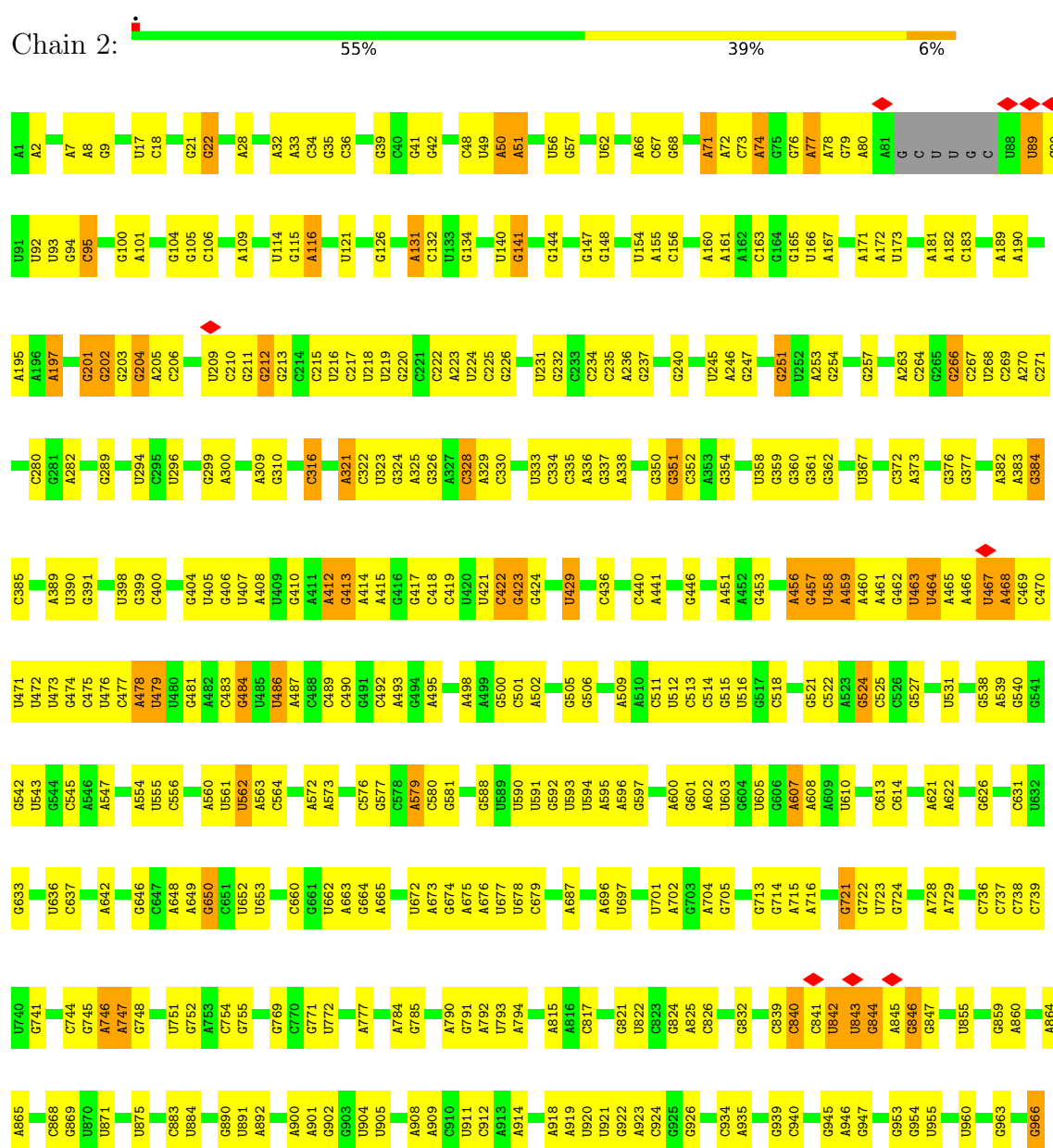
- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

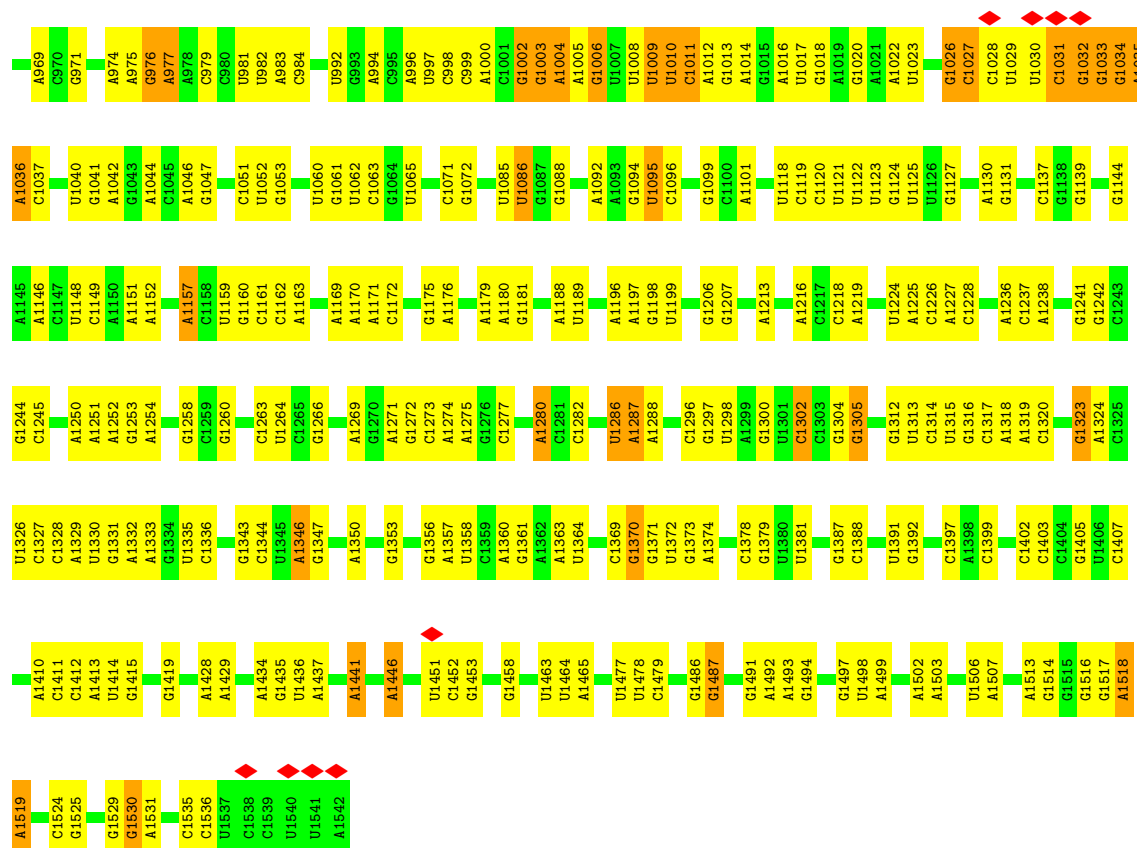
Mol	Chain	Residues	Atoms		AltConf
62	f	1	Total	Zn	0
			1	1	
62	a	1	Total	Zn	0
			1	1	

3 Residue-property plots

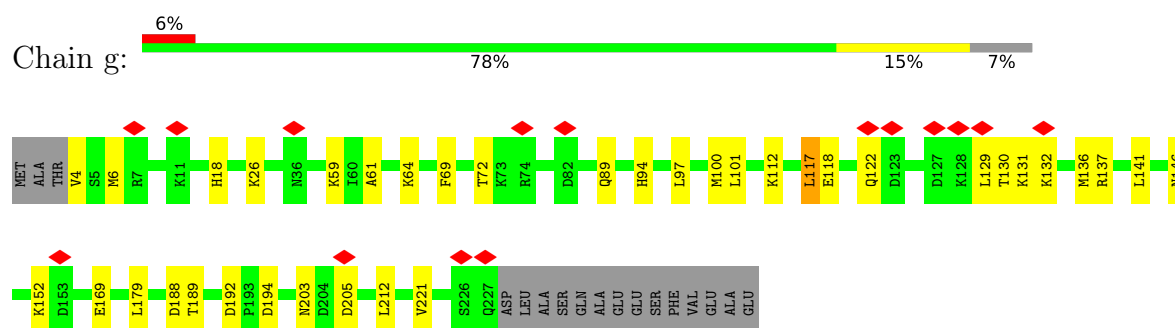
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

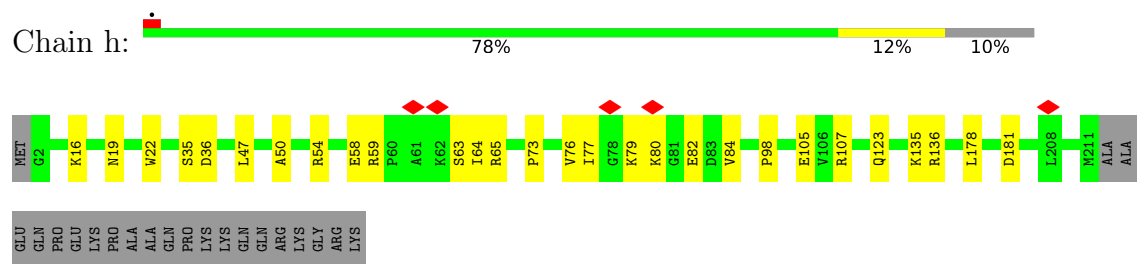




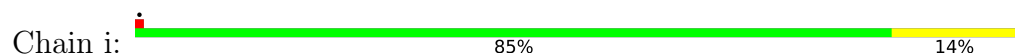
• Molecule 2: Small ribosomal subunit protein uS2

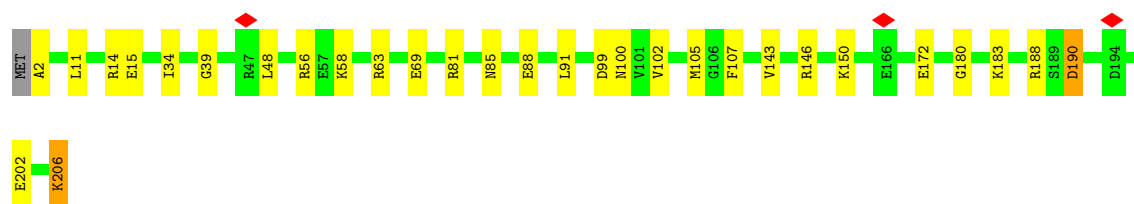


• Molecule 3: Small ribosomal subunit protein uS3



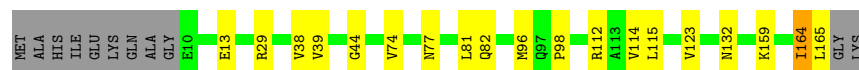
• Molecule 4: Small ribosomal subunit protein uS4





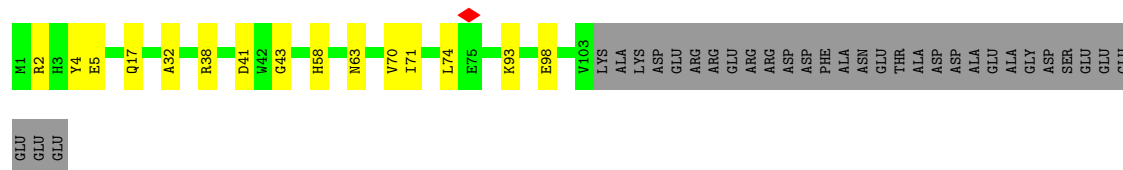
- Molecule 5: Small ribosomal subunit protein uS5

Chain j: 82% 11% 7%



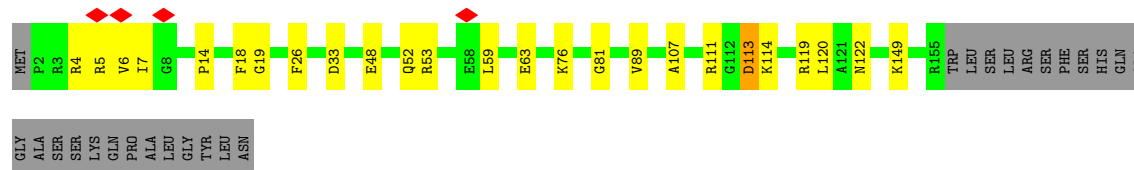
- Molecule 6: 30S ribosomal protein S6

Chain k: 65% 11% 24%



- Molecule 7: 30S ribosomal protein S7

Chain l: 72% 13% 14%



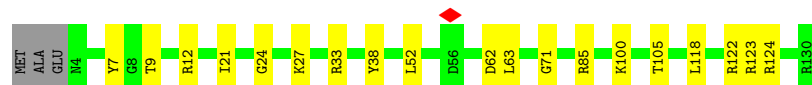
- Molecule 8: Small ribosomal subunit protein uS8

Chain m: 85% 14% 1%

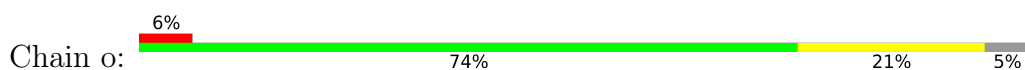


- Molecule 9: Small ribosomal subunit protein uS9

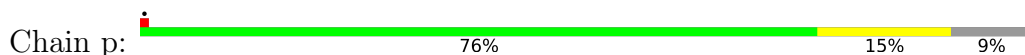
Chain n: 83% 15% 2%



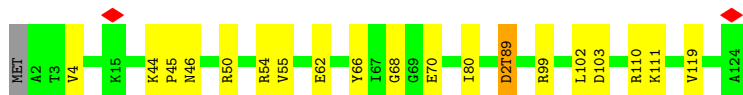
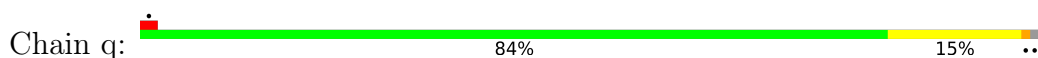
- Molecule 10: Small ribosomal subunit protein uS10



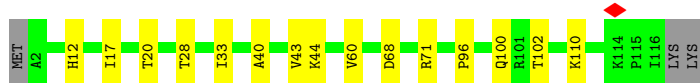
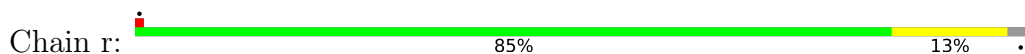
- Molecule 11: Small ribosomal subunit protein uS11



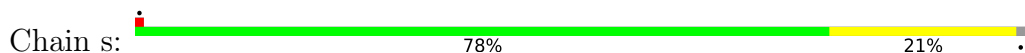
- Molecule 12: Small ribosomal subunit protein uS12



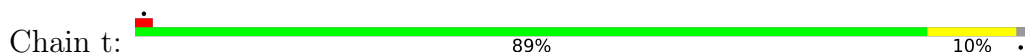
- Molecule 13: Small ribosomal subunit protein uS13



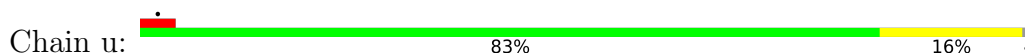
- Molecule 14: Small ribosomal subunit protein uS14



- Molecule 15: Small ribosomal subunit protein uS15

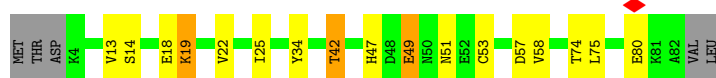


- Molecule 16: Small ribosomal subunit protein bS16

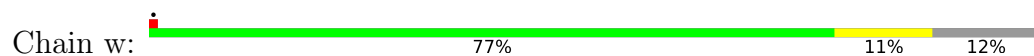




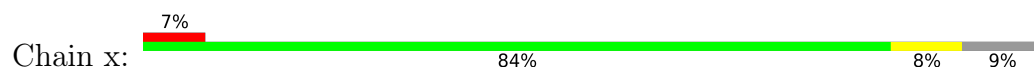
- Molecule 17: Small ribosomal subunit protein uS17



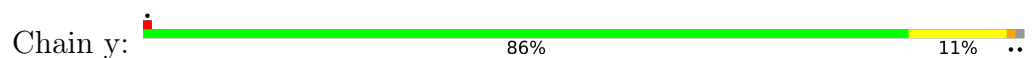
- Molecule 18: Small ribosomal subunit protein bS18



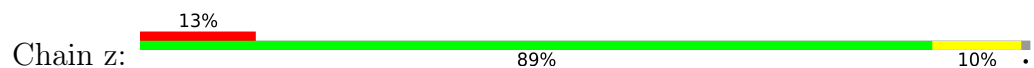
- Molecule 19: Small ribosomal subunit protein uS19



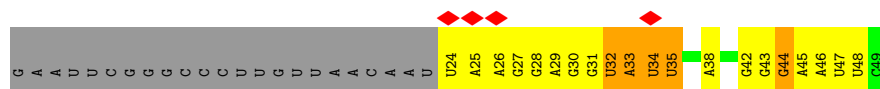
- Molecule 20: Small ribosomal subunit protein bS20



- Molecule 21: Small ribosomal subunit protein bS21



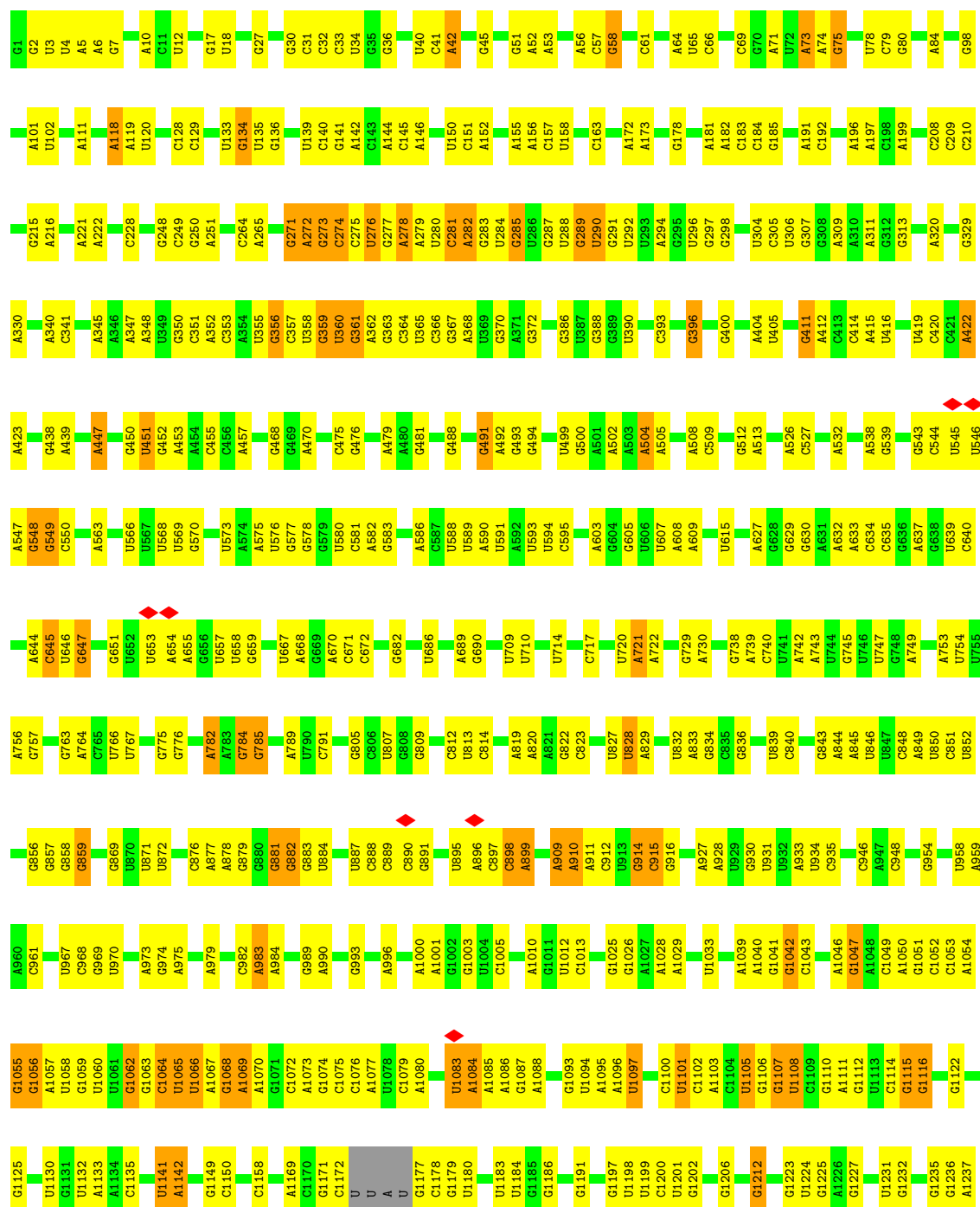
- Molecule 22: mRNA



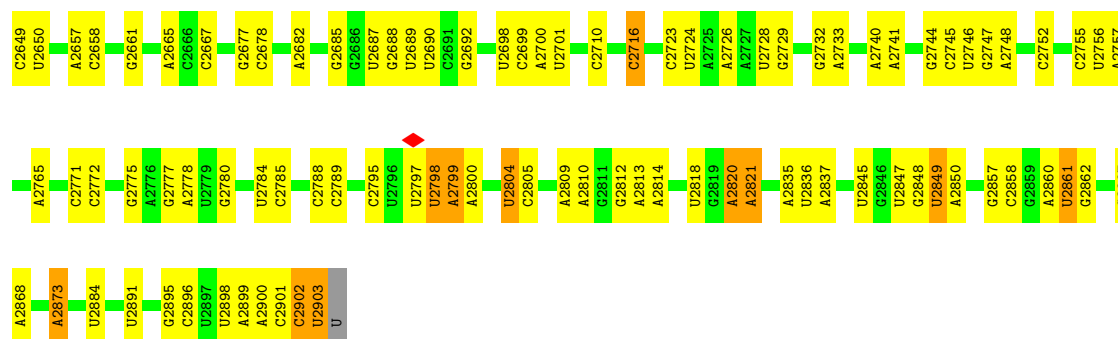
- Molecule 23: tRNA(fMet)



Chain 1: 60% 35% 5%



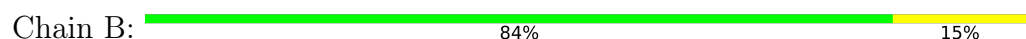
G2535	U2441	G2316	C2226	C2150	U2086	G1992	U1883	C1771	G1645	G1540	G1444	A1354	U1242
G2536	G2447	A2317	A2227	U2151	G2087	U1993	G1884	A1772	C1646	C1541	G1452	G1360	C1243
C2538	A2448	A2322	U2229	G2152	A1889	C1997	A1890	A1773	U1647	U1542	A1453	G1361	
G2543	C2452	G2325	U2233	C2153	G2093	G2012	A1900	U1732	U1648	A1544	C1454	G1362	U1248
G2544	A2453	C2326	G2234	U2154	C2096	A2013	A1786	A1787	A1650	G1546	G1455	G1363	U1249
A2547	A2456	A2327	G2238	U2155	A2097	A2014	U1788	C1788	G1651	C1547	U1458	A1365	G1250
U2548	G2456	U2329	G2239	G2156	U2098	A2015	G1904	U1789	U1789	A1548	U1460	A1370	A1283
U2549	G2457	G2330	G2240	G2157	G2100	G2018	G1905	C1790	A1668	A1549	U1371	G1371	U1285
U2552	U2443	G2331	U2243	U2158	G2102	A2019	G1907	A1791	G1674	U1554	C1463	U1375	G1256
G2553	U2444	G2332	U2244	G2159	C2103	A2020	G1910	A1794	C1675	U1559	G1464	U1376	G1266
U2554	A2461	A2333	U2245	C2160	C2023	G2023	U1911	C1795	A1676	U1560	G1465	A1378	U1267
U2555	C2462	U2334	G2246	C2161	G2024	A2024	A1912	U1796	A1677	U1563	A1469	U1379	A1268
C2556	A2469	A2335	U2247	G2162	U2105	C2025	A1913	G1797	U1682	C1564	A1470	A1383	A1269
G2557	G2470	A2336	C2248	A2163	U2106	U2026	G1914	U1798	U1683	C1565	G1471		C1270
C2558		G2337	U2249	C2164	G2107	G2027	3TD1915	G1799	U1684	A1566	G1475	C1386	A1272
		C2338	G2250	C2165	A2108		A1916	C1800				A1387	U1273
A2566	A2476	C2339	G2251	C2166	U2109	A2030	U1917	C1801	G1703	A1569	G1478	G1388	
G2567	U2477	A2340	U2257	U2167	G2110	A2031	A1918	A1802	C1704	A1570		A1392	C1278
U2568	A2478	G2341	C2258	U2167	G2110	G2032	A1919	A1803		A1571	G1482	A1393	G1279
G2573	G2481	G2345	U2259	G2168	U2111	A2033	C1920		G1710	A1572	G1483	U1394	G1280
G2574	A2482	A2346	A2266	A2169	G2112	C2036	A1928	A1808	A1711		G1484	A1395	G1281
U2580	C2483	C2347	A2267	A2170	U2113	A2037	G1929	A1809	U1712	U1578	U1486		U1282
G2581	G2484	C2350	A2268	A2171	A2114	G2038	G1930	C1816	U1713	A1583	C1493	U1405	G1293
G2582	U2491	U2172	A2273	U2172	G2115	U2039	U1932	U1827	U1714	U1584	A1494	U1406	U1294
G2583		C2173	A2273	A2173	G2116	G2040	A1932	A1828	G1715	C1585	A1496	G1295	C1295
U2584	G2494	G2361	A2274	C2174	A2117	C2043	G1933	A1829	U1716	U1586	A1497	G1407	C1297
U2585	C2495	G2373		C2175	U2118	G2049	A1936	C1830	A1717	U1589	C1498	U1411	
U2586	C2496	C2374	G2279	A2176	G2119	C2050	A1937	G1840	U1720	A1590		A1412	G1300
A2590	A2497	A2381	C2283	C2177	G2120	A2051	U1939	U1841	G1731	A1591	U1506	A1413	A1301
G2591	C2498	G2382	A2284	C2178	A2120	A2052	U1940	G1842	U1729	U1594	C1507	A1414	A1302
G2592	U2500	G2383	C2285	C2179	G2121	A2052	C1941	U1843	C1730	C1595	A1508	U1415	
	C2503	U2384	G2286	U2180	U2122	C2055		C1847	C1732	C1596	G1510	G1416	C1306
G2599	G2502	C2385	A2287	U2181	G2123	G2056	G1945	A1853	A1735	A1597	G1511	A1417	A1307
A2602	A2503	G2400	G2288	U2182	C2124	A2060	U1946	A1854	U1736	A1598	C1512	A1418	
G2603	G2505	U2401	G2289	U2183	G2125	G2061	U1955	U1855	G1737	U1599	U1513	A1419	C1315
U2609	U2506	U2402	U2291	A2184	A2126	A2062	U1956	U1856	G1738	C1600	G1514	A1420	G1316
	C2507		U2292	U2185	G2127	C2063	C1957	G1857	A1739	G1601	A1515	G1421	G1317
U2613	U2514	A2406	A2298	G2186	C2128	C2064	U1963	A1858		U1602	C1526	A1427	U1318
A2614	C2515	A2407	U2299	U2187	U2130	C2065	G1964	C1868	G1743	A1603	G1527	C1428	G1320
U2615	A2516	G2409	C2300	U2189	U2131	A2070	C1965	G1869	A1744	C1607	A1528	G1429	A1321
	C2517	G2410	C2301	G2190	G2132	A2071	A1966	C1870	A1745	A1608	G1529	G1430	A1322
C2626	U2518	U2419	G2304	A2191	G2133	C2072	C1967	A1871	U1747	G1613	G1530	A1431	C1323
U2629	C2520	C2420	C2305	U2192	A2134	C2073	A1970	A1872	C1748	G1631	C1531	A1432	A1327
G2638	G2525	A2425	G2307	U2195	A2135	C2074	U1971	G1873		U1534	C1532	A1433	A1328
A2639			G2308	U2198	G2136	U2075	G1972	C1874	A1754	G1631	C1533	G1435	U1329
G2640	G2529	A2430	U2312	A2199	U2137	U2076	G1984	G1875		U1634	U1535	U1440	G1338
G2641	C2532	A2435	C2313	A2204	G2138	U2077	U1881	U1880	C1760	A1635	A1536	G1441	U1352
C2646	U2533		G2315	A2205	U2139	C2078	U1991	U1882	C1764	U1637	C1537	U1442	A1353
	A2534			C2206	G2140	U2079							
				A2211	G2141								
				G2216	A2142								
				G2217	C2143								
				A2225	G2144								
					C2145								
					C2146								
					A2147								
					G2148								
					U2149								



• Molecule 25: 5S rRNA



• Molecule 26: 50S ribosomal protein L2



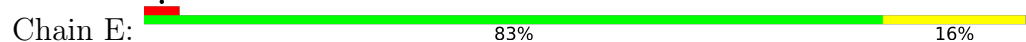
• Molecule 27: 50S ribosomal protein L3

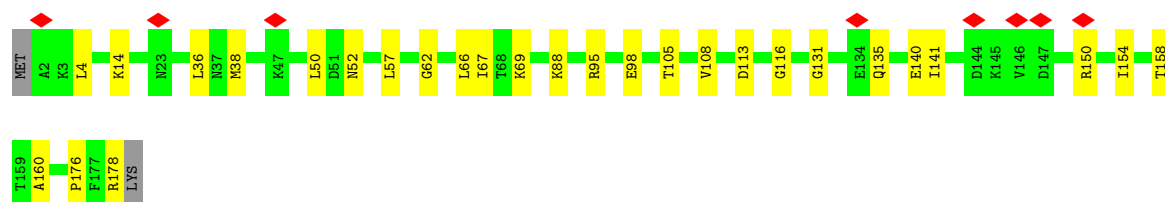


• Molecule 28: 50S ribosomal protein L4

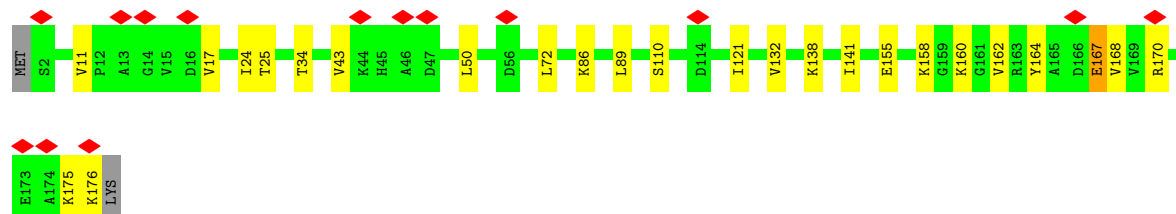
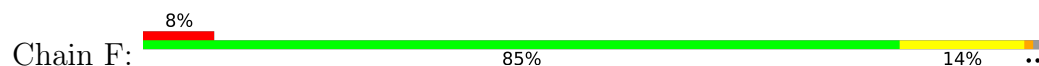


• Molecule 29: 50S ribosomal protein L5

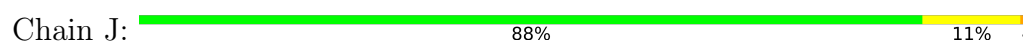




- Molecule 30: 50S ribosomal protein L6



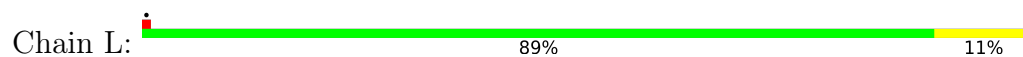
- Molecule 31: 50S ribosomal protein L13



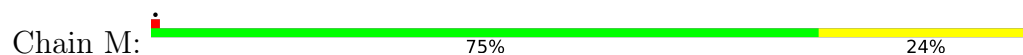
- Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15



- Molecule 34: Large ribosomal subunit protein uL16



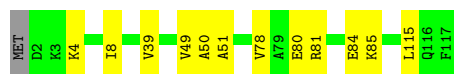
- Molecule 35: 50S ribosomal protein L17

Chain N:  82% 10% 7%



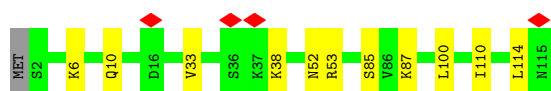
- Molecule 36: 50S ribosomal protein L18

Chain O:  89% 10% 1%



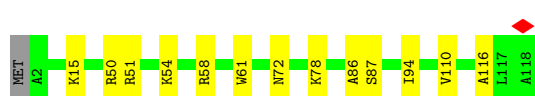
- Molecule 37: 50S ribosomal protein L19

Chain P:  90% 10% 1%



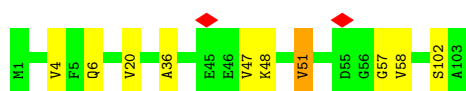
- Molecule 38: 50S ribosomal protein L20

Chain Q:  88% 11% 1%



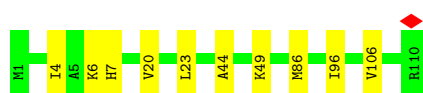
- Molecule 39: 50S ribosomal protein L21

Chain R:  90% 9% 1%



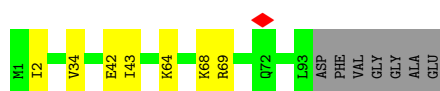
- Molecule 40: 50S ribosomal protein L22

Chain S:  91% 9% 1%



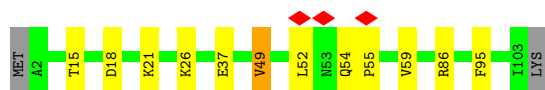
- Molecule 41: 50S ribosomal protein L23

Chain T:  86% 7% 7%



- Molecule 42: 50S ribosomal protein L24

Chain U:  87% 11% ..



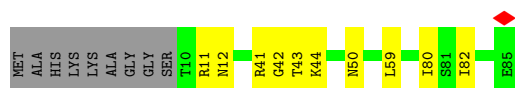
- Molecule 43: 50S ribosomal protein L25

Chain V:  86% 13% .



- Molecule 44: 50S ribosomal protein L27

Chain W:  78% 12% 11%



- Molecule 45: 50S ribosomal protein L28

Chain X:  82% 15% ..



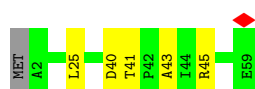
- Molecule 46: 50S ribosomal protein L29

Chain Y:  87% 10% ..



- Molecule 47: 50S ribosomal protein L30

Chain Z:  90% 8% .

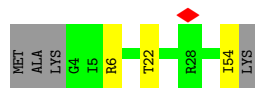
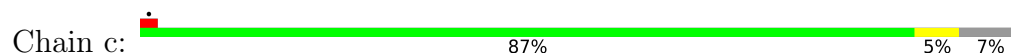


- Molecule 48: 50S ribosomal protein L32

Chain b:  89% 9% .



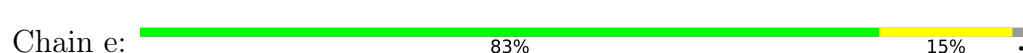
- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34



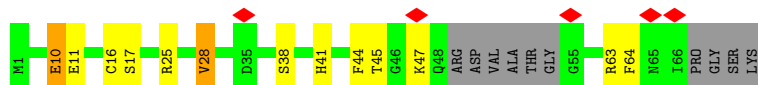
- Molecule 51: 50S ribosomal protein L35



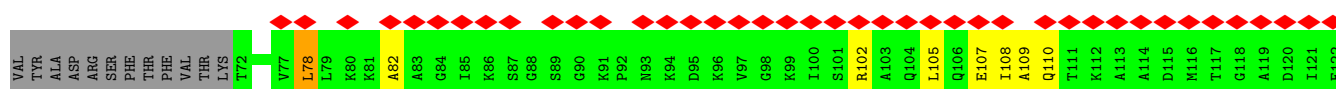
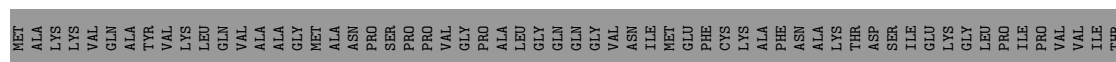
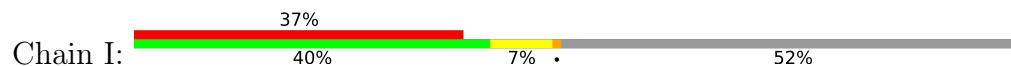
- Molecule 52: 50S ribosomal protein L36

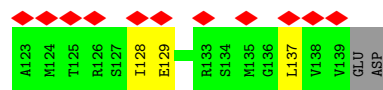


- Molecule 53: Large ribosomal subunit protein bL31A

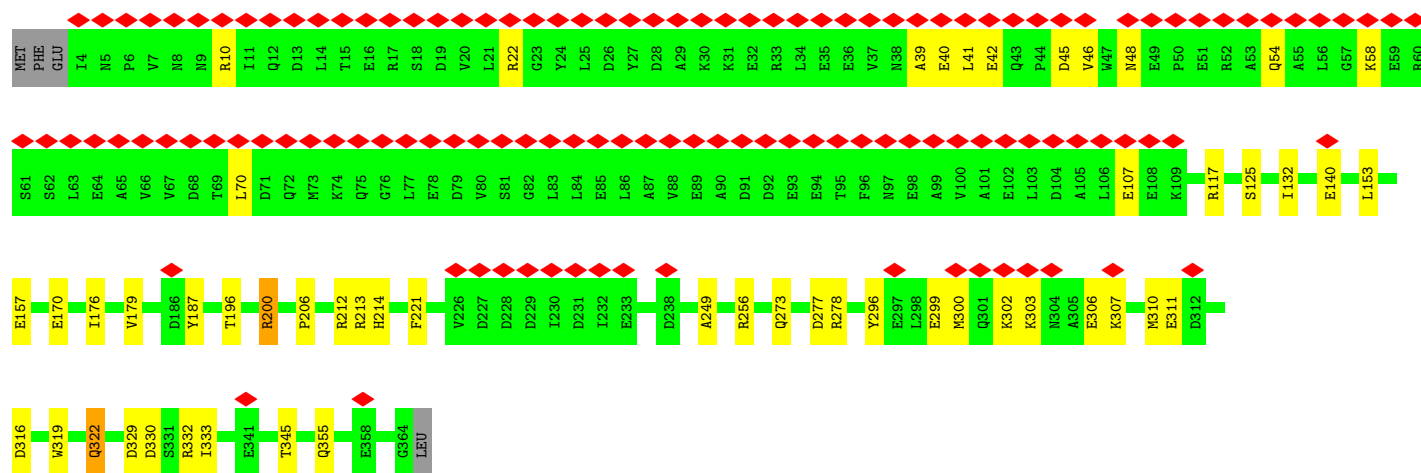
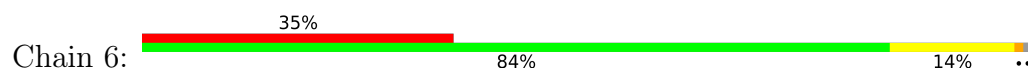


- Molecule 54: 50S ribosomal protein L11

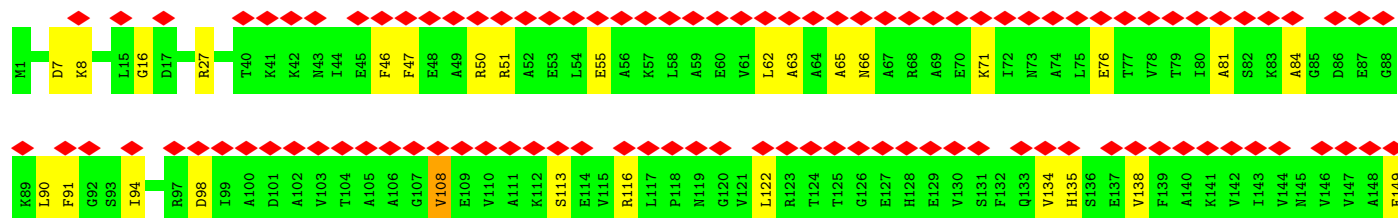
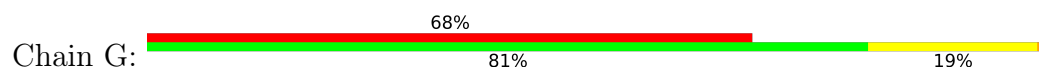




• Molecule 55: Peptide chain release factor RF2



• Molecule 56: 50S ribosomal protein L9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21843	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 ($e^-/\text{\AA}^2$)	38.14	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.263	Depositor
Minimum map value	-0.392	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	433.44598, 433.44598, 433.44598	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83355, 0.83355, 0.83355	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4D4, 1MG, OMC, IAS, 3TD, OMG, ZN, MG, UR3, K, 6MZ, OMU, PSU, H2U, MA6, 4OC, 2MA, G7M, D2T, PUT, MS6, MEQ, 5MU, 2MG, SPM, SPD, 5MC

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	2	0.27	0/36631	0.30	0/57136
2	g	0.18	0/1784	0.31	0/2403
3	h	0.21	0/1675	0.29	0/2256
4	i	0.20	0/1665	0.27	0/2227
5	j	0.23	0/1165	0.32	0/1568
6	k	0.20	0/858	0.29	0/1160
7	l	0.18	0/1230	0.30	0/1649
8	m	0.23	0/989	0.28	0/1326
9	n	0.19	0/1034	0.29	0/1375
10	o	0.21	0/796	0.33	0/1077
11	p	0.20	0/884	0.34	0/1191
12	q	0.23	0/960	0.30	0/1286
13	r	0.18	0/900	0.27	0/1204
14	s	0.20	0/817	0.26	0/1088
15	t	0.20	0/722	0.28	0/964
16	u	0.22	0/653	0.30	0/877
17	v	0.20	0/650	0.30	0/871
18	w	0.21	0/553	0.29	0/742
19	x	0.18	0/685	0.25	0/922
20	y	0.21	0/676	0.27	0/895
21	z	0.20	0/597	0.28	0/792
22	4	0.20	0/630	0.35	0/981
23	5	0.24	0/1813	0.29	0/2825
24	1	0.30	0/69147	0.31	0/107869
25	3	0.24	0/2850	0.26	0/4444
26	B	0.27	0/2121	0.33	0/2852
27	C	0.26	0/1576	0.31	0/2119
28	D	0.24	0/1571	0.31	0/2113
29	E	0.18	0/1434	0.30	0/1926
30	F	0.19	0/1333	0.31	0/1805
31	J	0.24	0/1152	0.27	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	K	0.25	0/955	0.33	0/1279
33	L	0.24	0/1062	0.29	0/1413
34	M	0.25	0/1073	0.30	0/1433
35	N	0.26	0/958	0.33	0/1281
36	O	0.20	0/902	0.31	0/1209
37	P	0.25	0/929	0.30	0/1242
38	Q	0.27	0/960	0.29	0/1278
39	R	0.25	0/829	0.36	0/1107
40	S	0.25	0/864	0.30	0/1156
41	T	0.21	0/744	0.31	0/994
42	U	0.21	0/787	0.33	0/1051
43	V	0.22	0/766	0.33	0/1025
44	W	0.26	0/589	0.32	0/779
45	X	0.26	0/635	0.30	0/848
46	Y	0.19	0/502	0.24	0/667
47	Z	0.23	0/453	0.34	0/605
48	b	0.24	0/450	0.28	0/599
49	c	0.23	0/424	0.30	0/565
50	d	0.27	0/380	0.29	0/498
51	e	0.25	0/513	0.31	0/676
52	f	0.25	0/303	0.30	0/397
53	a	0.15	0/488	0.31	0/649
54	I	0.15	0/486	0.37	0/650
55	6	0.19	0/2895	0.31	0/3899
56	G	0.16	0/1122	0.34	0/1515
All	All	0.27	0/159620	0.30	0/238309

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	32966	0	16606	450	0
2	g	1753	0	1780	19	0
3	h	1648	0	1722	15	0
4	i	1643	0	1707	23	0
5	j	1152	0	1196	14	0
6	k	839	0	833	10	0
7	l	1214	0	1267	17	0
8	m	979	0	1031	13	0
9	n	1022	0	1070	15	0
10	o	786	0	828	13	0
11	p	877	0	884	12	0
12	q	957	0	1017	13	0
13	r	891	0	952	10	0
14	s	805	0	844	15	0
15	t	714	0	734	6	0
16	u	643	0	661	8	0
17	v	641	0	682	9	0
18	w	544	0	565	6	0
19	x	668	0	693	4	0
20	y	670	0	719	7	0
21	z	589	0	629	4	0
22	4	562	0	279	21	0
23	5	1623	0	825	12	0
24	1	62252	0	31311	656	0
25	3	2549	0	1291	25	0
26	B	2082	0	2154	29	0
27	C	1566	0	1618	11	0
28	D	1552	0	1619	12	0
29	E	1410	0	1444	20	0
30	F	1313	0	1358	15	0
31	J	1129	0	1162	13	0
32	K	946	0	1023	6	0
33	L	1053	0	1129	10	0
34	M	1075	0	1145	23	0
35	N	945	0	989	10	0
36	O	892	0	923	6	0
37	P	917	0	962	8	0
38	Q	947	0	1019	9	0
39	R	816	0	839	4	0
40	S	857	0	922	7	0
41	T	738	0	807	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	U	779	0	830	7	0
43	V	753	0	780	10	0
44	W	582	0	599	8	0
45	X	625	0	652	9	0
46	Y	501	0	531	5	0
47	Z	449	0	488	3	0
48	b	444	0	458	4	0
49	c	417	0	451	2	0
50	d	377	0	418	3	0
51	e	504	0	572	6	0
52	f	302	0	340	1	0
53	a	480	0	478	10	0
54	I	484	0	521	6	0
55	6	2863	0	2769	36	0
56	G	1111	0	1148	17	0
57	1	223	0	0	0	0
57	2	95	0	0	0	0
57	3	5	0	0	0	0
57	5	2	0	0	0	0
57	B	1	0	0	0	0
57	C	1	0	0	0	0
57	Q	1	0	0	0	0
57	b	1	0	0	0	0
57	s	1	0	0	0	0
58	1	110	0	209	1	0
58	2	20	0	38	3	0
59	1	93	0	0	0	0
59	2	35	0	0	0	0
60	1	66	0	132	5	0
60	2	12	0	24	2	0
61	1	14	0	26	0	0
62	a	1	0	0	0	0
62	f	1	0	0	0	0
All	All	148578	0	100703	1571	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 6.

All (1571) 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)
24:1:1056:G:H4'	24:1:1086:A:H8	1.37	0.86
24:1:2100:G:H1	24:1:2189:U:H3	1.24	0.86
1:2:1028:C:N4	1:2:1033:G:O6	2.08	0.85
24:1:568:U:H1'	24:1:2030:6MZ:H9C1	1.59	0.83
34:M:77:PRO:HG2	34:M:80:VAL:HG21	1.61	0.81
1:2:673:A:H2'	1:2:674:G:C8	2.17	0.79
1:2:324:G:O2'	58:2:1691:SPD:N10	2.19	0.76
24:1:1105:U:H2'	24:1:1106:G:H8	1.49	0.76
1:2:1009:U:H3	1:2:1020:G:H1	1.32	0.76
29:E:158:THR:HG22	29:E:160:ALA:H	1.50	0.75
24:1:1105:U:H2'	24:1:1106:G:C8	2.21	0.75
24:1:1469:A:H2'	24:1:1470:A:C8	2.21	0.75
24:1:1802:A:H2'	24:1:1803:A:C8	2.22	0.74
4:i:48:LEU:HD21	4:i:56:ARG:HG3	1.68	0.74
26:B:107:PRO:HD2	26:B:110:LEU:HD22	1.70	0.73
1:2:664:G:H22	1:2:741:G:H1	1.36	0.73
4:i:172:GLU:HG3	4:i:183:LYS:HD2	1.70	0.73
16:u:4:ILE:HG12	16:u:21:VAL:HG22	1.71	0.72
24:1:2134:A:N6	24:1:2157:G:O2'	2.22	0.72
43:V:2:PHE:HB2	43:V:61:LEU:HD12	1.71	0.72
3:h:35:SER:OG	3:h:59:ARG:NH2	2.22	0.72
24:1:2133:G:O2'	24:1:2157:G:N2	2.23	0.71
1:2:754:C:OP1	15:t:72:ARG:NH2	2.23	0.71
42:U:26:LYS:HD3	42:U:37:GLU:HB3	1.73	0.71
24:1:1063:G:O2'	24:1:1064:C:O5'	2.07	0.71
24:1:1178:C:H2'	24:1:1179:G:H8	1.56	0.70
3:h:58:GLU:OE1	3:h:65:ARG:NH1	2.24	0.70
26:B:29:PRO:HG2	26:B:34:LEU:HD11	1.74	0.70
30:F:24:ILE:HD11	30:F:43:VAL:HG11	1.73	0.70
1:2:946:A:H2'	1:2:947:G:C8	2.26	0.70
1:2:1297:G:O2'	7:l:114:LYS:NZ	2.20	0.70
24:1:1478:G:H1	24:1:1513:U:H3	1.40	0.70
1:2:1312:G:OP2	53:a:63:ARG:NH2	2.24	0.69
24:1:1069:A:O2'	24:1:1073:A:N6	2.25	0.69
1:2:269:C:H2'	1:2:270:A:C8	2.28	0.69
25:3:1:U:H2'	25:3:2:G:H8	1.57	0.69
24:1:954:G:OP2	34:M:16:ARG:NH1	2.26	0.68
56:G:84:ALA:HB2	56:G:90:LEU:HD23	1.75	0.68
45:X:74:ARG:NH1	45:X:76:GLU:OE2	2.27	0.68
9:n:52:LEU:HD11	9:n:63:LEU:HD11	1.75	0.68
24:1:1058:U:H2'	24:1:1059:G:C8	2.28	0.68
56:G:81:ALA:HB1	56:G:149:GLU:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:l:5:ARG:NH2	7:l:7:ILE:O	2.27	0.68
24:1:1434:A:H2'	24:1:1435:G:C8	2.30	0.67
24:1:2336:A:H61	44:W:43:THR:HG21	1.58	0.67
26:B:120:VAL:HG22	56:G:91:PHE:HB3	1.77	0.67
17:v:19:LYS:HA	17:v:51:ASN:HD21	1.59	0.67
24:1:1102:C:H2'	24:1:1103:A:H8	1.56	0.67
24:1:2304:G:H22	24:1:2312:U:H3	1.41	0.67
24:1:1799:G:OP1	26:B:258:ARG:NH1	2.28	0.66
24:1:1434:A:H2'	24:1:1435:G:H8	1.59	0.66
1:2:999:C:N3	1:2:1042:A:N6	2.43	0.66
24:1:75:G:H22	24:1:111:A:H2	1.43	0.66
24:1:2328:A:H2'	24:1:2329:U:C6	2.30	0.66
25:3:36:C:N4	25:3:49:C:O2	2.29	0.66
24:1:284:U:H2'	24:1:285:G:C8	2.30	0.66
24:1:1796:U:H2'	24:1:1797:G:H8	1.62	0.65
1:2:677:U:H3	1:2:713:G:H22	1.45	0.65
14:s:34:VAL:O	14:s:41:ARG:NH2	2.29	0.65
1:2:405:U:O4	4:i:2:ALA:N	2.29	0.65
24:1:1469:A:H2'	24:1:1470:A:H8	1.61	0.65
3:h:77:ILE:HA	3:h:84:VAL:HG23	1.79	0.65
24:1:1300:G:H4'	24:1:1301:A:H5''	1.79	0.65
36:O:39:VAL:HB	36:O:49:VAL:HG22	1.79	0.64
24:1:1386:C:H2'	24:1:1387:A:C8	2.32	0.64
3:h:73:PRO:HG3	3:h:105:GLU:HG2	1.79	0.64
29:E:98:GLU:OE2	53:a:25:ARG:NH1	2.30	0.64
1:2:842:U:H4'	1:2:846:G:N1	2.11	0.64
24:1:2285:C:OP2	49:c:6:ARG:NH1	2.30	0.64
24:1:5:A:H2'	24:1:6:A:C8	2.33	0.64
24:1:1746:A:H2'	24:1:1747:U:C6	2.33	0.64
45:X:41:GLU:OE1	45:X:44:LYS:NZ	2.31	0.64
22:4:47:U:H5'	22:4:48:U:H5''	1.80	0.64
24:1:1102:C:H2'	24:1:1103:A:C8	2.33	0.63
31:J:125:TYR:OH	31:J:132:HIS:NE2	2.30	0.63
55:6:45:ASP:OD1	55:6:48:ASN:ND2	2.30	0.63
1:2:76:G:H1	1:2:93:U:H3	1.46	0.63
1:2:1027:C:H2'	1:2:1028:C:C6	2.33	0.63
56:G:71:LYS:HE3	56:G:108:VAL:HG13	1.79	0.63
1:2:1086:U:H3	1:2:1099:G:H22	1.45	0.63
34:M:53:MET:HG3	34:M:120:ALA:HB2	1.79	0.63
55:6:200:ARG:HB2	55:6:322:GLN:HB3	1.81	0.63
1:2:492:C:H2'	1:2:493:A:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:o:7:ARG:HD3	10:o:73:LEU:HD11	1.80	0.63
15:t:18:ASP:OD1	15:t:19:ALA:N	2.30	0.63
24:1:2193:G:H2'	24:1:2194:U:C6	2.34	0.62
1:2:310:G:H5''	16:u:31:ARG:HB2	1.80	0.62
1:2:1218:C:H2'	1:2:1219:A:C8	2.34	0.62
13:r:17:ILE:O	13:r:20:THR:OG1	2.17	0.62
24:1:1076:C:H2'	24:1:1077:A:C8	2.34	0.62
1:2:1032:G:H2'	1:2:1033:G:H4'	1.82	0.62
24:1:1941:C:OP2	60:1:3336:PUT:N1	2.32	0.62
25:3:76:G:OP1	43:V:9:ARG:NH1	2.32	0.62
27:C:1:MET:HB3	27:C:205:PRO:HG2	1.80	0.62
24:1:1084:A:H2'	24:1:1085:A:C8	2.35	0.62
1:2:1152:A:OP1	10:o:70:HIS:ND1	2.30	0.62
3:h:16:LYS:NZ	3:h:181:ASP:OD1	2.31	0.62
24:1:172:A:H2'	24:1:173:A:C8	2.34	0.62
24:1:848:C:H2'	24:1:849:A:H8	1.64	0.62
2:g:18:HIS:NE2	2:g:205:ASP:OD2	2.33	0.61
33:L:108:ALA:HB3	33:L:125:LEU:HD22	1.81	0.61
2:g:26:LYS:NZ	2:g:194:ASP:OD2	2.27	0.61
1:2:269:C:H2'	1:2:270:A:H8	1.64	0.61
1:2:147:G:H2'	1:2:148:G:C8	2.36	0.61
24:1:320:A:N3	28:D:163:ASN:ND2	2.49	0.61
24:1:1386:C:H2'	24:1:1387:A:H8	1.66	0.61
35:N:72:ASP:N	35:N:72:ASP:OD1	2.34	0.61
53:a:41:HIS:HB3	53:a:44:PHE:HD2	1.66	0.61
25:3:1:U:H2'	25:3:2:G:C8	2.36	0.61
1:2:1323:G:H2'	1:2:1324:A:C8	2.35	0.61
55:6:39:ALA:O	55:6:42:GLU:HG3	2.00	0.61
7:l:113:ASP:OD2	7:l:122:ASN:ND2	2.32	0.61
21:z:31:GLU:OE2	21:z:34:ARG:NH2	2.33	0.61
24:1:172:A:H2'	24:1:173:A:H8	1.65	0.61
1:2:662:U:H2'	1:2:663:A:C8	2.36	0.60
1:2:714:G:H2'	1:2:715:A:C8	2.36	0.60
1:2:1266:G:N2	1:2:1269:A:OP2	2.31	0.60
5:j:115:LEU:HD13	5:j:123:VAL:HG11	1.83	0.60
23:5:18:G:H21	23:5:58:A:H5'	1.65	0.60
1:2:475:C:H2'	1:2:476:U:C6	2.36	0.60
24:1:848:C:H2'	24:1:849:A:C8	2.36	0.60
24:1:1028:A:H2'	24:1:1029:A:C8	2.36	0.60
1:2:843:U:H3'	1:2:844:G:H5''	1.82	0.60
3:h:36:ASP:OD1	3:h:59:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1356:G:H2'	1:2:1357:A:C8	2.36	0.60
24:1:832:U:H2'	24:1:833:A:C8	2.35	0.60
24:1:2305:U:H5''	29:E:131:GLY:HA3	1.82	0.60
1:2:555:U:H2'	1:2:556:C:C6	2.36	0.60
1:2:1347:G:O6	9:n:12:ARG:NH2	2.34	0.60
24:1:2529:G:H4'	30:F:175:LYS:HG2	1.83	0.60
26:B:5:LYS:HD2	26:B:17:VAL:HG22	1.84	0.60
55:6:41:LEU:HA	55:6:46:VAL:HG11	1.82	0.60
4:i:202:GLU:OE1	5:j:112:ARG:NH1	2.34	0.60
24:1:494:G:H4'	40:S:6:LYS:HB2	1.84	0.60
1:2:466:A:H2'	1:2:468:A:C8	2.36	0.60
19:x:50:ALA:HB1	19:x:57:HIS:HB3	1.84	0.60
19:x:35:SER:OG	19:x:38:SER:OG	2.18	0.59
24:1:1590:A:H2'	24:1:1591:A:C8	2.37	0.59
1:2:219:U:H2'	1:2:220:G:H8	1.66	0.59
56:G:113:SER:O	56:G:116:ARG:NH1	2.31	0.59
1:2:842:U:H3'	1:2:843:U:H5''	1.84	0.59
17:v:18:GLU:O	17:v:51:ASN:ND2	2.35	0.59
24:1:639:U:H2'	24:1:640:C:C6	2.36	0.59
24:1:833:A:H2'	24:1:834:G:C8	2.37	0.59
1:2:1391:U:H2'	1:2:1392:G:C8	2.38	0.59
5:j:13:GLU:HG2	5:j:39:VAL:HG12	1.84	0.59
24:1:2327:A:H2'	24:1:2328:A:C8	2.38	0.59
24:1:2547:A:H2'	24:1:2548:U:C6	2.38	0.59
1:2:337:G:H2'	1:2:338:A:C8	2.38	0.59
24:1:272:A:H2'	24:1:273:G:C8	2.37	0.59
24:1:1083:U:O2'	24:1:1085:A:OP2	2.15	0.59
24:1:1720:U:H2'	24:1:1721:G:O4'	2.02	0.59
1:2:946:A:H2'	1:2:947:G:H8	1.65	0.59
43:V:4:ILE:HG12	43:V:50:MET:HE1	1.84	0.59
1:2:1031:C:O2'	1:2:1032:G:N2	2.35	0.59
30:F:89:LEU:HG	30:F:162:VAL:HG22	1.85	0.59
1:2:746:A:H2'	1:2:747:A:C8	2.37	0.59
1:2:1119:C:OP1	9:n:85:ARG:NH2	2.36	0.59
24:1:191:A:H2'	24:1:192:C:C6	2.38	0.59
24:1:356:G:H2'	24:1:357:C:C6	2.37	0.59
9:n:118:LEU:HD22	9:n:124:ARG:HG2	1.84	0.58
24:1:84:A:N1	24:1:98:G:O2'	2.34	0.58
24:1:832:U:H2'	24:1:833:A:H8	1.68	0.58
24:1:2243:U:H2'	24:1:2244:U:C6	2.37	0.58
1:2:842:U:H2'	1:2:844:G:H5'	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:93:U:H2'	1:2:95:C:C5	2.38	0.58
47:Z:41:THR:HG22	47:Z:43:ALA:H	1.68	0.58
12:q:68:GLY:O	12:q:99:ARG:NH1	2.35	0.58
1:2:843:U:H5	1:2:844:G:C4	2.22	0.58
24:1:549:G:H2'	24:1:550:C:C6	2.39	0.58
24:1:1365:A:OP1	45:X:3:ARG:NH1	2.35	0.58
34:M:66:ARG:NH1	34:M:104:GLU:OE2	2.36	0.58
1:2:93:U:H2'	1:2:95:C:H5	1.67	0.58
1:2:171:A:H2'	1:2:172:A:C8	2.38	0.58
1:2:1004:A:H2'	1:2:1005:A:O4'	2.04	0.58
12:q:110:ARG:HB3	12:q:119:VAL:HG21	1.84	0.58
54:I:105:LEU:HD13	54:I:129:GLU:HG2	1.85	0.58
7:l:113:ASP:HB2	7:l:119:ARG:HG3	1.85	0.58
24:1:1064:C:O2'	24:1:1065:U:H5'	2.03	0.58
24:1:1747:U:H2'	24:1:1748:C:C6	2.39	0.58
1:2:476:U:H2'	1:2:477:C:C6	2.38	0.58
24:1:1052:C:H2'	24:1:1053:C:C6	2.39	0.57
1:2:21:G:H2'	1:2:22:G:C8	2.39	0.57
1:2:316:C:H5'	60:2:1732:PUT:H32	1.87	0.57
24:1:2162:G:OP2	24:1:2164:C:N4	2.36	0.57
1:2:390:U:H2'	1:2:391:G:C8	2.38	0.57
1:2:475:C:H2'	1:2:476:U:H6	1.69	0.57
1:2:524:G:H2'	1:2:525:C:C6	2.39	0.57
1:2:1011:C:H2'	1:2:1012:A:C8	2.40	0.57
1:2:1071:C:H2'	1:2:1072:G:H8	1.69	0.57
5:j:164:ILE:O	8:m:114:ARG:NH2	2.37	0.57
22:4:29:A:H2'	22:4:30:G:H8	1.68	0.57
24:1:2193:G:H2'	24:1:2194:U:H6	1.68	0.57
1:2:613:C:OP1	4:i:81:ARG:NH1	2.34	0.57
1:2:673:A:H2'	1:2:674:G:H8	1.67	0.57
24:1:1084:A:N3	24:1:1105:U:O2'	2.31	0.57
24:1:1796:U:H2'	24:1:1797:G:C8	2.39	0.57
24:1:2329:U:H2'	24:1:2330:G:C8	2.38	0.57
33:L:57:LEU:HD22	51:e:54:ASP:HB3	1.86	0.57
24:1:1794:A:H2'	24:1:1795:C:C6	2.40	0.57
24:1:2514:U:H2'	24:1:2515:C:C6	2.39	0.57
1:2:17:U:H2'	1:2:18:C:C6	2.39	0.57
12:q:55:VAL:HG21	12:q:80:ILE:HD11	1.86	0.57
24:1:1301:A:O2'	24:1:1302:A:H3'	2.04	0.57
24:1:155:A:H2'	24:1:156:A:C8	2.39	0.57
24:1:2086:U:H2'	24:1:2087:G:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:k:41:ASP:OD1	6:k:58:HIS:NE2	2.34	0.57
38:Q:86:ALA:HB2	38:Q:116:ALA:HB2	1.87	0.57
15:t:17:ARG:NH1	15:t:26:GLU:OE1	2.38	0.56
1:2:1535:C:H2'	1:2:1536:C:C6	2.39	0.56
24:1:447:A:O2'	58:1:3212:SPD:H82	2.05	0.56
24:1:1000:A:H2'	24:1:1001:A:C8	2.39	0.56
29:E:116:GLY:HA3	29:E:178:ARG:HB3	1.88	0.56
1:2:56:U:H2'	1:2:57:G:C8	2.40	0.56
1:2:126:G:OP1	1:2:605:U:O2'	2.18	0.56
1:2:473:U:H2'	1:2:474:G:H8	1.69	0.56
24:1:5:A:H2'	24:1:6:A:H8	1.68	0.56
24:1:351:C:H2'	24:1:352:A:C8	2.40	0.56
24:1:414:C:H2'	24:1:415:A:C8	2.41	0.56
26:B:71:LYS:O	26:B:118:SER:OG	2.23	0.56
26:B:200:HIS:CE1	26:B:203:ARG:HH21	2.23	0.56
42:U:18:ASP:HB3	42:U:21:LYS:HD2	1.86	0.56
56:G:7:ASP:OD1	56:G:8:LYS:N	2.33	0.56
1:2:696:A:H2'	1:2:697:U:H6	1.70	0.56
24:1:475:C:O2	24:1:479:A:N6	2.31	0.56
24:1:1177:G:H2'	24:1:1178:C:C6	2.40	0.56
1:2:201:G:H1	1:2:216:U:H3	1.52	0.56
6:k:17:GLN:N	6:k:17:GLN:OE1	2.39	0.56
23:5:21:A:H61	23:5:46:G:H2'	1.71	0.56
24:1:2646:C:OP2	24:1:2732:G:O2'	2.24	0.56
29:E:52:ASN:HB2	29:E:150:ARG:HH22	1.71	0.56
1:2:1130:A:H2'	1:2:1131:G:H8	1.70	0.56
24:1:608:A:H2'	24:1:609:A:C8	2.41	0.56
24:1:839:U:H1'	24:1:1191:G:H1'	1.88	0.56
24:1:910:A:H2'	24:1:911:A:C8	2.40	0.56
24:1:1197:G:H2'	24:1:1198:U:H6	1.71	0.56
1:2:235:C:H2'	1:2:236:A:C8	2.41	0.56
1:2:1314:C:H2'	1:2:1315:U:C6	2.41	0.55
1:2:1530:G:H2'	1:2:1531:A:C8	2.41	0.55
24:1:1799:G:O2'	26:B:180:GLU:OE2	2.17	0.55
55:6:307:LYS:O	55:6:311:GLU:HG2	2.06	0.55
24:1:151:C:H2'	24:1:152:A:H8	1.71	0.55
24:1:1086:A:H4'	24:1:1103:A:C2	2.41	0.55
29:E:62:GLY:O	29:E:95:ARG:NH2	2.35	0.55
1:2:501:C:H2'	1:2:502:A:C8	2.41	0.55
1:2:1287:A:H2'	1:2:1288:A:C8	2.42	0.55
1:2:1463:U:H2'	1:2:1464:U:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:29:A:H2'	22:4:30:G:C8	2.41	0.55
24:1:1645:G:H5''	24:1:1646:C:H5'	1.88	0.55
24:1:1682:G:H2'	24:1:1683:U:C6	2.41	0.55
24:1:2096:C:H2'	24:1:2097:A:C8	2.42	0.55
2:g:69:PHE:HE1	2:g:89:GLN:HB2	1.72	0.55
24:1:887:U:O2'	24:1:889:C:OP2	2.20	0.55
32:K:7:MET:HE1	32:K:44:LYS:HG3	1.89	0.55
24:1:155:A:H2'	24:1:156:A:H8	1.70	0.55
1:2:840:C:N3	1:2:842:U:H5'	2.21	0.55
8:m:11:LEU:HD22	8:m:75:ILE:HD11	1.89	0.55
26:B:120:VAL:CG2	56:G:91:PHE:HB3	2.37	0.55
1:2:458:U:H2'	1:2:459:A:C8	2.42	0.55
24:1:594:U:H2'	24:1:595:C:C6	2.41	0.55
24:1:1062:G:H2'	24:1:1063:G:C8	2.41	0.55
24:1:1432:G:H2'	24:1:1433:A:C8	2.41	0.55
24:1:1913:A:H4'	24:1:1914:C:H5''	1.89	0.55
40:S:4:ILE:HG12	40:S:106:VAL:HG22	1.88	0.55
1:2:1314:C:H2'	1:2:1315:U:H6	1.72	0.55
24:1:581:C:H2'	24:1:582:A:C8	2.41	0.55
24:1:1178:C:H2'	24:1:1179:G:C8	2.38	0.55
1:2:28:A:O2'	1:2:296:U:OP1	2.22	0.55
24:1:249:C:O2	51:e:12:LYS:NZ	2.37	0.55
9:n:21:ILE:HG12	9:n:63:LEU:HD22	1.88	0.55
24:1:504:A:N3	24:1:504:A:H2'	2.21	0.55
24:1:1086:A:H4'	24:1:1103:A:H2	1.72	0.55
24:1:1475:G:O2'	24:1:1514:G:O6	2.25	0.55
24:1:2849:U:H4'	24:1:2868:A:C2	2.42	0.55
2:g:4:VAL:HG21	2:g:212:LEU:HD21	1.89	0.54
4:i:91:LEU:HD12	4:i:188:ARG:HD3	1.89	0.54
24:1:2014:A:H2'	24:1:2015:A:C8	2.43	0.54
24:1:2199:A:N1	24:1:2226:C:N4	2.55	0.54
24:1:2246:G:H2'	24:1:2247:A:C8	2.42	0.54
16:u:40:ASN:HB3	16:u:43:ALA:HB2	1.89	0.54
1:2:299:G:H2'	1:2:300:A:C8	2.42	0.54
1:2:501:C:H2'	1:2:502:A:H8	1.72	0.54
12:q:46:ASN:ND2	12:q:89:D2T:SB	2.80	0.54
20:y:59:ASP:OD1	20:y:76:LYS:NZ	2.40	0.54
24:1:210:C:OP1	50:d:29:GLN:NE2	2.40	0.54
24:1:742:A:H2'	24:1:743:A:C8	2.42	0.54
24:1:930:G:H1'	47:Z:25:LEU:HD11	1.88	0.54
7:l:59:LEU:O	7:l:63:GLU:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:1405:U:H2'	24:1:1406:U:C6	2.42	0.54
56:G:46:PHE:CZ	56:G:50:ARG:HD3	2.42	0.54
1:2:235:C:H2'	1:2:236:A:H8	1.72	0.54
1:2:745:G:H2'	1:2:746:A:C8	2.43	0.54
3:h:63:SER:OG	3:h:98:PRO:O	2.22	0.54
24:1:2420:C:OP1	51:e:34:THR:OG1	2.23	0.54
1:2:92:U:H2'	1:2:93:U:C6	2.42	0.54
24:1:357:C:H2'	24:1:358:U:C6	2.42	0.54
24:1:993:G:OP2	38:Q:51:ARG:NH2	2.38	0.54
24:1:1443:U:H2'	24:1:1444:G:H8	1.72	0.54
1:2:713:G:H2'	1:2:714:G:C8	2.43	0.54
1:2:1516:2MG:N2	1:2:1519:MA6:OP2	2.40	0.54
24:1:1083:U:O2'	24:1:1084:A:O5'	2.26	0.54
24:1:2537:U:H2'	24:1:2538:C:C6	2.43	0.54
1:2:376:G:H5''	16:u:5:ARG:HB2	1.90	0.54
24:1:1067:A:N1	55:6:54:GLN:HG2	2.23	0.54
24:1:2159:G:H2'	24:1:2160:C:C6	2.43	0.54
24:1:2557:G:H2'	24:1:2558:C:C6	2.43	0.54
24:1:2115:G:O2'	24:1:2117:A:N6	2.41	0.53
28:D:7:ASP:N	28:D:7:ASP:OD1	2.40	0.53
1:2:384:G:H2'	1:2:385:C:C6	2.44	0.53
12:q:4:VAL:HG23	17:v:34:TYR:HB3	1.90	0.53
25:3:66:A:H61	25:3:107:G:H2'	1.73	0.53
55:6:200:ARG:NE	55:6:322:GLN:OE1	2.41	0.53
1:2:539:A:H2'	1:2:540:G:C8	2.43	0.53
11:p:67:ALA:HB2	11:p:96:THR:HG23	1.90	0.53
22:4:42:G:H22	55:6:140:GLU:HG2	1.73	0.53
24:1:849:A:H2'	24:1:850:U:C6	2.44	0.53
24:1:1429:G:H2'	24:1:1430:G:H8	1.73	0.53
24:1:2233:U:H2'	24:1:2234:G:C8	2.43	0.53
24:1:2728:U:HO2'	24:1:2729:G:H8	1.55	0.53
1:2:868:C:H2'	1:2:869:G:O4'	2.08	0.53
1:2:1513:A:H2'	1:2:1514:G:C8	2.43	0.53
2:g:72:THR:OG1	2:g:169:GLU:OE2	2.17	0.53
24:1:1744:A:H3'	24:1:1745:A:H8	1.73	0.53
24:1:1794:A:H2'	24:1:1795:C:H6	1.73	0.53
1:2:463:U:H2'	1:2:464:U:C6	2.44	0.53
1:2:660:C:O2	1:2:745:G:N2	2.20	0.53
11:p:17:SER:HA	11:p:79:ILE:HA	1.90	0.53
24:1:2:G:H2'	24:1:3:U:C6	2.44	0.53
24:1:1248:G:OP1	28:D:44:ARG:NH1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:1494:A:H2'	24:1:1495:A:C8	2.44	0.53
24:1:2176:A:H2'	24:1:2177:C:C6	2.43	0.53
55:6:333:ILE:HG13	55:6:345:THR:HG22	1.91	0.53
24:1:52:A:H2'	24:1:53:A:C8	2.43	0.53
24:1:807:U:OP2	33:L:41:ARG:NH2	2.42	0.53
53:a:11:GLU:HA	53:a:25:ARG:HA	1.90	0.53
1:2:472:U:H2'	1:2:473:U:C6	2.43	0.53
12:q:70:GLU:N	12:q:70:GLU:OE1	2.42	0.53
24:1:709:U:H2'	24:1:710:U:C6	2.43	0.53
24:1:813:U:H2'	24:1:814:C:C6	2.44	0.53
24:1:1589:U:H2'	24:1:1590:A:H8	1.73	0.53
1:2:206:C:H42	1:2:213:G:H22	1.57	0.53
1:2:977:A:O2'	1:2:979:C:OP2	2.23	0.53
24:1:2602:A:C5	55:6:278:ARG:HG2	2.44	0.53
24:1:2901:C:H2'	24:1:2902:C:C6	2.44	0.53
5:j:164:ILE:HG22	5:j:165:LEU:HG	1.91	0.53
24:1:191:A:H2'	24:1:192:C:H6	1.74	0.53
24:1:2064:C:H2'	24:1:2065:C:C6	2.44	0.53
26:B:153:GLN:HA	26:B:156:ARG:HD3	1.91	0.53
29:E:140:GLU:HG3	53:a:28:VAL:HG12	1.90	0.53
39:R:36:ALA:HA	39:R:58:VAL:HG23	1.91	0.53
55:6:330:ASP:OD2	55:6:332:ARG:NH1	2.41	0.53
1:2:476:U:H2'	1:2:477:C:H6	1.73	0.52
24:1:1808:A:H3'	24:1:1809:A:C8	2.44	0.52
1:2:166:U:H2'	1:2:167:A:C8	2.44	0.52
1:2:660:C:N3	1:2:745:G:N1	2.37	0.52
52:f:16:ILE:HD13	52:f:25:VAL:HG22	1.90	0.52
1:2:1346:A:OP1	9:n:122:ARG:NH1	2.35	0.52
24:1:871:U:H2'	24:1:872:U:C6	2.45	0.52
11:p:87:LYS:HB2	11:p:113:VAL:HG23	1.91	0.52
24:1:281:C:H2'	24:1:282:A:C8	2.44	0.52
24:1:2483:C:N3	34:M:123:LYS:NZ	2.56	0.52
1:2:701:U:OP1	1:2:702:A:O2'	2.18	0.52
24:1:576:U:H2'	24:1:577:G:C8	2.44	0.52
1:2:1273:C:H2'	1:2:1274:A:O4'	2.10	0.52
1:2:1477:U:H2'	1:2:1478:U:C6	2.45	0.52
24:1:581:C:H2'	24:1:582:A:H8	1.73	0.52
24:1:1394:U:H2'	24:1:1395:A:O4'	2.10	0.52
24:1:2191:A:H2'	24:1:2192:U:C6	2.45	0.52
1:2:166:U:H2'	1:2:167:A:H8	1.73	0.52
7:l:113:ASP:N	7:l:113:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:p:85:MET:HE3	11:p:113:VAL:HG11	1.92	0.52
24:1:2692:G:H1'	24:1:2847:U:H1'	1.92	0.52
1:2:212:G:C4	1:2:213:G:C8	2.98	0.52
1:2:390:U:H2'	1:2:391:G:H8	1.75	0.52
24:1:288:U:H2'	24:1:289:G:C8	2.45	0.52
24:1:1059:G:H2'	24:1:1060:U:C5	2.45	0.52
24:1:1417:C:HO2'	24:1:1587:G:HO2'	1.43	0.52
24:1:2532:G:O2'	24:1:2657:A:N1	2.42	0.52
34:M:136:MET:HG2	43:V:77:VAL:HG12	1.91	0.52
1:2:1062:U:H2'	1:2:1063:C:C6	2.43	0.52
17:v:25:ILE:HB	17:v:42:THR:HG23	1.92	0.52
24:1:488:G:H1'	24:1:492:A:N6	2.25	0.52
24:1:1056:G:H4'	24:1:1086:A:C8	2.29	0.52
1:2:376:G:H2'	1:2:377:G:H8	1.74	0.52
8:m:77:ARG:NH1	8:m:79:SER:O	2.43	0.52
1:2:486:U:H2'	1:2:487:A:H8	1.73	0.51
1:2:1011:C:H2'	1:2:1012:A:H8	1.74	0.51
24:1:64:A:H2'	24:1:65:U:C6	2.45	0.51
24:1:306:U:H2'	24:1:307:G:O4'	2.10	0.51
24:1:629:G:N3	24:1:639:U:O2'	2.43	0.51
24:1:645:C:H2'	24:1:647:G:C8	2.45	0.51
24:1:849:A:H2'	24:1:850:U:H6	1.75	0.51
24:1:1278:C:H2'	24:1:1279:G:H8	1.74	0.51
24:1:2788:C:H2'	24:1:2789:C:C6	2.44	0.51
24:1:2591:C:H2'	24:1:2592:G:C8	2.45	0.51
28:D:21:ARG:HD3	28:D:106:LYS:HB3	1.90	0.51
1:2:728:A:H2'	1:2:729:A:C8	2.45	0.51
24:1:78:U:H2'	24:1:79:C:C6	2.46	0.51
24:1:543:G:H2'	24:1:544:C:O4'	2.11	0.51
1:2:131:A:H2'	1:2:132:C:C6	2.45	0.51
1:2:674:G:H2'	1:2:675:A:H8	1.75	0.51
1:2:1119:C:H2'	1:2:1120:C:H6	1.75	0.51
6:k:38:ARG:NH1	6:k:98:GLU:O	2.43	0.51
13:r:33:ILE:HD13	13:r:60:VAL:HG22	1.90	0.51
24:1:414:C:H2'	24:1:415:A:H8	1.74	0.51
24:1:2328:A:H2'	24:1:2329:U:H6	1.74	0.51
27:C:25:THR:HG21	27:C:193:VAL:HG22	1.92	0.51
51:e:62:LEU:HB3	51:e:65:ALA:HB2	1.93	0.51
1:2:1124:G:N2	1:2:1125:U:O4	2.38	0.51
24:1:851:C:H2'	24:1:852:U:C6	2.46	0.51
24:1:1141:U:H4'	24:1:1142:A:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:2192:U:H2'	24:1:2193:G:C8	2.45	0.51
24:1:2804:U:H2'	24:1:2805:C:C6	2.46	0.51
1:2:842:U:H4'	1:2:846:G:C2	2.44	0.51
7:l:76:LYS:HE3	7:l:89:VAL:HG21	1.92	0.51
24:1:588:U:H2'	24:1:589:U:C6	2.46	0.51
24:1:2071:A:H2'	24:1:2072:C:C6	2.46	0.51
1:2:35:G:H2'	1:2:36:C:C6	2.46	0.51
10:o:25:ILE:HG13	10:o:92:LEU:HD11	1.93	0.51
24:1:639:U:H2'	24:1:640:C:H6	1.76	0.51
24:1:1353:A:H2'	24:1:1354:A:C8	2.45	0.51
1:2:621:A:H2'	1:2:622:A:C8	2.46	0.51
24:1:1231:U:H2'	24:1:1232:G:H8	1.75	0.51
24:1:2291:U:H2'	24:1:2292:U:C6	2.46	0.51
34:M:42:THR:HG22	34:M:93:VAL:HG12	1.92	0.51
37:P:6:LYS:O	37:P:10:GLN:HG2	2.11	0.51
1:2:204:G:C4	1:2:205:A:C8	2.99	0.51
1:2:1120:C:H2'	1:2:1121:U:H6	1.75	0.51
31:J:34:ARG:HG3	31:J:39:LYS:HB2	1.93	0.51
1:2:197:A:N1	1:2:220:G:O2'	2.37	0.50
1:2:1304:G:H1'	1:2:1333:A:H61	1.76	0.50
24:1:1594:U:H2'	24:1:1595:C:C6	2.46	0.50
24:1:2099:U:H3	24:1:2190:G:H1	1.58	0.50
25:3:66:A:N6	25:3:107:G:H2'	2.26	0.50
1:2:223:A:H2'	1:2:224:U:C6	2.46	0.50
24:1:3:U:H2'	24:1:4:U:C6	2.46	0.50
24:1:538:A:O2'	31:J:9:GLU:OE2	2.24	0.50
24:1:1853:A:H2'	24:1:1854:A:C8	2.46	0.50
24:1:2698:U:H2'	24:1:2699:C:C6	2.46	0.50
24:1:2847:U:H2'	24:1:2848:G:O4'	2.11	0.50
25:3:95:U:H2'	25:3:96:G:C8	2.46	0.50
26:B:71:LYS:NZ	26:B:98:ASP:OD2	2.43	0.50
55:6:10:ARG:NH1	55:6:107:GLU:OE1	2.36	0.50
1:2:538:G:H5''	12:q:111:LYS:HB2	1.94	0.50
1:2:1402:4OC:HM22	1:2:1403:C:H5'	1.93	0.50
1:2:1441:A:N1	37:P:114:LEU:HD12	2.26	0.50
22:4:47:U:H5'	22:4:48:U:C5'	2.42	0.50
24:1:644:A:H2'	24:1:645:C:O4'	2.11	0.50
24:1:2052:A:H4'	27:C:148:GLN:O	2.11	0.50
24:1:2590:A:H2'	24:1:2591:C:C6	2.46	0.50
31:J:114:LEU:HG	31:J:118:MET:HE3	1.93	0.50
55:6:170:GLU:HA	55:6:176:ILE:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:G:63:ALA:HA	56:G:66:ASN:HD22	1.76	0.50
1:2:34:C:H2'	1:2:35:G:H8	1.77	0.50
1:2:875:U:O2'	8:m:15:ARG:NH1	2.42	0.50
1:2:1530:G:H2'	1:2:1531:A:H8	1.77	0.50
11:p:81:ASN:OD1	11:p:106:ARG:HB3	2.12	0.50
24:1:548:G:H2'	24:1:549:G:H1'	1.92	0.50
24:1:1527:G:N1	24:1:1544:A:OP2	2.38	0.50
24:1:1564:C:H2'	24:1:1565:C:C6	2.46	0.50
24:1:2809:A:H2'	24:1:2810:A:C8	2.47	0.50
1:2:1010:U:H2'	1:2:1011:C:C6	2.47	0.50
1:2:1121:U:H2'	1:2:1122:U:H6	1.77	0.50
6:k:32:ALA:HB2	6:k:70:VAL:HG11	1.93	0.50
24:1:739:A:H1'	24:1:740:C:H5	1.77	0.50
24:1:2567:G:H2'	24:1:2568:U:C6	2.47	0.50
28:D:170:ARG:NH1	28:D:176:ASP:OD1	2.36	0.50
1:2:842:U:H3'	1:2:843:U:C5'	2.42	0.50
24:1:667:U:H2'	24:1:668:A:O4'	2.11	0.50
24:1:1589:U:H2'	24:1:1590:A:C8	2.47	0.50
30:F:25:THR:HG22	30:F:34:THR:HG23	1.93	0.50
1:2:337:G:H2'	1:2:338:A:H8	1.76	0.50
24:1:2243:U:H2'	24:1:2244:U:H6	1.77	0.50
24:1:2246:G:H2'	24:1:2247:A:H8	1.76	0.50
37:P:100:LEU:HD11	37:P:110:ILE:HD11	1.94	0.50
1:2:56:U:H2'	1:2:57:G:H8	1.75	0.50
30:F:164:TYR:HB2	30:F:167:GLU:HB3	1.93	0.50
33:L:82:LEU:HD22	33:L:90:VAL:HG21	1.94	0.50
11:p:97:ILE:HG22	21:z:12:PHE:HZ	1.76	0.50
12:q:54:ARG:HH11	12:q:62:GLU:HG2	1.76	0.50
23:5:74:C:H3'	55:6:278:ARG:NH2	2.27	0.50
24:1:275:C:H2'	24:1:276:U:O4'	2.12	0.50
24:1:296:U:H2'	24:1:297:G:C8	2.47	0.50
24:1:580:U:H2'	24:1:581:C:C6	2.47	0.50
24:1:634:C:H2'	24:1:635:C:C6	2.46	0.50
31:J:128:ASN:ND2	31:J:128:ASN:O	2.45	0.50
1:2:202:G:O2'	1:2:468:A:N3	2.45	0.49
1:2:769:G:H4'	1:2:1513:A:H4'	1.94	0.49
1:2:1151:A:HO2'	1:2:1152:A:H8	1.58	0.49
1:2:1286:U:H2'	1:2:1287:A:H5'	1.93	0.49
9:n:27:LYS:HE3	9:n:62:ASP:HB3	1.93	0.49
24:1:1441:G:H2'	24:1:1442:U:C6	2.47	0.49
24:1:1506:U:H2'	24:1:1507:C:C6	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:L:132:ARG:HG3	33:L:142:ILE:HD12	1.94	0.49
53:a:10:GLU:OE1	53:a:11:GLU:N	2.42	0.49
2:g:97:LEU:H	2:g:100:MET:HE3	1.76	0.49
8:m:50:LYS:HE2	8:m:52:GLU:HG2	1.94	0.49
24:1:274:C:H2'	24:1:275:C:O4'	2.11	0.49
24:1:859:G:O2'	24:1:916:G:O6	2.28	0.49
1:2:236:A:H2'	1:2:237:G:C8	2.47	0.49
3:h:63:SER:OG	3:h:64:ILE:N	2.43	0.49
24:1:279:A:C2	24:1:362:A:H5'	2.48	0.49
30:F:138:LYS:O	30:F:141:ILE:HG13	2.13	0.49
1:2:77:A:H2'	1:2:78:A:C8	2.46	0.49
1:2:922:G:H2'	1:2:923:A:C8	2.48	0.49
1:2:1017:U:H2'	1:2:1018:G:C8	2.47	0.49
24:1:1107:G:H2'	24:1:1108:U:C6	2.48	0.49
24:1:2131:U:H5'	24:1:2132:U:H5''	1.94	0.49
24:1:2780:G:OP2	31:J:120:ARG:HD3	2.11	0.49
24:1:2898:U:H2'	24:1:2899:A:H8	1.78	0.49
30:F:50:LEU:HD13	30:F:72:LEU:HD23	1.93	0.49
1:2:76:G:H2'	1:2:77:A:C8	2.47	0.49
1:2:460:A:H2'	1:2:461:A:H8	1.76	0.49
1:2:600:A:H2'	1:2:601:G:H8	1.77	0.49
1:2:715:A:H2'	1:2:716:A:C8	2.47	0.49
1:2:1405:G:HO2'	1:2:1518:MA6:HO2'	1.60	0.49
1:2:1463:U:H2'	1:2:1464:U:H6	1.76	0.49
2:g:117:LEU:HD21	2:g:137:ARG:HB3	1.93	0.49
12:q:44:LYS:HG2	12:q:45:PRO:HA	1.94	0.49
24:1:30:G:H2'	24:1:31:C:C6	2.47	0.49
24:1:1315:C:O2'	24:1:1392:A:N3	2.45	0.49
24:1:1361:G:H2'	24:1:1362:C:C6	2.47	0.49
29:E:108:VAL:HG11	29:E:176:PRO:HG2	1.95	0.49
40:S:86:MET:HB2	40:S:96:ILE:HG12	1.95	0.49
1:2:204:G:H3'	1:2:205:A:H8	1.77	0.49
1:2:335:C:H2'	1:2:336:A:H8	1.77	0.49
1:2:593:U:H3	1:2:646:G:H1	1.58	0.49
24:1:813:U:H2'	24:1:814:C:H6	1.77	0.49
24:1:2373:G:H2'	24:1:2374:C:C6	2.47	0.49
24:1:2857:G:N2	24:1:2860:A:OP2	2.28	0.49
55:6:221:PHE:HZ	55:6:310:MET:HE2	1.78	0.49
1:2:234:C:H2'	1:2:235:C:H6	1.78	0.49
1:2:470:C:H2'	1:2:471:U:C6	2.47	0.49
1:2:1171:A:H2'	1:2:1172:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:k:5:GLU:OE1	18:w:23:TYR:OH	2.22	0.49
24:1:851:C:H2'	24:1:852:U:H6	1.77	0.49
24:1:1101:U:H2'	24:1:1102:C:O4'	2.12	0.49
24:1:2087:G:H2'	24:1:2088:A:H8	1.77	0.49
24:1:2430:A:N3	24:1:2430:A:H2'	2.26	0.49
37:P:85:SER:OG	37:P:87:LYS:NZ	2.45	0.49
1:2:1118:U:H2'	1:2:1119:C:H6	1.78	0.49
2:g:94:HIS:ND1	2:g:146:ASN:O	2.45	0.49
24:1:6:A:H2'	24:1:7:G:C8	2.48	0.49
24:1:927:A:H2'	24:1:928:A:C8	2.47	0.49
24:1:1084:A:H8	24:1:1084:A:OP1	1.96	0.49
24:1:1198:U:H2'	24:1:1199:U:C6	2.48	0.49
24:1:1484:U:H2'	24:1:1485:U:C6	2.48	0.49
24:1:2273:A:H2'	24:1:2274:A:C8	2.47	0.49
24:1:2590:A:H2'	24:1:2591:C:H6	1.76	0.49
25:3:48:U:H2'	25:3:49:C:C6	2.48	0.49
1:2:206:C:N4	1:2:213:G:H22	2.11	0.49
1:2:1032:G:C6	1:2:1033:G:H1'	2.47	0.49
22:4:24:U:H2'	22:4:25:A:H8	1.76	0.49
24:1:1028:A:N6	24:1:1125:G:H2'	2.28	0.49
32:K:40:LYS:HE3	32:K:57:VAL:HG12	1.93	0.49
1:2:189:A:H2'	1:2:190:A:C8	2.48	0.49
24:1:589:U:H2'	24:1:590:A:C8	2.47	0.49
24:1:2895:G:H2'	24:1:2896:C:C6	2.48	0.49
25:3:29:A:H2'	25:3:30:C:C6	2.48	0.49
34:M:50:ARG:HD3	34:M:65:ILE:HD11	1.95	0.49
1:2:206:C:H42	1:2:213:G:H1	1.60	0.48
5:j:159:LYS:HB2	5:j:164:ILE:HD13	1.94	0.48
20:y:67:ILE:HB	20:y:71:LYS:HD3	1.96	0.48
24:1:1443:U:H2'	24:1:1444:G:C8	2.47	0.48
24:1:1528:A:OP2	24:1:1543:G:N2	2.40	0.48
24:1:2452:C:H2'	24:1:2453:A:C8	2.48	0.48
24:1:2599:G:C8	26:B:236:GLU:HG2	2.48	0.48
26:B:133:ARG:HB3	26:B:186:ALA:HB1	1.96	0.48
22:4:32:U:H4'	22:4:33:A:OP1	2.12	0.48
24:1:356:G:H2'	24:1:357:C:H6	1.77	0.48
24:1:1046:A:H3'	24:1:1047:G:H5'	1.94	0.48
24:1:1062:G:C6	24:1:1077:A:C6	3.02	0.48
24:1:1096:A:H2'	24:1:1097:U:O4'	2.13	0.48
55:6:140:GLU:OE1	55:6:206:PRO:HD2	2.13	0.48
1:2:62:U:H3	1:2:105:G:H1	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:613:C:H2'	1:2:614:C:C6	2.48	0.48
1:2:1332:A:H2'	1:2:1333:A:C8	2.49	0.48
4:i:172:GLU:O	4:i:180:GLY:HA2	2.13	0.48
24:1:355:U:H2'	24:1:356:G:C8	2.49	0.48
24:1:843:G:H2'	24:1:844:A:C8	2.49	0.48
24:1:1442:U:H2'	24:1:1443:U:C6	2.49	0.48
24:1:2331:G:O2'	44:W:43:THR:HG22	2.13	0.48
30:F:17:VAL:HG11	30:F:50:LEU:HD21	1.96	0.48
1:2:41:G:H2'	1:2:42:G:H8	1.78	0.48
1:2:1026:G:O2'	1:2:1027:C:OP1	2.29	0.48
1:2:1198:G:H2'	1:2:1199:U:C6	2.48	0.48
1:2:1436:U:H2'	1:2:1437:A:C8	2.48	0.48
4:i:190:ASP:OD1	4:i:190:ASP:N	2.45	0.48
10:o:88:MET:HE1	10:o:100:ILE:HG21	1.95	0.48
24:1:151:C:H2'	24:1:152:A:C8	2.48	0.48
24:1:1321:A:C4	24:1:1322:A:C8	3.02	0.48
24:1:1631:G:H1'	24:1:1635:A:H61	1.78	0.48
24:1:2039:U:H2'	24:1:2040:G:C8	2.49	0.48
24:1:2250:G:O2'	24:1:2496:C:OP1	2.32	0.48
1:2:67:C:H2'	1:2:68:G:C8	2.49	0.48
1:2:554:A:H2'	1:2:555:U:C6	2.48	0.48
24:1:457:A:N1	24:1:470:A:H5''	2.28	0.48
24:1:2149:U:H2'	24:1:2150:C:C6	2.49	0.48
24:1:2845:U:H5''	37:P:52:ASN:O	2.14	0.48
1:2:100:G:H2'	1:2:101:A:O4'	2.13	0.48
1:2:1360:A:OP2	14:s:75:ARG:NH2	2.47	0.48
17:v:53:CYS:SG	17:v:75:LEU:HD11	2.54	0.48
24:1:2204:G:H4'	26:B:150:LYS:HD3	1.95	0.48
1:2:215:C:H2'	1:2:216:U:C6	2.48	0.48
23:5:26:G:H22	23:5:44:A:H2	1.62	0.48
24:1:422:A:H2'	24:1:423:A:C8	2.49	0.48
24:1:1318:U:H2'	24:1:1319:C:C6	2.48	0.48
29:E:36:LEU:HD22	29:E:154:ILE:HG12	1.95	0.48
46:Y:9:LYS:HB2	46:Y:14:LEU:HD13	1.96	0.48
1:2:216:U:H4'	1:2:464:U:H4'	1.95	0.48
1:2:1120:C:H2'	1:2:1121:U:C6	2.48	0.48
24:1:582:A:H2'	24:1:583:G:C8	2.49	0.48
24:1:1710:G:H4'	24:1:2858:C:O2	2.14	0.48
35:N:28:LEU:HD23	35:N:48:VAL:HG21	1.96	0.48
1:2:545:C:H5'	4:i:69:GLU:HB2	1.96	0.48
24:1:372:G:O2'	24:1:400:G:O6	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:729:G:C6	26:B:207:LYS:HB2	2.49	0.48
24:1:1548:A:H2'	24:1:1549:A:C8	2.49	0.48
24:1:1590:A:H2'	24:1:1591:A:H8	1.79	0.48
27:C:56:LYS:HB2	27:C:59:ARG:HB2	1.96	0.48
48:b:43:ILE:HG22	48:b:49:TYR:HB2	1.96	0.48
56:G:62:LEU:O	56:G:66:ASN:ND2	2.46	0.48
1:2:389:A:H3'	1:2:390:U:H6	1.79	0.48
1:2:1250:A:H2'	1:2:1251:A:C8	2.49	0.48
1:2:1513:A:H2'	1:2:1514:G:H8	1.79	0.48
24:1:197:A:N6	24:1:2430:A:O2'	2.46	0.48
24:1:2554:U:H2'	24:1:2555:U:C6	2.48	0.48
36:O:51:ALA:HB3	36:O:78:VAL:HB	1.95	0.48
55:6:319:TRP:CD1	55:6:319:TRP:H	2.32	0.48
1:2:190:A:O5'	1:2:190:A:H8	1.97	0.47
1:2:412:A:O2'	1:2:413:G:H4'	2.14	0.47
1:2:459:A:H2'	1:2:460:A:C8	2.49	0.47
1:2:600:A:H2'	1:2:601:G:C8	2.48	0.47
1:2:891:U:H2'	1:2:892:A:H8	1.79	0.47
1:2:945:G:C2	1:2:946:A:C8	3.02	0.47
1:2:1360:A:H2'	1:2:1361:G:C8	2.49	0.47
22:4:34:U:H4'	22:4:35:U:C6	2.49	0.47
24:1:1266:G:O2'	24:1:2012:G:O6	2.22	0.47
24:1:1563:U:H2'	24:1:1564:C:C6	2.49	0.47
29:E:38:MET:HE3	29:E:57:LEU:HD13	1.96	0.47
55:6:299:GLU:HG2	55:6:303:LYS:HE3	1.95	0.47
1:2:350:G:H2'	1:2:351:G:C8	2.49	0.47
1:2:562:U:H5'	1:2:563:A:C5	2.49	0.47
1:2:939:G:H2'	1:2:940:C:C6	2.49	0.47
1:2:1008:U:C2	1:2:1022:A:C2	3.03	0.47
24:1:52:A:H2'	24:1:53:A:H8	1.79	0.47
24:1:128:C:H2'	24:1:129:C:C6	2.48	0.47
24:1:720:U:H2'	24:1:721:A:C8	2.49	0.47
30:F:86:LYS:HG2	30:F:132:VAL:HG22	1.96	0.47
37:P:33:VAL:HG22	37:P:38:LYS:HG3	1.95	0.47
55:6:41:LEU:HD23	55:6:46:VAL:HG21	1.95	0.47
1:2:451:A:O2'	58:2:1690:SPD:N1	2.47	0.47
1:2:976:G:OP2	1:2:1358:U:O2'	2.32	0.47
9:n:33:ARG:HE	9:n:38:TYR:HD1	1.62	0.47
24:1:549:G:H2'	24:1:550:C:H6	1.78	0.47
24:1:1790:C:H2'	24:1:1791:A:C5	2.49	0.47
38:Q:15:LYS:HB3	38:Q:15:LYS:HE2	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:505:G:H2'	1:2:506:G:C8	2.49	0.47
1:2:1121:U:H2'	1:2:1122:U:C6	2.50	0.47
24:1:856:G:H2'	24:1:857:G:C8	2.49	0.47
24:1:1417:C:O2'	24:1:1587:G:O2'	2.20	0.47
24:1:1683:U:H2'	24:1:1684:G:C8	2.48	0.47
24:1:2460:U:C2	24:1:2461:A:C8	3.03	0.47
24:1:2747:G:O6	24:1:2755:C:H5''	2.15	0.47
53:a:16:CYS:SG	53:a:17:SER:N	2.88	0.47
53:a:45:THR:O	53:a:47:LYS:NZ	2.46	0.47
1:2:642:A:N7	8:m:107:SER:HA	2.30	0.47
1:2:983:A:H5'	1:2:984:C:OP2	2.15	0.47
1:2:1435:G:H2'	1:2:1436:U:C6	2.49	0.47
6:k:38:ARG:HB3	6:k:63:ASN:HB2	1.96	0.47
8:m:39:VAL:HG21	8:m:110:VAL:HG12	1.96	0.47
17:v:58:VAL:HB	17:v:80:GLU:HB2	1.96	0.47
24:1:145:C:H2'	24:1:146:A:C8	2.50	0.47
24:1:839:U:H2'	24:1:840:C:C6	2.49	0.47
24:1:1049:C:C2	24:1:1050:A:C8	3.03	0.47
24:1:1242:U:H2'	24:1:1243:C:C6	2.49	0.47
24:1:1889:A:H2'	24:1:1890:A:C8	2.50	0.47
24:1:2469:A:H2'	24:1:2470:G:O4'	2.15	0.47
55:6:153:LEU:O	55:6:157:GLU:HG2	2.15	0.47
9:n:7:TYR:HH	9:n:9:THR:HG1	1.62	0.47
24:1:1387:A:H2'	24:1:1388:G:H8	1.80	0.47
24:1:1597:A:H5''	24:1:1598:A:H5'	1.96	0.47
24:1:1631:G:H1'	24:1:1635:A:N6	2.30	0.47
24:1:1717:A:H61	24:1:1743:G:H1'	1.79	0.47
26:B:203:ARG:NH1	26:B:205:LEU:HD21	2.30	0.47
54:I:78:LEU:HD13	54:I:108:ILE:HG23	1.96	0.47
1:2:477:C:H2'	1:2:478:A:C8	2.49	0.47
1:2:522:C:H41	12:q:50:ARG:NH2	2.12	0.47
1:2:664:G:OP1	18:w:57:ARG:NH2	2.37	0.47
1:2:736:C:H2'	1:2:737:C:C6	2.50	0.47
1:2:982:U:H4'	1:2:983:A:O4'	2.14	0.47
1:2:1216:A:H5''	14:s:5:SER:HB3	1.96	0.47
23:5:21:A:N6	23:5:46:G:H2'	2.28	0.47
24:1:1075:C:H2'	24:1:1076:C:O4'	2.15	0.47
24:1:1485:U:H2'	24:1:1486:U:C6	2.50	0.47
25:3:2:G:H2'	25:3:3:C:H6	1.79	0.47
25:3:106:G:H2'	25:3:107:G:O4'	2.15	0.47
26:B:72:ASP:OD1	26:B:72:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:152:PRO:HG3	27:C:156:PHE:CZ	2.50	0.47
30:F:170:ARG:NH1	30:F:170:ARG:HA	2.30	0.47
34:M:20:LEU:HD13	43:V:81:PRO:HG2	1.96	0.47
1:2:216:U:H1'	1:2:466:A:H61	1.78	0.47
1:2:1060:U:H2'	1:2:1061:G:H8	1.80	0.47
1:2:1088:G:H4'	21:z:70:LEU:HD13	1.96	0.47
18:w:11:CYS:HB2	18:w:48:ARG:HD3	1.97	0.47
22:4:43:G:H1	55:6:213[B]:ARG:HH11	1.63	0.47
24:1:279:A:H61	24:1:360:U:C2'	2.28	0.47
24:1:1047:G:HO2'	24:1:1110:G:H1	1.61	0.47
24:1:2184:A:H2'	24:1:2185:U:O4'	2.14	0.47
35:N:8:ARG:HD2	35:N:43:GLU:HG2	1.96	0.47
1:2:842:U:H2'	1:2:844:G:C5'	2.44	0.47
3:h:47:LEU:HB3	3:h:50:ALA:HB3	1.96	0.47
5:j:81:LEU:HD11	5:j:96:MET:HB3	1.95	0.47
13:r:12:HIS:O	13:r:44:LYS:NZ	2.30	0.47
24:1:969:G:H2'	24:1:970:U:C6	2.49	0.47
24:1:2185:U:H2'	24:1:2186:G:C8	2.50	0.47
24:1:2848:G:O2'	24:1:2867:G:N2	2.35	0.47
1:2:89:U:H2'	1:2:90:C:C6	2.50	0.47
1:2:224:U:H2'	1:2:225:C:C6	2.50	0.47
1:2:382:A:H2'	1:2:383:A:C8	2.50	0.47
1:2:1005:A:H4'	1:2:1037:C:H1'	1.96	0.47
1:2:1008:U:H2'	1:2:1009:U:O4'	2.15	0.47
1:2:1123:U:O2'	1:2:1124:G:H5'	2.15	0.47
7:l:48:GLU:O	7:l:52:GLN:HG2	2.15	0.47
11:p:86:VAL:HG21	11:p:97:ILE:HD11	1.96	0.47
22:4:26:A:H2'	22:4:27:G:H8	1.80	0.47
24:1:491:G:O6	40:S:49:LYS:NZ	2.39	0.47
24:1:878:A:N7	24:1:899:A:H2	2.13	0.47
24:1:1433:A:H2'	24:1:1434:A:C8	2.50	0.47
24:1:1485:U:H2'	24:1:1486:U:H6	1.80	0.47
24:1:2461:A:H2'	24:1:2462:C:C6	2.50	0.47
24:1:2836:U:H2'	24:1:2837:A:C8	2.50	0.47
33:L:78:ARG:HG2	33:L:113:ALA:HB3	1.97	0.47
38:Q:87:SER:HB2	39:R:51:VAL:HG23	1.97	0.47
40:S:20:VAL:HG11	40:S:44:ALA:HA	1.97	0.47
1:2:49:U:O2	1:2:362:G:H1'	2.15	0.46
24:1:347:A:H2'	24:1:348:A:C8	2.50	0.46
24:1:2020:A:H5'	48:b:9:THR:CG2	2.45	0.46
46:Y:12:GLU:CD	46:Y:12:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:205:A:H2'	1:2:206:C:C6	2.50	0.46
1:2:216:U:H2'	1:2:217:C:C6	2.50	0.46
1:2:652:U:O4	1:2:752:G:O2'	2.28	0.46
2:g:118:GLU:O	2:g:122:GLN:HG2	2.15	0.46
3:h:19:ASN:OD1	3:h:54:ARG:NH2	2.48	0.46
4:i:11:LEU:HB3	4:i:63:ARG:HD3	1.97	0.46
7:l:53:ARG:NH2	7:l:122:ASN:OD1	2.47	0.46
24:1:967:U:H2'	24:1:968:C:C6	2.49	0.46
24:1:1484:U:H2'	24:1:1485:U:H6	1.78	0.46
43:V:2:PHE:HB3	43:V:50:MET:HE3	1.97	0.46
1:2:461:A:H2'	1:2:462:G:H8	1.80	0.46
1:2:470:C:H2'	1:2:471:U:H6	1.80	0.46
1:2:1013:G:N2	1:2:1016:A:OP2	2.40	0.46
1:2:1051:C:H2'	1:2:1052:U:C6	2.50	0.46
1:2:1228:C:OP2	13:r:110:LYS:NZ	2.44	0.46
1:2:1263:C:H2'	1:2:1264:U:C6	2.50	0.46
1:2:1428:A:H2'	1:2:1429:A:O4'	2.16	0.46
4:i:102:VAL:HG13	4:i:107:PHE:HB2	1.96	0.46
24:1:17:G:H2'	24:1:18:U:C6	2.50	0.46
24:1:526:A:O2'	24:1:2043:C:O2	2.33	0.46
34:M:75:GLU:HB2	34:M:90:GLU:HG3	1.97	0.46
24:1:305:C:H2'	24:1:306:U:C6	2.50	0.46
24:1:504:A:O2'	24:1:1235:G:OP1	2.32	0.46
24:1:593:U:H2'	24:1:594:U:C6	2.50	0.46
24:1:632:A:H2'	24:1:633:A:C8	2.51	0.46
24:1:1802:A:H2'	24:1:1803:A:H8	1.78	0.46
24:1:2175:C:H2'	24:1:2176:A:C8	2.50	0.46
1:2:459:A:H2'	1:2:460:A:H8	1.80	0.46
1:2:545:C:OP1	4:i:58:LYS:NZ	2.48	0.46
1:2:607:A:H2'	1:2:608:A:C8	2.51	0.46
1:2:1458:G:OP1	20:y:30:THR:OG1	2.28	0.46
24:1:1636:U:H2'	24:1:1637:A:C8	2.50	0.46
24:1:2484:G:OP1	34:M:44:ARG:NH1	2.42	0.46
24:1:2820:A:H2'	24:1:2820:A:N3	2.30	0.46
28:D:6:LYS:HA	28:D:9:GLN:HE21	1.81	0.46
1:2:560:A:H4'	1:2:561:U:H5''	1.97	0.46
1:2:855:U:OP2	1:2:871:U:N3	2.39	0.46
1:2:1035:A:C4	1:2:1036:A:C2	3.04	0.46
24:1:150:U:H2'	24:1:151:C:C6	2.51	0.46
24:1:476:G:H4'	24:1:502:A:N1	2.31	0.46
24:1:1107:G:H2'	24:1:1108:U:H6	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:1464:G:H2'	24:1:1465:G:C8	2.51	0.46
25:3:93:C:H2'	25:3:94:A:H8	1.80	0.46
1:2:790:A:H2'	1:2:791:G:C8	2.51	0.46
1:2:844:G:H3'	1:2:844:G:N3	2.30	0.46
1:2:1464:U:H2'	1:2:1465:A:H8	1.80	0.46
3:h:135:LYS:HE3	3:h:135:LYS:HB2	1.81	0.46
24:1:589:U:H2'	24:1:590:A:H8	1.81	0.46
24:1:668:A:H2'	24:1:670:A:H62	1.81	0.46
24:1:1353:A:H2'	24:1:1354:A:H8	1.80	0.46
45:X:3:ARG:O	45:X:12:PRO:HD3	2.15	0.46
51:e:26:HIS:NE2	51:e:48:ALA:HB2	2.30	0.46
1:2:51:A:N7	1:2:114:U:O2'	2.48	0.46
1:2:246:A:C2	1:2:282:A:C5	3.03	0.46
1:2:562:U:H5'	1:2:563:A:C4	2.51	0.46
1:2:1092:A:H5''	7:l:4:ARG:NH2	2.31	0.46
1:2:1315:U:H2'	1:2:1316:G:O4'	2.15	0.46
14:s:79:LEU:HB2	14:s:84:VAL:HG23	1.98	0.46
20:y:57:ILE:O	20:y:61:GLN:HG2	2.15	0.46
24:1:2657:A:O3'	30:F:160:LYS:NZ	2.47	0.46
33:L:10:GLU:H	33:L:10:GLU:CD	2.23	0.46
54:I:82:ALA:HB2	54:I:108:ILE:HD11	1.98	0.46
55:6:196:THR:HG23	55:6:221:PHE:HA	1.98	0.46
1:2:473:U:H2'	1:2:474:G:C8	2.51	0.46
1:2:555:U:H2'	1:2:556:C:H6	1.81	0.46
1:2:1251:A:H2'	1:2:1252:A:C8	2.50	0.46
24:1:671:C:H2'	24:1:672:C:C6	2.51	0.46
24:1:898:C:H2'	24:1:899:A:O4'	2.15	0.46
24:1:1387:A:H2'	24:1:1388:G:C8	2.50	0.46
24:1:1754:A:N1	24:1:2716:C:O2'	2.44	0.46
25:3:94:A:H2'	25:3:95:U:O4'	2.16	0.46
1:2:140:U:H2'	1:2:141:G:O4'	2.15	0.46
1:2:839:C:H2'	1:2:840:C:C6	2.50	0.46
24:1:1570:A:H2'	24:1:1571:A:C8	2.51	0.46
24:1:1920:C:H6	24:1:1920:C:O5'	1.99	0.46
30:F:155:GLU:OE2	30:F:160:LYS:HB2	2.16	0.46
34:M:53:MET:HE1	34:M:103:TYR:CD1	2.50	0.46
1:2:105:G:H2'	1:2:106:C:C6	2.51	0.45
1:2:1296:C:H4'	1:2:1302:C:N4	2.30	0.45
2:g:64:LYS:HD3	2:g:64:LYS:HA	1.76	0.45
24:1:1370:C:H2'	24:1:1371:G:O4'	2.16	0.45
24:1:2186:G:H2'	24:1:2187:U:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:2658:C:OP1	30:F:158:LYS:NZ	2.42	0.45
24:1:2740:A:H2'	24:1:2741:A:C8	2.51	0.45
41:T:34:VAL:HG21	41:T:43:ILE:HD11	1.97	0.45
1:2:360:G:H2'	1:2:361:G:C8	2.51	0.45
1:2:883:C:O2'	1:2:884:U:H5'	2.17	0.45
1:2:999:C:H2'	1:2:1000:A:H8	1.81	0.45
1:2:1162:C:H2'	1:2:1163:A:H8	1.81	0.45
24:1:2:G:N1	24:1:2902:C:N3	2.64	0.45
24:1:419:U:H2'	24:1:420:C:C6	2.51	0.45
24:1:689:A:H2'	24:1:690:G:C8	2.52	0.45
24:1:1039:A:H2'	24:1:1040:A:O4'	2.16	0.45
24:1:1540:G:C6	24:1:1541:C:C4	3.04	0.45
24:1:1840:G:H2'	24:1:1841:U:C6	2.52	0.45
24:1:1957:C:H5'	24:1:1984:G:O2'	2.16	0.45
24:1:2641:G:H5''	31:J:78:THR:HB	1.98	0.45
24:1:2649:C:H2'	24:1:2650:U:H6	1.80	0.45
41:T:2:ILE:HD13	41:T:42:GLU:HG2	1.99	0.45
1:2:73:C:C2	1:2:74:A:C8	3.04	0.45
1:2:1014:A:C2	1:2:1219:A:H1'	2.51	0.45
24:1:590:A:H2'	24:1:591:U:C6	2.51	0.45
24:1:1197:G:H2'	24:1:1198:U:C6	2.51	0.45
36:O:4:LYS:O	36:O:8:ILE:HG12	2.17	0.45
1:2:465:A:H2'	1:2:466:A:C8	2.52	0.45
1:2:1118:U:H2'	1:2:1119:C:C6	2.51	0.45
1:2:1171:A:H2'	1:2:1172:C:H6	1.82	0.45
15:t:88:ARG:NH2	24:1:714:U:OP2	2.49	0.45
17:v:47:HIS:HB3	17:v:74:THR:HG22	1.98	0.45
24:1:990:A:N6	24:1:1186:G:H1'	2.31	0.45
32:K:71:ARG:HA	32:K:71:ARG:HD3	1.82	0.45
1:2:335:C:H2'	1:2:336:A:C8	2.51	0.45
1:2:384:G:H2'	1:2:385:C:H6	1.82	0.45
1:2:505:G:H2'	1:2:506:G:H8	1.82	0.45
1:2:904:U:H2'	1:2:905:U:C6	2.51	0.45
24:1:144:A:H2'	24:1:145:C:C6	2.51	0.45
24:1:340:A:H2'	24:1:341:C:O4'	2.16	0.45
24:1:548:G:H2'	24:1:549:G:C1'	2.46	0.45
24:1:1532:A:C6	24:1:1540:G:C6	3.04	0.45
24:1:2087:G:H2'	24:1:2088:A:C8	2.50	0.45
24:1:2333:A:H5'	24:1:2335:A:H1'	1.98	0.45
42:U:86:ARG:HG3	42:U:95:PHE:CE1	2.51	0.45
24:1:657:U:H2'	24:1:658:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:1429:G:H2'	24:1:1430:G:C8	2.52	0.45
24:1:1470:A:H2'	24:1:1471:G:O4'	2.17	0.45
24:1:1529:G:H2'	24:1:1530:G:C8	2.52	0.45
24:1:1649:G:O2'	35:N:106:ASP:OD2	2.18	0.45
24:1:2065:C:H2'	24:1:2066:C:H6	1.81	0.45
24:1:2533:U:OP1	24:1:2665:A:O2'	2.35	0.45
24:1:2902:C:H3'	24:1:2903:U:C6	2.51	0.45
25:3:90:C:H5'	34:M:18:ARG:HG2	1.99	0.45
26:B:145:GLU:HG2	26:B:151:GLY:C	2.42	0.45
42:U:49:VAL:HG23	42:U:52:LEU:O	2.16	0.45
1:2:636:U:H2'	1:2:637:C:C6	2.52	0.45
4:i:105:MET:HE1	4:i:143:VAL:HB	1.99	0.45
24:1:547:A:H4'	24:1:548:G:O4'	2.16	0.45
24:1:577:G:O2'	24:1:1254:A:OP1	2.31	0.45
24:1:784:G:H5'	24:1:785:G:OP1	2.17	0.45
24:1:1064:C:O2'	24:1:1065:U:C6	2.66	0.45
24:1:1509:A:O2'	24:1:1510:G:H8	1.99	0.45
24:1:1526:C:H2'	24:1:1527:G:O4'	2.17	0.45
25:3:2:G:H2'	25:3:3:C:C6	2.51	0.45
25:3:49:C:H2'	25:3:50:A:C8	2.52	0.45
26:B:120:VAL:HG23	26:B:134:ASN:OD1	2.17	0.45
46:Y:37:LEU:HG	46:Y:39:GLN:O	2.17	0.45
56:G:16:GLY:HA3	56:G:51:ARG:NH2	2.32	0.45
1:2:321:A:N7	1:2:328:C:O2'	2.47	0.45
1:2:410:G:H2'	1:2:429:U:C5	2.52	0.45
1:2:1017:U:H2'	1:2:1018:G:H8	1.82	0.45
1:2:1407:5MC:O2'	24:1:1912:A:N1	2.46	0.45
22:4:33:A:H4'	22:4:34:U:N3	2.31	0.45
24:1:1231:U:H2'	24:1:1232:G:C8	2.52	0.45
24:1:1747:U:H2'	24:1:1748:C:H6	1.82	0.45
24:1:2469:A:N6	24:1:2481:G:O2'	2.43	0.45
24:1:2543:G:H2'	24:1:2544:G:C8	2.52	0.45
24:1:2798:U:H4'	24:1:2799:A:H5'	1.97	0.45
32:K:66:LYS:HE2	32:K:66:LYS:HB3	1.80	0.45
40:S:23:LEU:HD22	48:b:24:ALA:HB2	1.98	0.45
1:2:41:G:H2'	1:2:42:G:C8	2.52	0.45
1:2:594:U:H2'	1:2:595:A:O4'	2.17	0.45
1:2:1144:G:N2	1:2:1146:A:H62	2.14	0.45
1:2:1335:U:H5''	1:2:1336:C:H5'	1.99	0.45
1:2:1387:G:H2'	1:2:1388:C:C6	2.52	0.45
1:2:1486:G:H2'	1:2:1487:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:l:18:PHE:HB3	7:l:59:LEU:HD11	1.99	0.45
23:5:63:G:H2'	23:5:64:G:H8	1.81	0.45
24:1:364:C:H2'	24:1:365:U:C6	2.52	0.45
24:1:1571:A:H2'	24:1:1572:A:C8	2.51	0.45
55:6:302:LYS:O	55:6:306:GLU:HG2	2.17	0.45
4:i:188:ARG:HD2	4:i:188:ARG:HA	1.76	0.45
23:5:16:C:H3'	23:5:17:C:C6	2.52	0.45
23:5:18:G:N2	23:5:58:A:OP2	2.50	0.45
24:1:351:C:H2'	24:1:352:A:H8	1.81	0.45
24:1:671:C:H2'	24:1:672:C:H6	1.82	0.45
24:1:1712:U:H3'	24:1:1713:A:H2'	1.99	0.45
24:1:2820:A:O2'	24:1:2821:A:OP1	2.31	0.45
28:D:46:GLN:O	28:D:88:ARG:NH2	2.50	0.45
38:Q:50:ARG:O	38:Q:54:LYS:NZ	2.43	0.45
1:2:73:C:HO2'	1:2:74:A:C5'	2.29	0.44
1:2:253:A:H2'	1:2:254:G:C8	2.52	0.44
1:2:270:A:H2'	1:2:271:C:C6	2.52	0.44
1:2:399:G:H2'	1:2:400:C:C6	2.51	0.44
1:2:721:G:H4'	1:2:722:G:O4'	2.17	0.44
1:2:1162:C:H2'	1:2:1163:A:C8	2.52	0.44
7:l:107:ALA:O	7:l:111:ARG:HG3	2.17	0.44
10:o:59:LYS:HE2	10:o:62:ARG:NH2	2.32	0.44
24:1:764:A:H5'	26:B:209:GLY:HA2	1.98	0.44
24:1:1115:G:O2'	24:1:1116:G:O5'	2.35	0.44
24:1:1545:A:H2'	24:1:1546:G:O4'	2.17	0.44
24:1:2018:G:OP1	60:1:3333:PUT:N1	2.49	0.44
24:1:2153:C:H2'	24:1:2154:A:H8	1.82	0.44
24:1:2313:C:H5''	29:E:88:LYS:HD3	1.99	0.44
44:W:41:ARG:HA	44:W:41:ARG:HD3	1.73	0.44
1:2:71:A:C6	1:2:72:A:N7	2.85	0.44
1:2:134:G:H1'	1:2:325:A:C5	2.52	0.44
1:2:160:A:H2'	1:2:161:A:O4'	2.18	0.44
1:2:322:C:H2'	1:2:323:U:C6	2.53	0.44
1:2:486:U:H2'	1:2:487:A:C8	2.52	0.44
1:2:1005:A:C5	1:2:1006:G:H1'	2.52	0.44
1:2:1304:G:H1'	1:2:1333:A:N6	2.32	0.44
1:2:1405:G:O2'	1:2:1518:MA6:O2'	2.33	0.44
1:2:1478:U:H2'	1:2:1479:C:C6	2.52	0.44
5:j:38:VAL:HG11	5:j:114:VAL:HG22	1.99	0.44
7:l:14:PRO:HB2	7:l:19:GLY:HA2	1.99	0.44
24:1:499:U:H2'	24:1:500:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:756:A:H2'	24:1:757:G:O4'	2.17	0.44
24:1:833:A:H2'	24:1:834:G:H8	1.80	0.44
24:1:1072:C:H2'	24:1:1093:G:O6	2.17	0.44
24:1:1883:U:H2'	24:1:1884:G:O4'	2.17	0.44
24:1:2455:G:H2'	24:1:2456:C:C6	2.52	0.44
27:C:181:ASP:HB3	27:C:186:LEU:HB2	1.99	0.44
1:2:71:A:C2	1:2:72:A:C8	3.05	0.44
1:2:602:A:H2'	1:2:603:U:C6	2.52	0.44
1:2:696:A:H2'	1:2:697:U:C6	2.51	0.44
1:2:1271:A:H2'	1:2:1272:G:C8	2.53	0.44
13:r:96:PRO:HB2	13:r:100:GLN:OE1	2.17	0.44
24:1:645:C:H2'	24:1:647:G:N7	2.33	0.44
24:1:766:U:H2'	24:1:767:U:C6	2.52	0.44
24:1:828:U:H2'	24:1:829:A:C8	2.53	0.44
24:1:2339:C:H2'	24:1:2340:A:C8	2.52	0.44
44:W:50:ASN:HB2	44:W:82:ILE:HB	1.99	0.44
1:2:294:U:OP1	1:2:610:U:O2'	2.26	0.44
1:2:500:G:H2'	1:2:501:C:C6	2.52	0.44
1:2:745:G:O2'	1:2:746:A:H5'	2.17	0.44
1:2:1009:U:O2	1:2:1020:G:N2	2.39	0.44
1:2:1086:U:H3	1:2:1099:G:H1	1.65	0.44
1:2:1122:U:H2'	1:2:1123:U:C6	2.53	0.44
10:o:84:VAL:O	10:o:88:MET:HG2	2.18	0.44
24:1:739:A:N3	24:1:740:C:N4	2.53	0.44
24:1:2873:A:C2	35:N:5:LYS:HG3	2.52	0.44
24:1:2895:G:H2'	24:1:2896:C:H6	1.81	0.44
25:3:77:U:OP1	43:V:21:ARG:NH1	2.39	0.44
42:U:54:GLN:HG2	42:U:55:PRO:HD3	1.98	0.44
1:2:459:A:C6	1:2:474:G:C6	3.06	0.44
1:2:908:A:H2'	1:2:909:A:C8	2.52	0.44
1:2:999:C:H2'	1:2:1000:A:C8	2.53	0.44
1:2:1095:U:H2'	1:2:1096:C:C6	2.52	0.44
1:2:1305:G:N2	1:2:1331:G:H1'	2.33	0.44
1:2:1436:U:H2'	1:2:1437:A:H8	1.81	0.44
14:s:47:LYS:O	14:s:50:THR:OG1	2.31	0.44
22:4:44:G:OP2	55:6:212:ARG:NH1	2.48	0.44
24:1:290:U:H3	24:1:350:G:H1	1.65	0.44
24:1:1055:G:H3'	24:1:1056:G:H8	1.83	0.44
24:1:1588:G:H2'	24:1:1589:U:C6	2.52	0.44
24:1:2070:A:H2'	24:1:2071:A:C8	2.53	0.44
24:1:2251:OMG:H1'	24:1:2251:OMG:HM23	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:2259:U:OP1	60:1:3330:PUT:H42	2.17	0.44
38:Q:78:LYS:HE3	38:Q:78:LYS:HB3	1.88	0.44
1:2:73:C:O2'	1:2:74:A:H8	2.01	0.44
1:2:966:2MG:C2	23:5:34:C:H5'	2.52	0.44
1:2:1218:C:H2'	1:2:1219:A:H8	1.81	0.44
6:k:43:GLY:HA2	6:k:58:HIS:CE1	2.52	0.44
24:1:1874:C:H2'	24:1:1875:G:O4'	2.17	0.44
24:1:2109:U:H2'	24:1:2110:G:C8	2.53	0.44
24:1:2812:G:H2'	24:1:2813:A:C8	2.53	0.44
24:1:2861:U:H2'	24:1:2862:G:H8	1.82	0.44
31:J:76:HIS:CE1	31:J:85:LYS:HB2	2.52	0.44
55:6:22:ARG:HG2	55:6:70:LEU:HD13	2.00	0.44
1:2:66:A:C2	1:2:104:G:H1'	2.53	0.44
1:2:219:U:H2'	1:2:220:G:C8	2.49	0.44
1:2:918:A:H2'	1:2:919:A:C8	2.53	0.44
1:2:1130:A:H2'	1:2:1131:G:C8	2.50	0.44
1:2:1397:C:OP2	5:j:29:ARG:NH2	2.51	0.44
9:n:100:LYS:HE3	9:n:100:LYS:HB3	1.63	0.44
11:p:113:VAL:HG12	18:w:73:ARG:HD3	1.99	0.44
24:1:75:G:N3	24:1:75:G:H2'	2.31	0.44
24:1:118:A:N3	24:1:178:G:H1'	2.33	0.44
1:2:864:A:H2'	1:2:865:A:C8	2.53	0.44
1:2:1169:A:H2'	1:2:1170:A:C8	2.52	0.44
1:2:1319:A:C8	1:2:1323:G:C6	3.06	0.44
10:o:66:GLU:OE2	10:o:68:ARG:NE	2.47	0.44
17:v:47:HIS:HE2	17:v:49:GLU:HG2	1.81	0.44
24:1:208:C:H2'	24:1:209:C:C6	2.53	0.44
24:1:1059:G:H3'	24:1:1060:U:H2'	1.99	0.44
24:1:1278:C:H2'	24:1:1279:G:C8	2.53	0.44
24:1:1529:G:H2'	24:1:1530:G:H8	1.83	0.44
24:1:2025:C:H2'	24:1:2026:U:C6	2.52	0.44
24:1:2667:C:N3	30:F:110:SER:OG	2.50	0.44
24:1:2728:U:O2'	24:1:2729:G:H8	2.00	0.44
25:3:5:U:H2'	25:3:6:G:H8	1.83	0.44
45:X:60:ASP:OD2	56:G:27:ARG:NH2	2.49	0.44
1:2:50:A:O2'	1:2:360:G:N2	2.50	0.44
1:2:79:G:H22	1:2:90:C:H42	1.66	0.44
1:2:514:C:H2'	1:2:515:G:H8	1.81	0.44
1:2:826:C:O2	8:m:16:ASN:ND2	2.50	0.44
21:z:24:GLU:OE2	22:4:29:A:O2'	2.17	0.44
22:4:31:G:H2'	22:4:32:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:12:U:O2	24:1:2626:C:H4'	2.18	0.44
24:1:128:C:H2'	24:1:129:C:H6	1.82	0.44
24:1:276:U:HO2'	24:1:278:A:H8	1.64	0.44
24:1:279:A:H2'	24:1:280:U:O4'	2.18	0.44
24:1:1316:U:H2'	24:1:1317:G:H8	1.81	0.44
24:1:1735:A:H2'	24:1:1736:U:C6	2.53	0.44
24:1:2340:A:H2'	24:1:2341:G:C8	2.53	0.44
24:1:2898:U:H2'	24:1:2899:A:C8	2.53	0.44
31:J:125:TYR:HH	31:J:132:HIS:CD2	2.36	0.44
34:M:41:LEU:HG	34:M:96:ILE:HG13	2.00	0.44
1:2:591:U:H2'	1:2:592:G:H8	1.83	0.43
1:2:824:G:H2'	1:2:825:A:H8	1.82	0.43
1:2:994:A:C4	1:2:1216:A:H4'	2.52	0.43
1:2:1127:G:H5'	1:2:1280:A:O2'	2.17	0.43
2:g:112:LYS:HE3	2:g:112:LYS:HB3	1.83	0.43
10:o:37:ARG:HB2	10:o:75:ASP:HB2	1.99	0.43
14:s:33:ASP:HB3	14:s:36:ALA:HB2	1.99	0.43
22:4:25:A:H2'	22:4:26:A:H8	1.83	0.43
24:1:57:C:H2'	24:1:58:G:O4'	2.18	0.43
24:1:271:G:O2'	24:1:272:A:O5'	2.33	0.43
24:1:297:G:H2'	24:1:298:G:O4'	2.18	0.43
24:1:729:G:C5	26:B:207:LYS:HB2	2.53	0.43
24:1:1536:C:H4'	24:1:1537:G:C4	2.53	0.43
24:1:2745:C:H2'	24:1:2746:U:C6	2.53	0.43
34:M:14:LYS:HE2	34:M:14:LYS:HB3	1.82	0.43
34:M:50:ARG:HA	34:M:53:MET:HE3	1.99	0.43
55:6:132:ILE:HB	55:6:179:VAL:HG12	1.99	0.43
56:G:135:HIS:HB3	56:G:138:VAL:HG12	2.00	0.43
1:2:672:U:H2'	1:2:673:A:C8	2.53	0.43
1:2:737:C:H2'	1:2:738:C:H6	1.83	0.43
1:2:842:U:C6	1:2:843:U:H5''	2.53	0.43
1:2:1329:A:C5	1:2:1330:U:C5	3.06	0.43
2:g:26:LYS:HD2	2:g:192:ASP:OD1	2.18	0.43
11:p:87:LYS:HD3	11:p:115:PRO:HD3	2.00	0.43
22:4:27:G:H2'	22:4:28:G:H8	1.83	0.43
24:1:6:A:H2'	24:1:7:G:H8	1.82	0.43
24:1:58:G:O2'	24:1:73:A:N1	2.47	0.43
24:1:1292:G:H2'	24:1:1293:C:C6	2.53	0.43
24:1:1676:A:H2'	24:1:1677:A:O4'	2.18	0.43
24:1:1683:U:H2'	24:1:1684:G:H8	1.82	0.43
24:1:1703:G:H2'	24:1:1704:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:1842:G:H2'	24:1:1843:C:C6	2.52	0.43
24:1:2038:G:H2'	24:1:2039:U:O4'	2.18	0.43
24:1:2064:C:H2'	24:1:2065:C:H6	1.83	0.43
24:1:2329:U:H2'	24:1:2330:G:H8	1.80	0.43
36:O:50:ALA:O	36:O:81:ARG:NH1	2.48	0.43
56:G:65:ALA:HB1	56:G:135:HIS:HB2	1.99	0.43
1:2:334:C:H2'	1:2:335:C:H6	1.83	0.43
1:2:923:A:H2'	1:2:924:C:C6	2.52	0.43
1:2:1326:U:H2'	1:2:1327:C:C6	2.53	0.43
1:2:1498:UR3:O4'	1:2:1519:MA6:H2	2.18	0.43
1:2:1524:C:H2'	1:2:1525:G:C8	2.53	0.43
9:n:123:ARG:NH1	9:n:124:ARG:O	2.51	0.43
24:1:4:U:H2'	24:1:5:A:H8	1.83	0.43
24:1:78:U:H2'	24:1:79:C:H6	1.82	0.43
24:1:304:U:H3	24:1:313:G:H1	1.67	0.43
24:1:1224:U:H2'	24:1:1225:G:C8	2.52	0.43
24:1:2408:U:H2'	24:1:2409:G:C8	2.53	0.43
24:1:2469:A:H4'	34:M:55:ARG:CD	2.48	0.43
30:F:121:ILE:HD12	30:F:141:ILE:HG22	2.00	0.43
46:Y:14:LEU:HB3	46:Y:57:LEU:HD21	1.99	0.43
1:2:407:U:H2'	1:2:408:A:H8	1.83	0.43
1:2:422:C:O2	1:2:423:G:N1	2.51	0.43
1:2:676:A:H2'	1:2:677:U:H6	1.84	0.43
1:2:900:A:H2'	1:2:901:A:C8	2.53	0.43
1:2:1350:A:O2'	7:l:33:ASP:OD1	2.30	0.43
1:2:1356:G:H2'	1:2:1357:A:H8	1.80	0.43
11:p:35:THR:HG22	11:p:41:ALA:HA	2.00	0.43
22:4:34:U:H4'	22:4:35:U:H6	1.82	0.43
22:4:42:G:C2	55:6:214:HIS:HB3	2.53	0.43
24:1:278:A:C6	24:1:362:A:C8	3.06	0.43
24:1:721:A:H2'	24:1:722:A:C8	2.54	0.43
24:1:1068:G:N2	24:1:1095:A:O2'	2.51	0.43
1:2:154:U:H2'	1:2:155:A:C8	2.54	0.43
1:2:514:C:C2	1:2:515:G:C8	3.06	0.43
1:2:1009:U:H2'	1:2:1010:U:C6	2.54	0.43
1:2:1250:A:N3	1:2:1370:G:O2'	2.50	0.43
24:1:1412:U:H2'	24:1:1413:A:C8	2.53	0.43
24:1:2316:G:H2'	24:1:2317:A:H8	1.84	0.43
26:B:2:ALA:N	26:B:20:VAL:O	2.52	0.43
29:E:52:ASN:CB	29:E:150:ARG:HH22	2.30	0.43
32:K:107:LEU:HB2	32:K:116:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:I:109:ALA:HB2	54:I:128:ILE:HD12	2.01	0.43
1:2:201:G:H2'	1:2:202:G:O4'	2.19	0.43
1:2:253:A:H2'	1:2:254:G:H8	1.83	0.43
1:2:1040:U:H2'	1:2:1041:G:C8	2.53	0.43
4:i:85:ASN:HB3	4:i:88:GLU:HG3	2.00	0.43
24:1:566:U:H5''	33:L:29:LYS:HE3	2.00	0.43
24:1:1179:G:H2'	24:1:1180:U:C6	2.53	0.43
24:1:1306:C:H2'	24:1:1307:A:H8	1.82	0.43
24:1:1496:A:H2'	24:1:1498:C:C5	2.53	0.43
24:1:2591:C:H2'	24:1:2592:G:H8	1.82	0.43
36:O:115:LEU:HD23	36:O:115:LEU:HA	1.83	0.43
1:2:321:A:H2'	1:2:322:C:C6	2.53	0.43
1:2:649:A:H2'	1:2:650:G:O4'	2.18	0.43
1:2:745:G:H2'	1:2:746:A:H8	1.83	0.43
1:2:1148:U:H2'	1:2:1149:C:O4'	2.18	0.43
1:2:1188:A:H2'	1:2:1189:U:O4'	2.18	0.43
1:2:1206:G:H2'	1:2:1207:2MG:O4'	2.18	0.43
7:l:81:GLY:C	22:4:34:U:H5'	2.43	0.43
10:o:10:LEU:HD11	10:o:25:ILE:HD12	2.00	0.43
24:1:279:A:C6	24:1:361:G:H1'	2.53	0.43
24:1:359:G:H2'	24:1:360:U:H5'	1.99	0.43
24:1:388:G:H2'	24:1:390:U:C5	2.54	0.43
24:1:493:G:O2'	40:S:7:HIS:HA	2.19	0.43
24:1:819:A:H5''	24:1:973:A:N1	2.34	0.43
24:1:1268:A:H2'	24:1:1269:A:O4'	2.18	0.43
24:1:1281:G:H2'	24:1:1282:U:C6	2.54	0.43
24:1:1544:A:H2'	24:1:1545:A:C8	2.53	0.43
24:1:1651:G:OP1	35:N:40:LYS:NZ	2.47	0.43
24:1:2419:U:H4'	49:c:22:THR:HG21	2.00	0.43
28:D:111:GLU:OE1	28:D:115:GLN:NE2	2.46	0.43
29:E:105:THR:HA	53:a:38:SER:HB2	1.99	0.43
33:L:112:LEU:HD12	33:L:130:GLY:HA3	2.00	0.43
55:6:125:SER:HA	55:6:187:TYR:HA	2.01	0.43
1:2:513:C:H2'	1:2:514:C:C6	2.54	0.43
1:2:859:G:H2'	1:2:860:A:C8	2.54	0.43
1:2:974:A:OP1	14:s:69:ARG:NH2	2.51	0.43
4:i:146:ARG:O	4:i:150:LYS:HG3	2.18	0.43
24:1:933:A:H5'	24:1:934:U:OP2	2.19	0.43
24:1:1771:C:H2'	24:1:1772:A:C8	2.54	0.43
24:1:2247:A:H2'	24:1:2248:C:H6	1.84	0.43
60:1:3332:PUT:H42	60:1:3332:PUT:H11	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1022:A:H2'	1:2:1023:U:O4'	2.18	0.43
24:1:41:C:H2'	24:1:42:A:O4'	2.18	0.43
24:1:208:C:H2'	24:1:209:C:H6	1.83	0.43
24:1:580:U:H2'	24:1:581:C:H6	1.83	0.43
24:1:782:A:N7	26:B:220:VAL:HG21	2.34	0.43
24:1:909:A:H2'	24:1:912:C:H5	1.84	0.43
24:1:979:A:H2'	24:1:982:C:H42	1.83	0.43
24:1:1414:C:H2'	24:1:1415:U:O4'	2.19	0.43
24:1:1880:U:H2'	24:1:1881:C:C6	2.53	0.43
24:1:2639:A:H2'	24:1:2640:G:O4'	2.19	0.43
25:3:42:C:C6	29:E:66:LEU:HB2	2.54	0.43
34:M:8:LYS:H	34:M:8:LYS:HG2	1.60	0.43
1:2:1160:G:C2	1:2:1161:C:C6	3.07	0.43
1:2:1414:U:H2'	1:2:1415:G:H8	1.84	0.43
24:1:492:A:H2'	24:1:493:G:O4'	2.19	0.43
24:1:990:A:C6	24:1:1186:G:H1'	2.54	0.43
24:1:1003:G:O2'	24:1:1010:A:N1	2.51	0.43
24:1:2330:G:H21	44:W:42:GLY:HA2	1.84	0.43
26:B:68:LYS:NZ	26:B:149:GLY:O	2.51	0.43
27:C:35:THR:HG22	27:C:73:VAL:HG21	2.01	0.43
56:G:16:GLY:HA2	56:G:47:PHE:CE2	2.54	0.43
1:2:251:G:C6	1:2:266:G:C6	3.07	0.42
1:2:456:A:H3'	1:2:457:G:H8	1.84	0.42
1:2:771:G:H2'	1:2:772:U:C6	2.54	0.42
1:2:1031:C:H4'	1:2:1032:G:N1	2.34	0.42
2:g:132:LYS:O	2:g:136:MET:HG3	2.19	0.42
14:s:10:GLU:HG3	14:s:63:ARG:HD2	2.01	0.42
16:u:9:HIS:HD2	16:u:18:GLN:HG3	1.84	0.42
24:1:468:G:N7	50:d:39:ARG:NH2	2.58	0.42
24:1:682:G:H5'	50:d:26:ASN:CG	2.44	0.42
24:1:1076:C:H2'	24:1:1077:A:H8	1.83	0.42
24:1:1079:C:H2'	24:1:1080:A:C8	2.53	0.42
24:1:1946:U:H2'	24:1:1947:C:C6	2.54	0.42
24:1:2339:C:H2'	24:1:2340:A:H8	1.84	0.42
28:D:12:LEU:HD11	28:D:194:LYS:HE3	2.00	0.42
37:P:53:ARG:HD3	37:P:53:ARG:HA	1.80	0.42
55:6:296:TYR:CZ	55:6:300:MET:HE3	2.54	0.42
1:2:34:C:H2'	1:2:35:G:C8	2.54	0.42
1:2:231:U:H2'	1:2:232:G:H8	1.84	0.42
1:2:263:A:H2'	1:2:264:C:C6	2.54	0.42
10:o:10:LEU:HD12	10:o:22:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:t:29:VAL:HG13	15:t:63:ARG:HG3	2.01	0.42
24:1:30:G:H2'	24:1:31:C:H6	1.83	0.42
24:1:629:G:H1'	24:1:639:U:H1'	2.01	0.42
24:1:876:C:H2'	24:1:877:A:O4'	2.17	0.42
24:1:934:U:H2'	24:1:935:C:C6	2.54	0.42
24:1:1997:C:OP2	27:C:129:THR:OG1	2.28	0.42
24:1:2074:U:H2'	24:1:2075:U:C6	2.54	0.42
24:1:2183:A:H2'	24:1:2184:A:C8	2.55	0.42
24:1:2649:C:H2'	24:1:2650:U:C6	2.53	0.42
1:2:483:C:H2'	1:2:484:G:C8	2.55	0.42
1:2:1226:C:O2'	13:r:102:THR:O	2.31	0.42
4:i:11:LEU:O	4:i:15:GLU:HG2	2.18	0.42
5:j:164:ILE:HD12	5:j:164:ILE:HA	1.85	0.42
8:m:7:ILE:O	8:m:11:LEU:HG	2.19	0.42
11:p:34:ILE:HB	11:p:74:VAL:HG11	2.01	0.42
15:t:10:LYS:HE2	15:t:10:LYS:HB3	1.85	0.42
22:4:28:G:H2'	22:4:29:A:H8	1.84	0.42
24:1:605:G:H1'	24:1:657:U:H1'	2.01	0.42
24:1:749:A:H4'	24:1:1271:G:N3	2.34	0.42
24:1:1094:U:H1'	24:1:1097:U:H5	1.84	0.42
24:1:1361:G:H2'	24:1:1362:C:H6	1.83	0.42
24:1:2518:A:H2'	24:1:2518:A:N3	2.34	0.42
26:B:181:MET:HB3	26:B:268:VAL:HB	2.01	0.42
27:C:55:LYS:HD3	27:C:60:VAL:HG22	2.02	0.42
44:W:11:ARG:O	44:W:12:ASN:ND2	2.52	0.42
46:Y:19:LEU:HD23	46:Y:19:LEU:HA	1.79	0.42
1:2:115:G:H1'	1:2:116:A:N7	2.35	0.42
1:2:593:U:H2'	1:2:594:U:H6	1.84	0.42
1:2:751:U:H2'	1:2:752:G:O4'	2.20	0.42
1:2:821:G:H2'	1:2:822:U:C6	2.54	0.42
1:2:842:U:H4'	1:2:846:G:C6	2.54	0.42
1:2:979:C:O2	14:s:59:ARG:HD2	2.18	0.42
1:2:1047:G:H5''	14:s:4:GLN:HG3	2.01	0.42
1:2:1277:C:H1'	1:2:1282:C:O2	2.19	0.42
24:1:569:U:O2'	24:1:983:A:N1	2.48	0.42
24:1:577:G:H2'	24:1:578:G:C8	2.54	0.42
24:1:871:U:H2'	24:1:872:U:H6	1.82	0.42
24:1:2050:C:H2'	24:1:2051:A:C8	2.54	0.42
24:1:2723:C:H2'	24:1:2724:U:O4'	2.20	0.42
56:G:94:ILE:HB	56:G:122:LEU:HB2	2.00	0.42
1:2:109:A:H2'	1:2:326:G:N2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:542:G:H5'	4:i:39:GLY:HA3	2.01	0.42
1:2:1346:A:N1	1:2:1374:A:H5''	2.35	0.42
1:2:1371:G:O3'	9:n:71:GLY:HA3	2.20	0.42
13:r:40:ALA:HB3	13:r:43:VAL:HG23	2.00	0.42
14:s:83:LYS:HA	14:s:83:LYS:HD3	1.85	0.42
24:1:182:A:H2'	24:1:183:C:H6	1.84	0.42
24:1:281:C:H2'	24:1:282:A:H8	1.83	0.42
24:1:586:A:N1	24:1:809:G:O2'	2.45	0.42
24:1:1059:G:C2	24:1:1080:A:C2	3.07	0.42
24:1:2233:U:H2'	24:1:2234:G:H8	1.84	0.42
24:1:2298:A:H2'	24:1:2299:U:O4'	2.20	0.42
34:M:53:MET:HE3	34:M:53:MET:HB2	1.86	0.42
1:2:321:A:H2'	1:2:322:C:H6	1.84	0.42
1:2:839:C:H2'	1:2:840:C:H6	1.85	0.42
1:2:908:A:H2'	1:2:909:A:H8	1.85	0.42
1:2:1315:U:O2	1:2:1360:A:H2	2.02	0.42
1:2:1343:G:H2'	1:2:1344:C:C6	2.54	0.42
1:2:1372:U:H2'	1:2:1373:G:O4'	2.20	0.42
2:g:130:THR:OG1	2:g:131:LYS:N	2.53	0.42
24:1:27:G:N2	24:1:512:G:H1'	2.35	0.42
24:1:69:C:O2	24:1:73:A:O2'	2.34	0.42
24:1:279:A:H1'	24:1:362:A:H4'	2.01	0.42
24:1:820:A:H4'	24:1:836:G:H22	1.85	0.42
24:1:1870:C:O2'	24:1:1871:A:O4'	2.32	0.42
24:1:2345:G:N3	24:1:2381:A:H2'	2.35	0.42
35:N:24:MET:HE1	35:N:40:LYS:HD3	2.01	0.42
37:P:114:LEU:HD23	37:P:114:LEU:HA	1.83	0.42
1:2:981:U:OP1	14:s:9:ARG:NH1	2.49	0.42
1:2:1319:A:O2'	1:2:1323:G:N7	2.45	0.42
4:i:99:ASP:OD1	4:i:100:ASN:N	2.53	0.42
7:l:149:LYS:HE2	7:l:149:LYS:HB2	1.86	0.42
14:s:74:LEU:HD12	14:s:84:VAL:HG21	2.01	0.42
19:x:9:PRO:HD3	53:a:64:PHE:CG	2.54	0.42
24:1:2:G:H2'	24:1:3:U:H6	1.82	0.42
24:1:184:C:H2'	24:1:185:G:H8	1.84	0.42
24:1:570:G:H2'	24:1:2030:6MZ:N7	2.34	0.42
24:1:1599:U:H2'	24:1:1600:C:C6	2.55	0.42
24:1:2266:A:H4'	24:1:2267:A:N3	2.35	0.42
24:1:2305:U:H2'	24:1:2306:C:C6	2.55	0.42
24:1:2314:A:H2'	24:1:2315:G:C8	2.55	0.42
55:6:213[B]:ARG:HH21	55:6:329:ASP:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:358:U:H2'	1:2:359:G:C8	2.55	0.42
1:2:543:U:OP1	4:i:14:ARG:HD2	2.20	0.42
1:2:997:U:H2'	1:2:998:C:O4'	2.20	0.42
1:2:1033:G:C8	1:2:1034:G:C8	3.07	0.42
2:g:61:ALA:CB	2:g:221:VAL:HG13	2.50	0.42
3:h:79:LYS:HA	3:h:79:LYS:HD3	1.86	0.42
5:j:77:ASN:HB2	5:j:82:GLN:CD	2.45	0.42
16:u:6:LEU:HB3	16:u:17:TYR:HB3	2.01	0.42
24:1:279:A:C6	24:1:280:U:C2	3.08	0.42
24:1:538:A:H5''	31:J:7:LYS:HE3	2.02	0.42
24:1:959:A:N3	24:1:2457:PSU:O2'	2.48	0.42
24:1:1042:G:H2'	24:1:1043:C:C6	2.54	0.42
24:1:1062:G:C2	24:1:1063:G:C5	3.07	0.42
24:1:1212:G:H1'	24:1:1237:A:N6	2.35	0.42
24:1:1440:U:H2'	24:1:1441:G:C8	2.54	0.42
24:1:1511:G:H2'	24:1:1512:C:H6	1.85	0.42
24:1:1602:U:OP2	41:T:64:LYS:NZ	2.48	0.42
24:1:2638:G:O2'	24:1:2775:G:N2	2.50	0.42
29:E:14:LYS:H	29:E:14:LYS:HD2	1.85	0.42
33:L:77:ILE:HD13	33:L:108:ALA:HB1	2.01	0.42
39:R:57:GLY:HA2	39:R:102:SER:O	2.19	0.42
1:2:35:G:H2'	1:2:36:C:H6	1.85	0.42
1:2:195:A:H1'	1:2:222:C:O2'	2.19	0.42
1:2:236:A:H2'	1:2:237:G:H8	1.84	0.42
1:2:920:U:H2'	1:2:921:U:C6	2.54	0.42
1:2:996:A:H2'	1:2:997:U:C6	2.55	0.42
9:n:33:ARG:HH21	9:n:38:TYR:HA	1.85	0.42
12:q:50:ARG:HB3	12:q:66:TYR:HE1	1.85	0.42
24:1:65:U:H2'	24:1:66:C:H6	1.85	0.42
24:1:753:A:H2'	24:1:754:U:C6	2.55	0.42
24:1:1394:U:H4'	24:1:1603:A:H4'	2.02	0.42
24:1:1668:A:O2'	24:1:1674:G:N7	2.44	0.42
24:1:1917:PSU:H2'	24:1:1918:A:O4'	2.20	0.42
34:M:110:GLU:O	34:M:114:ARG:HG3	2.19	0.42
34:M:136:MET:O	43:V:79:ARG:NH2	2.29	0.42
1:2:205:A:C6	1:2:206:C:N4	2.88	0.42
24:1:742:A:H2'	24:1:743:A:H8	1.84	0.42
24:1:1042:G:H2'	24:1:1043:C:H6	1.85	0.42
24:1:1509:A:HO2'	24:1:1510:G:H8	1.63	0.42
24:1:1932:A:H2'	24:1:1933:G:O4'	2.19	0.42
24:1:2185:U:H2'	24:1:2186:G:N7	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:1:3334:PUT:H12	60:1:3334:PUT:H41	1.91	0.42
29:E:135:GLN:HG2	29:E:141:ILE:HG21	2.00	0.42
35:N:47:VAL:O	35:N:51:LEU:HD23	2.20	0.42
1:2:8:A:N6	4:i:206:LYS:HB3	2.35	0.41
1:2:1125:U:C2	1:2:1127:G:C8	3.09	0.41
1:2:1236:A:H2'	1:2:1237:C:C6	2.55	0.41
2:g:188:ASP:OD1	2:g:189:THR:N	2.43	0.41
3:h:123:GLN:NE2	3:h:136:ARG:HH21	2.18	0.41
24:1:40:U:H2'	24:1:41:C:C6	2.55	0.41
24:1:411:G:OP2	24:1:2406:A:O2'	2.36	0.41
24:1:527:C:N4	24:1:2777:G:O2'	2.47	0.41
24:1:1068:G:O6	24:1:1069:A:N6	2.52	0.41
24:1:1149:G:H2'	24:1:1150:C:C6	2.55	0.41
24:1:1406:U:H2'	24:1:1407:G:H8	1.84	0.41
24:1:2183:A:H2'	24:1:2184:A:H8	1.84	0.41
24:1:2216:G:H2'	24:1:2217:G:H8	1.85	0.41
24:1:2615:U:C2	48:b:4:GLN:HA	2.55	0.41
36:O:80:GLU:O	36:O:84:GLU:HG2	2.19	0.41
54:I:102:ARG:HA	54:I:105:LEU:HD12	2.02	0.41
1:2:626:G:OP1	16:u:35:ARG:NH2	2.53	0.41
1:2:678:U:H2'	1:2:679:C:H6	1.85	0.41
4:i:91:LEU:HD23	4:i:91:LEU:HA	1.85	0.41
8:m:69:LYS:HB3	8:m:69:LYS:HE3	1.78	0.41
23:5:15:G:H2'	23:5:59:A:N1	2.34	0.41
24:1:32:C:H2'	24:1:33:C:C6	2.56	0.41
24:1:296:U:H2'	24:1:297:G:H8	1.85	0.41
24:1:488:G:N2	24:1:491:G:H5''	2.36	0.41
24:1:651:G:H5'	51:e:19:LYS:HG3	2.02	0.41
24:1:1065:U:HO2'	24:1:1066:U:P	2.43	0.41
24:1:1966:A:N3	24:1:2592:G:O2'	2.53	0.41
24:1:2516:A:O2'	24:1:2517:C:H5'	2.20	0.41
24:1:2700:A:H2'	24:1:2701:U:H6	1.84	0.41
24:1:2861:U:H2'	24:1:2862:G:C8	2.55	0.41
1:2:1244:G:H2'	1:2:1245:C:C6	2.55	0.41
1:2:1369:C:H2'	1:2:1370:G:C8	2.55	0.41
6:k:32:ALA:CB	6:k:70:VAL:HG11	2.50	0.41
8:m:50:LYS:HE3	8:m:50:LYS:HB2	1.73	0.41
24:1:4:U:H2'	24:1:5:A:C8	2.55	0.41
24:1:157:C:H2'	24:1:158:U:O4'	2.20	0.41
24:1:250:G:H2'	24:1:251:A:C8	2.55	0.41
24:1:2194:U:H2'	24:1:2195:U:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:200:HIS:HE1	26:B:203:ARG:HH21	1.66	0.41
34:M:54:THR:HG22	34:M:59:ARG:HG2	2.01	0.41
45:X:40:VAL:HG22	45:X:43:GLU:H	1.84	0.41
1:2:155:A:H2'	1:2:156:C:C6	2.55	0.41
1:2:911:U:H2'	1:2:912:C:C6	2.56	0.41
1:2:1071:C:H2'	1:2:1072:G:C8	2.52	0.41
1:2:1446:A:H8	1:2:1446:A:OP1	2.02	0.41
14:s:3:LYS:HB2	14:s:6:MET:HG2	2.02	0.41
24:1:273:G:C6	24:1:274:C:C4	3.09	0.41
24:1:630:G:N2	24:1:633:A:OP2	2.40	0.41
24:1:1063:G:O2'	24:1:1064:C:C6	2.74	0.41
24:1:1295:C:C2	24:1:1296:G:C8	3.08	0.41
24:1:1297:C:OP1	24:1:2710:C:H4'	2.20	0.41
24:1:1327:A:H2'	24:1:1328:A:O4'	2.20	0.41
24:1:1364:G:P	45:X:50:ARG:HH12	2.43	0.41
24:1:1412:U:H2'	24:1:1413:A:H8	1.85	0.41
24:1:1842:G:H2'	24:1:1843:C:H6	1.85	0.41
26:B:155:ALA:HB2	26:B:162:VAL:HG23	2.02	0.41
1:2:268:U:H2'	1:2:269:C:C6	2.56	0.41
1:2:739:C:OP2	6:k:2:ARG:NH2	2.47	0.41
1:2:1175:G:H2'	1:2:1176:A:C8	2.56	0.41
1:2:1313:U:H2'	1:2:1314:C:C6	2.56	0.41
24:1:822:G:H2'	24:1:823:C:C6	2.56	0.41
24:1:948:C:H1'	24:1:984:A:C8	2.55	0.41
24:1:1829:A:C8	24:1:1830:C:C5	3.09	0.41
24:1:2205:A:H2'	24:1:2206:C:C6	2.55	0.41
24:1:2771:C:H2'	24:1:2772:C:H6	1.85	0.41
25:3:93:C:H2'	25:3:94:A:C8	2.56	0.41
35:N:70:THR:O	35:N:70:THR:OG1	2.37	0.41
55:6:40:GLU:O	55:6:46:VAL:HB	2.21	0.41
1:2:440:C:C2	1:2:441:A:C8	3.08	0.41
1:2:489:C:H2'	1:2:490:C:C6	2.56	0.41
1:2:744:C:H2'	1:2:745:G:H8	1.85	0.41
1:2:1180:A:OP1	9:n:105:THR:OG1	2.26	0.41
13:r:68:ASP:OD1	13:r:71:ARG:NH1	2.53	0.41
20:y:44:LYS:HD3	20:y:87:ALA:HA	2.02	0.41
23:5:23:C:H2'	23:5:24:U:C6	2.56	0.41
24:1:1322:A:C5	24:1:1323:C:C5	3.09	0.41
24:1:1936:A:H61	24:1:1963:U:H3	1.68	0.41
1:2:592:G:H2'	1:2:593:U:C6	2.56	0.41
1:2:704:A:C4	1:2:705:G:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:844:G:C2	1:2:846:G:H1'	2.55	0.41
1:2:954:G:H2'	1:2:955:U:C6	2.56	0.41
1:2:1319:A:C8	1:2:1323:G:C5	3.09	0.41
1:2:1360:A:H2'	1:2:1361:G:H8	1.85	0.41
12:q:54:ARG:NH1	12:q:62:GLU:HG2	2.34	0.41
13:r:71:ARG:NH2	29:E:113:ASP:OD1	2.54	0.41
24:1:307:G:N2	24:1:309:A:H3'	2.36	0.41
24:1:538:A:H2'	24:1:539:G:O4'	2.20	0.41
24:1:1114:C:O2'	24:1:1115:G:H5'	2.20	0.41
24:1:1199:U:H2'	24:1:1200:C:H6	1.86	0.41
24:1:1721:G:O2'	24:1:1739:A:N6	2.52	0.41
24:1:2336:A:H61	44:W:43:THR:CG2	2.31	0.41
24:1:2552:OMU:HM23	24:1:2554:U:C6	2.56	0.41
24:1:2813:A:H2'	24:1:2814:A:H8	1.84	0.41
1:2:466:A:C2	1:2:468:A:C4	3.08	0.41
1:2:512:U:H2'	1:2:513:C:C6	2.55	0.41
1:2:687:A:C2	1:2:704:A:C5	3.08	0.41
1:2:1120:C:C2	1:2:1121:U:C5	3.08	0.41
2:g:59:LYS:HE2	2:g:59:LYS:HB2	1.93	0.41
18:w:57:ARG:O	18:w:61:ARG:HG3	2.21	0.41
24:1:145:C:H2'	24:1:146:A:H8	1.84	0.41
24:1:476:G:N1	24:1:479:A:OP2	2.49	0.41
24:1:1463:C:H2'	24:1:1464:G:C8	2.56	0.41
24:1:1736:U:H2'	24:1:1737:G:O4'	2.20	0.41
24:1:2547:A:H4'	32:K:29:HIS:NE2	2.36	0.41
24:1:2813:A:H2'	24:1:2814:A:C8	2.55	0.41
26:B:245:VAL:HG12	26:B:251:GLN:HA	2.02	0.41
27:C:12:THR:HG22	27:C:13:ARG:H	1.86	0.41
43:V:72:VAL:HB	43:V:91:PHE:HB3	2.02	0.41
45:X:59:ILE:HG12	45:X:67:VAL:HG21	2.02	0.41
1:2:33:A:H2'	1:2:34:C:C6	2.56	0.41
1:2:333:U:OP1	20:y:2:ALA:N	2.54	0.41
1:2:360:G:C6	1:2:361:G:C6	3.08	0.41
1:2:404:G:O2'	1:2:498:A:N1	2.47	0.41
1:2:410:G:H2'	1:2:429:U:C4	2.55	0.41
1:2:579:A:H2'	1:2:580:C:C6	2.55	0.41
1:2:1179:A:H2'	1:2:1180:A:O4'	2.20	0.41
1:2:1241:G:H2'	1:2:1242:G:H8	1.85	0.41
1:2:1330:U:C4	1:2:1331:G:C6	3.09	0.41
1:2:1412:C:H2'	1:2:1413:A:C8	2.56	0.41
4:i:85:ASN:HB3	4:i:88:GLU:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:l:26:PHE:HZ	7:l:120:LEU:HD11	1.86	0.41
19:x:80:TYR:CZ	19:x:82:GLY:HA2	2.56	0.41
20:y:55:GLN:HG3	20:y:76:LYS:HD2	2.02	0.41
23:5:75:C:H2'	23:5:76:A:C8	2.56	0.41
24:1:56:A:H2'	24:1:57:C:O4'	2.21	0.41
24:1:133:U:H2'	24:1:134:G:C8	2.56	0.41
24:1:367:G:H2'	24:1:368:A:C8	2.56	0.41
24:1:659:G:O5'	28:D:95:LYS:HD3	2.20	0.41
24:1:720:U:H2'	24:1:721:A:H8	1.86	0.41
24:1:881:G:H2'	24:1:882:G:C8	2.55	0.41
24:1:909:A:H2'	24:1:912:C:C5	2.55	0.41
24:1:1183:U:H2'	24:1:1184:U:C6	2.56	0.41
24:1:2062:A:HO2'	24:1:2063:C:H6	1.68	0.41
24:1:2100:G:C6	24:1:2190:G:C6	3.09	0.41
24:1:2104:C:N4	24:1:2186:G:O6	2.54	0.41
25:3:49:C:H2'	25:3:50:A:H8	1.85	0.41
25:3:112:G:H2'	25:3:113:C:C6	2.55	0.41
28:D:118:LEU:HD11	28:D:188:MET:SD	2.61	0.41
31:J:9:GLU:CD	31:J:9:GLU:H	2.28	0.41
34:M:17:ASN:OD1	34:M:97:GLN:NE2	2.45	0.41
55:6:355:GLN:H	55:6:355:GLN:HG2	1.71	0.41
1:2:590:U:H2'	1:2:591:U:C6	2.56	0.41
1:2:1157:A:C2	1:2:1181:G:C4	3.09	0.41
1:2:1434:A:H2'	1:2:1435:G:O4'	2.21	0.41
3:h:50:ALA:HB1	3:h:76:VAL:HG22	2.02	0.41
5:j:81:LEU:HB2	5:j:98:PRO:HG3	2.03	0.41
6:k:4:TYR:CE1	6:k:71:ILE:HG13	2.56	0.41
10:o:10:LEU:HD22	10:o:98:VAL:HG22	2.03	0.41
10:o:52:LEU:HB2	14:s:81:ARG:HD2	2.02	0.41
24:1:64:A:H2'	24:1:65:U:H6	1.86	0.41
24:1:228:C:N4	24:1:2407:A:N3	2.65	0.41
24:1:415:A:H2'	24:1:416:U:C6	2.55	0.41
24:1:1100:C:H2'	24:1:1101:U:O4'	2.21	0.41
24:1:1223:G:C6	24:1:1227:G:C6	3.09	0.41
24:1:1856:U:H2'	24:1:1857:G:O4'	2.20	0.41
24:1:2498:OMC:HM22	24:1:2499:C:H5'	2.03	0.41
25:3:45:A:C4	25:3:46:A:C8	3.09	0.41
55:6:277:ASP:OD1	55:6:278:ARG:N	2.54	0.41
1:2:580:C:H2'	1:2:581:G:C8	2.56	0.40
1:2:1175:G:H2'	1:2:1176:A:H8	1.86	0.40
1:2:1253:G:H2'	1:2:1254:A:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:m:90:ASP:OD1	8:m:91:GLU:HG3	2.21	0.40
9:n:24:GLY:HA3	9:n:62:ASP:CG	2.47	0.40
16:u:3:THR:HG22	16:u:66:THR:OG1	2.21	0.40
17:v:14:SER:HB3	17:v:22:VAL:HB	2.02	0.40
24:1:184:C:H2'	24:1:185:G:C8	2.56	0.40
24:1:279:A:N6	24:1:361:G:H1'	2.36	0.40
24:1:1338:G:O2'	24:1:1393:A:N1	2.52	0.40
24:1:1428:C:C5	24:1:1569:A:H5''	2.56	0.40
24:1:1904:G:O2'	24:1:1928:A:N1	2.52	0.40
24:1:2300:C:H2'	24:1:2301:C:H6	1.86	0.40
24:1:2677:G:H2'	24:1:2678:C:C6	2.56	0.40
24:1:2687:U:H2'	24:1:2688:G:O4'	2.21	0.40
26:B:160:THR:HB	26:B:177:ARG:HG3	2.03	0.40
28:D:97:ASN:HB2	28:D:100:MET:HG3	2.03	0.40
29:E:50:LEU:HD11	29:E:67:ILE:HD12	2.03	0.40
38:Q:58:ARG:HA	38:Q:61:TRP:CE3	2.56	0.40
55:6:10:ARG:HD2	55:6:107:GLU:OE1	2.22	0.40
55:6:58:LYS:HE2	55:6:58:LYS:HB2	1.94	0.40
1:2:266:G:P	60:2:1731:PUT:H12	2.61	0.40
1:2:418:C:H2'	1:2:419:C:C6	2.56	0.40
1:2:466:A:H4'	1:2:467:U:C5	2.56	0.40
1:2:784:A:H2'	1:2:785:G:C8	2.56	0.40
1:2:842:U:N3	1:2:844:G:OP2	2.54	0.40
1:2:1002:G:C4	1:2:1003:G:C8	3.09	0.40
1:2:1328:C:H5''	13:r:28:THR:HG21	2.03	0.40
2:g:101:LEU:HB3	2:g:179:LEU:HD12	2.03	0.40
2:g:117:LEU:HD22	2:g:141:LEU:HD12	2.04	0.40
10:o:36:VAL:HG12	10:o:76:ILE:HD13	2.02	0.40
24:1:438:G:H2'	24:1:439:A:C8	2.56	0.40
24:1:451:U:H2'	24:1:453:A:OP2	2.21	0.40
24:1:607:U:N3	24:1:608:A:N7	2.68	0.40
24:1:1201:U:H2'	24:1:1202:G:C8	2.56	0.40
24:1:1536:C:H4'	24:1:1537:G:N3	2.36	0.40
24:1:2257:U:O2'	24:1:2258:C:H5'	2.21	0.40
24:1:2287:A:C8	24:1:2289:G:C8	3.09	0.40
24:1:2533:U:H2'	24:1:2534:A:O4'	2.22	0.40
24:1:2584:U:H4'	55:6:249:ALA:O	2.22	0.40
24:1:2784:U:H2'	24:1:2785:C:C6	2.57	0.40
31:J:95:ARG:HD3	31:J:96:ARG:NH1	2.36	0.40
44:W:59:LEU:HD12	44:W:80:ILE:HD12	2.03	0.40
56:G:94:ILE:HG23	56:G:98:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:309:A:H2'	1:2:310:G:H8	1.87	0.40
1:2:479:U:O4	58:2:1690:SPD:H72	2.22	0.40
1:2:1316:G:N2	1:2:1318:A:H3'	2.35	0.40
3:h:22:TRP:NE1	3:h:36:ASP:OD2	2.45	0.40
5:j:44:GLY:O	5:j:74:VAL:N	2.49	0.40
11:p:64:GLN:HG3	11:p:99:ALA:HB2	2.03	0.40
24:1:36:G:N3	24:1:450:G:O2'	2.53	0.40
24:1:359:G:H2'	24:1:359:G:N3	2.36	0.40
24:1:396:G:OP2	45:X:10:LYS:NZ	2.50	0.40
24:1:1637:A:H5'	24:1:1760:C:O2'	2.22	0.40
24:1:1881:C:H2'	24:1:1882:U:O4'	2.20	0.40
24:1:1993:U:H4'	27:C:133:THR:OG1	2.21	0.40
24:1:2447:G:C8	24:1:2500:U:H3'	2.56	0.40
25:3:79:G:O6	43:V:14:LYS:NZ	2.48	0.40
42:U:54:GLN:H	42:U:54:GLN:CD	2.29	0.40
54:I:107:GLU:O	54:I:110:GLN:HG2	2.21	0.40
1:2:18:C:OP1	5:j:132:ASN:ND2	2.43	0.40
1:2:77:A:H2'	1:2:78:A:O4'	2.21	0.40
1:2:217:C:H2'	1:2:218:U:C6	2.56	0.40
1:2:324:G:N2	1:2:326:G:H3'	2.37	0.40
1:2:398:U:H2'	1:2:399:G:C8	2.57	0.40
8:m:96:MET:HE2	8:m:99:LEU:HB2	2.04	0.40
18:w:32:TYR:HB3	18:w:55:LEU:HD21	2.04	0.40
22:4:24:U:H2'	22:4:25:A:C8	2.54	0.40
24:1:279:A:H61	24:1:360:U:H2'	1.86	0.40
24:1:975:A:H1'	24:1:990:A:C2	2.56	0.40
24:1:1827:U:H2'	24:1:1828:G:O4'	2.22	0.40
24:1:2039:U:H2'	24:1:2040:G:H8	1.85	0.40
24:1:2151:U:H2'	24:1:2152:G:H8	1.87	0.40
24:1:2228:G:H2'	24:1:2229:U:C6	2.56	0.40
24:1:2455:G:H2'	24:1:2456:C:H6	1.86	0.40
24:1:2537:U:H2'	24:1:2538:C:H6	1.84	0.40
25:3:111:U:H2'	25:3:112:G:H8	1.87	0.40
29:E:4:LEU:HD23	29:E:4:LEU:HA	1.79	0.40
29:E:69:LYS:HE3	29:E:69:LYS:HB3	1.86	0.40
38:Q:72:ASN:HB3	38:Q:110:VAL:HG11	2.04	0.40
38:Q:94:ILE:HG21	39:R:4:VAL:HG11	2.02	0.40
42:U:49:VAL:H	42:U:54:GLN:HA	1.86	0.40
47:Z:40:ASP:OD2	47:Z:45:ARG:NH2	2.46	0.40
1:2:1399:C:O2	1:2:1502:A:N6	2.55	0.40
1:2:1410:A:H2'	1:2:1411:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:102:LEU:HB3	12:q:103:ASP:H	1.80	0.40
24:1:858:G:N3	24:1:2268:A:H2'	2.36	0.40
24:1:914:G:H5'	24:1:915:C:OP2	2.22	0.40
24:1:1857:G:C2	24:1:1884:G:N3	2.90	0.40
24:1:1945:G:H2'	24:1:1946:U:C6	2.55	0.40
24:1:2078:C:H2'	24:1:2079:U:C6	2.56	0.40
24:1:2340:A:H2'	24:1:2341:G:H8	1.87	0.40
24:1:2756:U:H1'	24:1:2757:A:H5''	2.03	0.40
24:1:2771:C:H2'	24:1:2772:C:C6	2.56	0.40
24:1:2850:A:N7	24:1:2868:A:O2'	2.45	0.40
31:J:36:LEU:HD11	31:J:122:LEU:HB2	2.04	0.40
35:N:56:LYS:HE2	35:N:87:PHE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	g	222/241 (92%)	217 (98%)	5 (2%)	0	100	100
3	h	208/233 (89%)	204 (98%)	4 (2%)	0	100	100
4	i	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	j	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
6	k	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
7	l	152/179 (85%)	145 (95%)	7 (5%)	0	100	100
8	m	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	n	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	o	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	35
11	p	113/129 (88%)	110 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	q	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	r	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
14	s	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
15	t	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	u	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
17	v	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
18	w	64/75 (85%)	64 (100%)	0	0	100	100
19	x	82/92 (89%)	82 (100%)	0	0	100	100
20	y	84/87 (97%)	84 (100%)	0	0	100	100
21	z	68/71 (96%)	68 (100%)	0	0	100	100
26	B	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
27	C	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24	52
28	D	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
29	E	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
30	F	173/177 (98%)	166 (96%)	7 (4%)	0	100	100
31	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
32	K	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	L	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
34	M	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
35	N	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
36	O	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
37	P	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
38	Q	115/118 (98%)	115 (100%)	0	0	100	100
39	R	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	S	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
41	T	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
42	U	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
43	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
44	W	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	X	75/78 (96%)	75 (100%)	0	0	100	100
46	Y	60/63 (95%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
48	b	54/57 (95%)	54 (100%)	0	0	100	100
49	c	49/55 (89%)	49 (100%)	0	0	100	100
50	d	44/46 (96%)	44 (100%)	0	0	100	100
51	e	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
52	f	36/38 (95%)	36 (100%)	0	0	100	100
53	a	56/70 (80%)	54 (96%)	2 (4%)	0	100	100
54	I	66/142 (46%)	65 (98%)	1 (2%)	0	100	100
55	6	359/365 (98%)	356 (99%)	3 (1%)	0	100	100
56	G	147/149 (99%)	140 (95%)	6 (4%)	1 (1%)	18	44
All	All	6016/6420 (94%)	5884 (98%)	129 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	o	57	VAL
27	C	149	ASN
56	G	76	GLU

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	
2	g	186/199 (94%)	181 (97%)	5 (3%)	39	71
3	h	172/190 (90%)	168 (98%)	4 (2%)	44	75
4	i	172/173 (99%)	169 (98%)	3 (2%)	53	80
5	j	119/126 (94%)	118 (99%)	1 (1%)	73	89
6	k	90/116 (78%)	88 (98%)	2 (2%)	45	75
7	l	127/147 (86%)	125 (98%)	2 (2%)	55	81
8	m	104/105 (99%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	n	105/107 (98%)	105 (100%)	0	100	100
10	o	86/90 (96%)	85 (99%)	1 (1%)	63	84
11	p	89/98 (91%)	89 (100%)	0	100	100
12	q	102/103 (99%)	102 (100%)	0	100	100
13	r	93/96 (97%)	93 (100%)	0	100	100
14	s	83/84 (99%)	83 (100%)	0	100	100
15	t	76/77 (99%)	76 (100%)	0	100	100
16	u	65/65 (100%)	65 (100%)	0	100	100
17	v	73/78 (94%)	68 (93%)	5 (7%)	14	38
18	w	57/65 (88%)	57 (100%)	0	100	100
19	x	72/79 (91%)	72 (100%)	0	100	100
20	y	65/66 (98%)	64 (98%)	1 (2%)	57	81
21	z	60/61 (98%)	58 (97%)	2 (3%)	33	66
26	B	216/218 (99%)	215 (100%)	1 (0%)	81	92
27	C	163/163 (100%)	162 (99%)	1 (1%)	78	91
28	D	165/165 (100%)	165 (100%)	0	100	100
29	E	148/150 (99%)	148 (100%)	0	100	100
30	F	136/138 (99%)	132 (97%)	4 (3%)	37	70
31	J	116/116 (100%)	115 (99%)	1 (1%)	70	87
32	K	104/104 (100%)	103 (99%)	1 (1%)	68	86
33	L	103/103 (100%)	102 (99%)	1 (1%)	68	86
34	M	107/107 (100%)	103 (96%)	4 (4%)	30	62
35	N	98/103 (95%)	97 (99%)	1 (1%)	68	86
36	O	86/87 (99%)	85 (99%)	1 (1%)	63	84
37	P	99/100 (99%)	99 (100%)	0	100	100
38	Q	89/90 (99%)	89 (100%)	0	100	100
39	R	84/84 (100%)	79 (94%)	5 (6%)	17	43
40	S	93/93 (100%)	93 (100%)	0	100	100
41	T	80/84 (95%)	78 (98%)	2 (2%)	42	73
42	U	83/85 (98%)	80 (96%)	3 (4%)	31	63
43	V	78/78 (100%)	76 (97%)	2 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	W	58/63 (92%)	57 (98%)	1 (2%)	53	80
45	X	67/68 (98%)	66 (98%)	1 (2%)	57	81
46	Y	54/55 (98%)	53 (98%)	1 (2%)	50	78
47	Z	48/49 (98%)	48 (100%)	0	100	100
48	b	47/48 (98%)	47 (100%)	0	100	100
49	c	46/49 (94%)	45 (98%)	1 (2%)	45	75
50	d	38/38 (100%)	38 (100%)	0	100	100
51	e	51/52 (98%)	49 (96%)	2 (4%)	28	60
52	f	34/34 (100%)	34 (100%)	0	100	100
53	a	55/62 (89%)	53 (96%)	2 (4%)	31	63
54	I	50/110 (46%)	48 (96%)	2 (4%)	28	60
55	6	306/310 (99%)	300 (98%)	6 (2%)	48	77
56	G	114/114 (100%)	111 (97%)	3 (3%)	40	72
All	All	5012/5245 (96%)	4940 (99%)	72 (1%)	57	82

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	g	6	MET
2	g	117	LEU
2	g	129	LEU
2	g	152	LYS
2	g	203	ASN
3	h	80	LYS
3	h	82	GLU
3	h	107	ARG
3	h	178	LEU
4	i	34	ILE
4	i	190	ASP
4	i	206	LYS
5	j	164	ILE
6	k	74	LEU
6	k	93	LYS
7	l	6	VAL
7	l	113	ASP
10	o	90	LEU
17	v	13	VAL

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Mol	Chain	Res	Type
17	v	19	LYS
17	v	42	THR
17	v	49	GLU
17	v	57	ASP
20	y	76	LYS
21	z	3	VAL
21	z	49	LYS
26	B	242	LYS
27	C	12	THR
30	F	11	VAL
30	F	167	GLU
30	F	168	VAL
30	F	176	LYS
31	J	9	GLU
32	K	76	VAL
33	L	93	ASN
34	M	7	THR
34	M	14	LYS
34	M	51	ARG
34	M	135	VAL
35	N	72	ASP
36	O	85	LYS
39	R	6	GLN
39	R	20	VAL
39	R	47	VAL
39	R	48	LYS
39	R	51	VAL
41	T	68	LYS
41	T	69	ARG
42	U	15	THR
42	U	49	VAL
42	U	59	VAL
43	V	61	LEU
43	V	65	VAL
44	W	44	LYS
45	X	40	VAL
46	Y	14	LEU
49	c	54	ILE
51	e	30	ARG
51	e	31	HIS
53	a	10	GLU
53	a	28	VAL

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Mol	Chain	Res	Type
54	I	78	LEU
54	I	137	LEU
55	6	117	ARG
55	6	200	ARG
55	6	256	ARG
55	6	273	GLN
55	6	316	ASP
55	6	322	GLN
56	G	55	GLU
56	G	108	VAL
56	G	134	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
2	g	109	GLN
2	g	203	ASN
3	h	3	GLN
3	h	100	GLN
3	h	102	ASN
3	h	123	GLN
3	h	139	GLN
3	h	190	HIS
4	i	41	HIS
4	i	131	ASN
4	i	198	HIS
5	j	73	ASN
5	j	97	GLN
5	j	146	ASN
7	l	68	ASN
8	m	67	GLN
9	n	110	GLN
10	o	58	ASN
11	p	15	GLN
11	p	38	GLN
14	s	60	GLN
14	s	66	GLN
16	u	40	ASN
17	v	51	ASN
19	x	14	HIS
19	x	56	GLN
19	x	57	HIS

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Mol	Chain	Res	Type
20	y	13	GLN
26	B	90	ASN
26	B	117	GLN
26	B	200	HIS
28	D	9	GLN
28	D	115	GLN
30	F	45	HIS
30	F	111	HIS
31	J	58	ASN
31	J	86	GLN
31	J	128	ASN
31	J	138	GLN
34	M	13	HIS
35	N	18	GLN
35	N	73	ASN
37	P	52	ASN
37	P	66	ASN
38	Q	44	GLN
39	R	6	GLN
39	R	66	HIS
40	S	40	ASN
41	T	59	ASN
42	U	53	ASN
43	V	49	ASN
44	W	12	ASN
44	W	57	HIS
46	Y	27	ASN
46	Y	38	GLN
46	Y	39	GLN
46	Y	58	ASN
48	b	5	GLN
53	a	30	HIS
55	6	48	ASN
55	6	214	HIS
55	6	275	GLN
55	6	280	GLN
55	6	290	GLN
55	6	346	GLN
56	G	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1534/1542 (99%)	225 (14%)	5 (0%)
22	4	25/49 (51%)	7 (28%)	1 (4%)
23	5	75/76 (98%)	31 (41%)	1 (1%)
24	1	2897/2904 (99%)	455 (15%)	8 (0%)
25	3	118/120 (98%)	15 (12%)	0
All	All	4649/4691 (99%)	733 (15%)	15 (0%)

All (733) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	7	A
1	2	9	G
1	2	22	G
1	2	32	A
1	2	39	G
1	2	48	C
1	2	50	A
1	2	51	A
1	2	71	A
1	2	74	A
1	2	77	A
1	2	80	A
1	2	89	U
1	2	94	G
1	2	95	C
1	2	116	A
1	2	121	U
1	2	131	A
1	2	141	G
1	2	144	G
1	2	163	C
1	2	165	G
1	2	173	U
1	2	181	A
1	2	182	A
1	2	183	C
1	2	197	A
1	2	201	G
1	2	202	G
1	2	203	G
1	2	204	G
1	2	209	U

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Mol	Chain	Res	Type
1	2	210	C
1	2	211	G
1	2	212	G
1	2	226	G
1	2	240	G
1	2	245	U
1	2	247	G
1	2	251	G
1	2	257	G
1	2	266	G
1	2	267	C
1	2	280	C
1	2	289	G
1	2	316	C
1	2	321	A
1	2	328	C
1	2	329	A
1	2	330	C
1	2	351	G
1	2	352	C
1	2	354	G
1	2	367	U
1	2	372	C
1	2	373	A
1	2	384	G
1	2	406	G
1	2	412	A
1	2	413	G
1	2	414	A
1	2	415	A
1	2	417	G
1	2	421	U
1	2	422	C
1	2	423	G
1	2	424	G
1	2	429	U
1	2	436	C
1	2	446	G
1	2	453	G
1	2	456	A
1	2	457	G
1	2	458	U

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Mol	Chain	Res	Type
1	2	459	A
1	2	463	U
1	2	464	U
1	2	467	U
1	2	468	A
1	2	469	C
1	2	478	A
1	2	479	U
1	2	481	G
1	2	484	G
1	2	486	U
1	2	495	A
1	2	509	A
1	2	511	C
1	2	518	C
1	2	521	G
1	2	524	G
1	2	527	G7M
1	2	531	U
1	2	547	A
1	2	562	U
1	2	564	C
1	2	572	A
1	2	573	A
1	2	576	C
1	2	577	G
1	2	579	A
1	2	588	G
1	2	596	A
1	2	597	G
1	2	607	A
1	2	631	C
1	2	633	G
1	2	648	A
1	2	650	G
1	2	653	U
1	2	665	A
1	2	721	G
1	2	723	U
1	2	724	G
1	2	746	A
1	2	747	A

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Mol	Chain	Res	Type
1	2	748	G
1	2	755	G
1	2	777	A
1	2	792	A
1	2	793	U
1	2	794	A
1	2	815	A
1	2	817	C
1	2	832	G
1	2	840	C
1	2	841	C
1	2	842	U
1	2	843	U
1	2	844	G
1	2	845	A
1	2	846	G
1	2	847	G
1	2	890	G
1	2	902	G
1	2	914	A
1	2	926	G
1	2	934	C
1	2	935	A
1	2	953	G
1	2	960	U
1	2	963	G
1	2	966	2MG
1	2	969	A
1	2	971	G
1	2	975	A
1	2	976	G
1	2	977	A
1	2	992	U
1	2	1002	G
1	2	1003	G
1	2	1004	A
1	2	1006	G
1	2	1009	U
1	2	1010	U
1	2	1011	C
1	2	1027	C
1	2	1029	U

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Mol	Chain	Res	Type
1	2	1030	U
1	2	1031	C
1	2	1032	G
1	2	1033	G
1	2	1034	G
1	2	1036	A
1	2	1044	A
1	2	1046	A
1	2	1053	G
1	2	1065	U
1	2	1085	U
1	2	1086	U
1	2	1094	G
1	2	1095	U
1	2	1101	A
1	2	1137	C
1	2	1139	G
1	2	1157	A
1	2	1159	U
1	2	1196	A
1	2	1197	A
1	2	1213	A
1	2	1224	U
1	2	1225	A
1	2	1227	A
1	2	1238	A
1	2	1258	G
1	2	1260	G
1	2	1275	A
1	2	1280	A
1	2	1286	U
1	2	1287	A
1	2	1298	U
1	2	1300	G
1	2	1302	C
1	2	1305	G
1	2	1317	C
1	2	1320	C
1	2	1323	G
1	2	1346	A
1	2	1353	G
1	2	1363	A

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Mol	Chain	Res	Type
1	2	1364	U
1	2	1370	G
1	2	1378	C
1	2	1379	G
1	2	1381	U
1	2	1419	G
1	2	1441	A
1	2	1446	A
1	2	1451	U
1	2	1452	C
1	2	1453	G
1	2	1487	G
1	2	1491	G
1	2	1492	A
1	2	1493	A
1	2	1494	G
1	2	1497	G
1	2	1499	A
1	2	1503	A
1	2	1506	U
1	2	1507	A
1	2	1517	G
1	2	1529	G
1	2	1530	G
22	4	33	A
22	4	34	U
22	4	35	U
22	4	38	A
22	4	44	G
22	4	45	A
22	4	46	A
23	5	5	G
23	5	6	G
23	5	7	G
23	5	9	G
23	5	13	C
23	5	14	A
23	5	16	C
23	5	17	C
23	5	17(A)	U
23	5	18	G
23	5	19	G

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Mol	Chain	Res	Type
23	5	20	U
23	5	21	A
23	5	25	C
23	5	31	G
23	5	42	G
23	5	43	A
23	5	47	U
23	5	48	C
23	5	51	C
23	5	52	G
23	5	53	G
23	5	54	U
23	5	58	A
23	5	60	U
23	5	65	C
23	5	69	C
23	5	70	G
23	5	71	C
23	5	75	C
23	5	76	A
24	1	10	A
24	1	34	U
24	1	42	A
24	1	45	G
24	1	51	G
24	1	58	G
24	1	61	C
24	1	71	A
24	1	73	A
24	1	74	A
24	1	75	G
24	1	80	G
24	1	101	A
24	1	102	U
24	1	118	A
24	1	119	A
24	1	120	U
24	1	134	G
24	1	135	U
24	1	136	G
24	1	139	U
24	1	140	C

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Mol	Chain	Res	Type
24	1	141	G
24	1	142	A
24	1	163	C
24	1	181	A
24	1	196	A
24	1	199	A
24	1	215	G
24	1	216	A
24	1	221	A
24	1	222	A
24	1	248	G
24	1	264	C
24	1	265	A
24	1	271	G
24	1	272	A
24	1	273	G
24	1	274	C
24	1	276	U
24	1	277	G
24	1	278	A
24	1	281	C
24	1	282	A
24	1	283	G
24	1	285	G
24	1	287	G
24	1	289	G
24	1	290	U
24	1	291	G
24	1	292	U
24	1	294	A
24	1	311	A
24	1	329	G
24	1	330	A
24	1	345	A
24	1	353	C
24	1	356	G
24	1	359	G
24	1	360	U
24	1	361	G
24	1	363	G
24	1	366	C
24	1	370	G

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Mol	Chain	Res	Type
24	1	386	G
24	1	393	C
24	1	396	G
24	1	405	U
24	1	411	G
24	1	412	A
24	1	422	A
24	1	447	A
24	1	451	U
24	1	452	G
24	1	455	C
24	1	481	G
24	1	491	G
24	1	504	A
24	1	505	A
24	1	508	A
24	1	509	C
24	1	513	A
24	1	532	A
24	1	545	U
24	1	546	U
24	1	548	G
24	1	549	G
24	1	563	A
24	1	573	U
24	1	575	A
24	1	603	A
24	1	615	U
24	1	627	A
24	1	637	A
24	1	645	C
24	1	646	U
24	1	647	G
24	1	653	U
24	1	654	A
24	1	655	A
24	1	686	U
24	1	717	C
24	1	721	A
24	1	730	A
24	1	738	G
24	1	747	5MU

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Mol	Chain	Res	Type
24	1	763	G
24	1	775	G
24	1	776	G
24	1	782	A
24	1	784	G
24	1	785	G
24	1	789	A
24	1	791	C
24	1	805	G
24	1	812	C
24	1	827	U
24	1	828	U
24	1	845	A
24	1	846	U
24	1	859	G
24	1	869	G
24	1	879	G
24	1	881	G
24	1	882	G
24	1	883	G
24	1	884	U
24	1	888	C
24	1	890	C
24	1	891	G
24	1	895	U
24	1	896	A
24	1	897	C
24	1	898	C
24	1	899	A
24	1	909	A
24	1	910	A
24	1	914	G
24	1	915	C
24	1	931	U
24	1	946	C
24	1	958	U
24	1	961	C
24	1	974	G
24	1	983	A
24	1	989	G
24	1	996	A
24	1	1005	C

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Mol	Chain	Res	Type
24	1	1012	U
24	1	1013	C
24	1	1025	G
24	1	1026	G
24	1	1033	U
24	1	1041	G
24	1	1042	G
24	1	1047	G
24	1	1051	G
24	1	1054	A
24	1	1055	G
24	1	1056	G
24	1	1057	A
24	1	1062	G
24	1	1064	C
24	1	1065	U
24	1	1066	U
24	1	1068	G
24	1	1069	A
24	1	1070	A
24	1	1074	G
24	1	1083	U
24	1	1084	A
24	1	1087	G
24	1	1088	A
24	1	1097	U
24	1	1101	U
24	1	1105	U
24	1	1107	G
24	1	1108	U
24	1	1111	A
24	1	1112	G
24	1	1115	G
24	1	1116	G
24	1	1122	G
24	1	1130	U
24	1	1132	U
24	1	1133	A
24	1	1135	C
24	1	1141	U
24	1	1142	A
24	1	1158	C

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Mol	Chain	Res	Type
24	1	1169	A
24	1	1171	G
24	1	1172	C
24	1	1206	G
24	1	1212	G
24	1	1236	G
24	1	1242	U
24	1	1250	G
24	1	1253	A
24	1	1256	G
24	1	1271	G
24	1	1272	A
24	1	1273	U
24	1	1300	G
24	1	1301	A
24	1	1329	U
24	1	1352	U
24	1	1360	G
24	1	1365	A
24	1	1375	U
24	1	1378	A
24	1	1379	U
24	1	1383	A
24	1	1399	C
24	1	1411	U
24	1	1416	G
24	1	1419	A
24	1	1420	A
24	1	1421	G
24	1	1427	A
24	1	1428	C
24	1	1452	G
24	1	1453	A
24	1	1454	C
24	1	1455	G
24	1	1458	U
24	1	1460	U
24	1	1482	G
24	1	1486	U
24	1	1493	C
24	1	1497	U
24	1	1508	A

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Mol	Chain	Res	Type
24	1	1509	A
24	1	1510	G
24	1	1515	A
24	1	1529	G
24	1	1534	U
24	1	1535	A
24	1	1536	C
24	1	1537	G
24	1	1554	U
24	1	1559	U
24	1	1560	G
24	1	1566	A
24	1	1569	A
24	1	1578	U
24	1	1583	A
24	1	1584	U
24	1	1585	C
24	1	1586	A
24	1	1607	C
24	1	1608	A
24	1	1613	G
24	1	1634	A
24	1	1647	U
24	1	1648	U
24	1	1649	G
24	1	1667	G
24	1	1674	G
24	1	1715	G
24	1	1729	U
24	1	1730	C
24	1	1731	G
24	1	1732	C
24	1	1738	G
24	1	1764	C
24	1	1773	A
24	1	1782	U
24	1	1786	A
24	1	1788	C
24	1	1791	A
24	1	1800	C
24	1	1801	A
24	1	1808	A

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Mol	Chain	Res	Type
24	1	1816	C
24	1	1829	A
24	1	1847	A
24	1	1857	G
24	1	1858	A
24	1	1868	C
24	1	1870	C
24	1	1871	A
24	1	1873	G
24	1	1900	A
24	1	1906	G
24	1	1907	G
24	1	1910	G
24	1	1913	A
24	1	1914	C
24	1	1915	3TD
24	1	1929	G
24	1	1930	G
24	1	1937	A
24	1	1938	A
24	1	1939	5MU
24	1	1955	U
24	1	1965	C
24	1	1967	C
24	1	1970	A
24	1	1971	U
24	1	1972	G
24	1	1991	U
24	1	1992	G
24	1	1993	U
24	1	2023	C
24	1	2027	G
24	1	2031	A
24	1	2033	A
24	1	2036	C
24	1	2043	C
24	1	2049	G
24	1	2055	C
24	1	2056	G
24	1	2060	A
24	1	2061	G
24	1	2062	A

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Mol	Chain	Res	Type
24	1	2069	G7M
24	1	2093	G
24	1	2097	A
24	1	2098	U
24	1	2099	U
24	1	2100	G
24	1	2101	A
24	1	2102	G
24	1	2104	C
24	1	2110	G
24	1	2111	U
24	1	2113	U
24	1	2115	G
24	1	2116	G
24	1	2117	A
24	1	2118	U
24	1	2122	U
24	1	2124	G
24	1	2125	G
24	1	2126	A
24	1	2127	G
24	1	2128	G
24	1	2131	U
24	1	2132	U
24	1	2133	G
24	1	2134	A
24	1	2139	U
24	1	2147	A
24	1	2157	G
24	1	2158	A
24	1	2159	G
24	1	2162	G
24	1	2163	A
24	1	2164	C
24	1	2165	C
24	1	2171	A
24	1	2172	U
24	1	2182	U
24	1	2183	A
24	1	2185	U
24	1	2188	U
24	1	2190	G

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Mol	Chain	Res	Type
24	1	2191	A
24	1	2198	A
24	1	2204	G
24	1	2211	A
24	1	2225	A
24	1	2238	G
24	1	2239	G
24	1	2259	U
24	1	2268	A
24	1	2279	G
24	1	2283	C
24	1	2287	A
24	1	2288	A
24	1	2289	G
24	1	2305	U
24	1	2308	G
24	1	2322	A
24	1	2325	G
24	1	2333	A
24	1	2335	A
24	1	2336	A
24	1	2337	G
24	1	2345	G
24	1	2347	C
24	1	2350	C
24	1	2361	G
24	1	2383	G
24	1	2385	C
24	1	2400	G
24	1	2402	U
24	1	2406	A
24	1	2408	U
24	1	2410	G
24	1	2425	A
24	1	2429	G
24	1	2430	A
24	1	2435	A
24	1	2441	U
24	1	2448	A
24	1	2476	A
24	1	2478	A
24	1	2491	U

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Mol	Chain	Res	Type
24	1	2494	G
24	1	2498	OMC
24	1	2502	G
24	1	2505	G
24	1	2507	C
24	1	2518	A
24	1	2520	C
24	1	2525	G
24	1	2529	G
24	1	2535	G
24	1	2547	A
24	1	2566	A
24	1	2567	G
24	1	2573	C
24	1	2574	G
24	1	2582	G
24	1	2585	U
24	1	2586	U
24	1	2602	A
24	1	2603	G
24	1	2609	U
24	1	2613	U
24	1	2615	U
24	1	2629	U
24	1	2661	G
24	1	2682	A
24	1	2685	G
24	1	2689	U
24	1	2690	U
24	1	2716	C
24	1	2726	A
24	1	2733	A
24	1	2744	G
24	1	2748	A
24	1	2752	C
24	1	2765	A
24	1	2778	A
24	1	2795	C
24	1	2797	U
24	1	2798	U
24	1	2799	A
24	1	2800	A

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Mol	Chain	Res	Type
24	1	2804	U
24	1	2818	U
24	1	2820	A
24	1	2821	A
24	1	2835	A
24	1	2849	U
24	1	2861	U
24	1	2873	A
24	1	2884	U
24	1	2891	U
24	1	2900	A
24	1	2902	C
24	1	2903	U
25	3	9	G
25	3	13	G
25	3	24	G
25	3	33	G
25	3	35	C
25	3	36	C
25	3	45	A
25	3	56	G
25	3	57	A
25	3	58	A
25	3	67	G
25	3	89	U
25	3	90	C
25	3	99	A
25	3	109	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	182	A
1	2	209	U
1	2	467	U
1	2	1026	G
1	2	1035	A
22	4	32	U
23	5	19	G
24	1	277	G
24	1	404	A
24	1	451	U

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Mol	Chain	Res	Type
24	1	504	A
24	1	784	G
24	1	827	U
24	1	2146	C
24	1	2162	G

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	$\# Z > 2$
24	PSU	1	746	24,57	18,21,22	0.60	0	22,30,33	0.37	0
24	6MZ	1	2030	24	22,25,26	0.34	0	30,36,39	0.42	0
1	MA6	2	1518	1	23,26,27	0.34	0	34,38,41	0.69	1 (2%)
24	PSU	1	1911	24	18,21,22	0.53	0	22,30,33	0.57	0
24	PSU	1	2457	24	18,21,22	0.61	0	22,30,33	0.59	0
34	MS6	M	82	34	5,7,8	0.26	0	2,7,9	0.03	0
24	PSU	1	1917	24	18,21,22	0.57	0	22,30,33	0.56	0
1	2MG	2	1516	1	23,26,27	0.38	0	32,38,41	0.45	0
1	PSU	2	516	57,1	18,21,22	0.54	0	22,30,33	0.60	1 (4%)
1	4OC	2	1402	57,1	20,23,24	0.36	0	26,32,35	0.61	0
24	2MG	1	1835	24	23,26,27	0.35	0	32,38,41	0.30	0
24	OMC	1	2498	24,57	19,22,23	0.36	0	26,31,34	0.43	0
24	OMU	1	2552	24,57	19,22,23	0.34	0	26,31,34	0.42	0
1	5MC	2	967	1	18,22,23	0.32	0	26,32,35	0.41	0
24	6MZ	1	1618	24	22,25,26	0.31	0	30,36,39	0.45	0
27	MEQ	C	150	27	8,9,10	0.85	0	5,10,12	0.63	0
24	OMG	1	2251	24,59,23	23,26,27	0.37	0	33,38,41	0.34	0
24	PSU	1	955	24	18,21,22	0.60	0	22,30,33	0.59	0
1	2MG	2	1207	59,1	23,26,27	0.34	0	32,38,41	0.35	0
24	3TD	1	1915	24,57	19,22,23	0.53	0	21,32,35	0.78	0
24	PSU	1	2504	24,59	18,21,22	0.60	0	22,30,33	0.62	0
24	PSU	1	2580	24	18,21,22	0.64	1 (5%)	22,30,33	0.67	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	2MG	1	2445	24	23,26,27	0.43	0	32,38,41	0.34	0
1	G7M	2	527	59,1	23,26,27	0.36	0	35,39,42	0.51	0
1	5MC	2	1407	1	18,22,23	0.33	0	26,32,35	0.45	0
12	D2T	q	89	12	7,9,10	0.89	0	6,11,13	1.72	2 (33%)
24	5MU	1	747	24	19,22,23	0.35	0	28,32,35	0.34	0
24	H2U	1	2449	24	18,21,22	0.36	0	21,30,33	0.44	0
24	2MA	1	2503	24,57,59	22,25,26	1.03	1 (4%)	33,37,40	1.27	3 (9%)
24	5MU	1	1939	24,59	19,22,23	0.58	0	28,32,35	0.90	3 (10%)
1	2MG	2	966	1	23,26,27	0.32	0	32,38,41	0.35	0
1	UR3	2	1498	1	19,22,23	0.33	0	26,32,35	0.35	0
24	1MG	1	745	24	22,26,27	0.39	0	33,39,42	0.62	1 (3%)
24	G7M	1	2069	24,59	23,26,27	0.40	0	35,39,42	0.51	0
1	MA6	2	1519	1	23,26,27	0.34	0	34,38,41	0.74	1 (2%)
11	IAS	p	119	11	6,7,8	0.95	0	6,8,10	1.25	1 (16%)
24	PSU	1	2604	24	18,21,22	0.56	0	22,30,33	0.64	0
24	PSU	1	2605	24	18,21,22	0.56	0	22,30,33	0.67	0
24	5MC	1	1962	24,59	18,22,23	0.33	0	26,32,35	0.44	0
55	MEQ	6	252	55	8,9,10	0.90	0	5,10,12	0.64	0
34	4D4	M	81	34	9,11,12	0.67	0	8,13,15	1.90	3 (37%)

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
24	PSU	1	746	24,57	-	1/7/25/26	0/2/2/2
24	6MZ	1	2030	24	-	2/9/27/28	0/3/3/3
1	MA6	2	1518	1	-	0/11/29/30	0/3/3/3
24	PSU	1	1911	24	-	0/7/25/26	0/2/2/2
24	PSU	1	2457	24	-	0/7/25/26	0/2/2/2
34	MS6	M	82	34	-	1/4/6/8	-
24	PSU	1	1917	24	-	0/7/25/26	0/2/2/2
1	2MG	2	1516	1	-	0/9/27/28	0/3/3/3
1	PSU	2	516	57,1	-	0/7/25/26	0/2/2/2
1	4OC	2	1402	57,1	-	3/9/29/30	0/2/2/2
24	2MG	1	1835	24	-	0/9/27/28	0/3/3/3
24	OMC	1	2498	24,57	-	0/9/27/28	0/2/2/2
24	OMU	1	2552	24,57	-	0/9/27/28	0/2/2/2
1	5MC	2	967	1	-	0/7/25/26	0/2/2/2
24	6MZ	1	1618	24	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	MEQ	C	150	27	-	2/8/9/11	-
24	OMG	1	2251	24,59,23	-	1/9/27/28	0/3/3/3
24	PSU	1	955	24	-	0/7/25/26	0/2/2/2
1	2MG	2	1207	59,1	-	0/9/27/28	0/3/3/3
24	3TD	1	1915	24,57	-	2/7/25/26	0/2/2/2
24	PSU	1	2504	24,59	-	0/7/25/26	0/2/2/2
24	PSU	1	2580	24	-	0/7/25/26	0/2/2/2
24	2MG	1	2445	24	-	1/9/27/28	0/3/3/3
1	G7M	2	527	59,1	-	3/7/25/26	0/3/3/3
1	5MC	2	1407	1	-	0/7/25/26	0/2/2/2
12	D2T	q	89	12	-	3/7/12/14	-
24	5MU	1	747	24	-	0/7/25/26	0/2/2/2
24	H2U	1	2449	24	-	0/7/38/39	0/2/2/2
24	2MA	1	2503	24,57,59	-	2/7/25/26	0/3/3/3
24	5MU	1	1939	24,59	-	2/7/25/26	0/2/2/2
1	2MG	2	966	1	-	2/9/27/28	0/3/3/3
1	UR3	2	1498	1	-	0/7/25/26	0/2/2/2
24	1MG	1	745	24	-	0/7/25/26	0/3/3/3
24	G7M	1	2069	24,59	-	2/7/25/26	0/3/3/3
1	MA6	2	1519	1	-	1/11/29/30	0/3/3/3
11	IAS	p	119	11	-	1/7/7/8	-
24	PSU	1	2604	24	-	0/7/25/26	0/2/2/2
24	PSU	1	2605	24	-	0/7/25/26	0/2/2/2
24	5MC	1	1962	24,59	-	0/7/25/26	0/2/2/2
55	MEQ	6	252	55	-	2/8/9/11	-
34	4D4	M	81	34	-	2/11/12/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	2503	2MA	C6-N6	-3.77	1.24	1.34
24	1	2580	PSU	O4'-C1'	-2.17	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	2503	2MA	N6-C6-N1	4.19	122.95	117.03
24	1	2503	2MA	C2-N1-C6	3.71	123.86	118.08
34	M	81	4D4	NE-CZ-NH2	3.56	126.95	120.70
24	1	2503	2MA	C5-C6-N1	-3.36	113.22	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	M	81	4D4	O-C-CA	-3.04	116.80	124.78
12	q	89	D2T	O-C-CA	-2.85	117.31	124.78
24	1	745	1MG	C6-C5-C4	-2.72	116.96	119.97
24	1	1939	5MU	O4'-C1'-N1	2.55	114.18	108.36
34	M	81	4D4	NH1-CZ-NE	-2.52	113.39	119.19
11	p	119	IAS	OD1-CG-CB	-2.44	118.32	125.43
1	2	1518	MA6	C2-N1-C6	2.39	117.40	111.75
12	q	89	D2T	OD1-CG-CB	-2.38	117.45	122.44
1	2	1519	MA6	C2-N1-C6	2.38	117.37	111.75
24	1	2580	PSU	O4'-C1'-C2'	2.34	108.44	105.14
24	1	1939	5MU	C1'-N1-C6	2.32	124.99	121.12
24	1	1939	5MU	C1'-N1-C2	-2.16	113.66	117.57
1	2	516	PSU	O4'-C1'-C2'	2.07	108.06	105.14

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	1915	3TD	C3'-C4'-C5'-O5'
24	1	1915	3TD	O4'-C4'-C5'-O5'
24	1	1939	5MU	O4'-C4'-C5'-O5'
24	1	2030	6MZ	O4'-C4'-C5'-O5'
24	1	2251	OMG	C1'-C2'-O2'-CM2
1	2	527	G7M	C3'-C4'-C5'-O5'
24	1	1939	5MU	C3'-C4'-C5'-O5'
24	1	2030	6MZ	C3'-C4'-C5'-O5'
1	2	966	2MG	C3'-C4'-C5'-O5'
27	C	150	MEQ	NE2-CD-CG-CB
27	C	150	MEQ	OE1-CD-CG-CB
1	2	966	2MG	O4'-C4'-C5'-O5'
1	2	527	G7M	O4'-C4'-C5'-O5'
34	M	82	MS6	CB-CG-SD-CE
55	6	252	MEQ	OE1-CD-CG-CB
55	6	252	MEQ	NE2-CD-CG-CB
12	q	89	D2T	CG-CB-SB-CB1
12	q	89	D2T	CA-CB-CG-OD2
34	M	81	4D4	OB-CB-CG-CD
24	1	2445	2MG	C3'-C4'-C5'-O5'
1	2	1402	4OC	O4'-C4'-C5'-O5'
1	2	1519	MA6	O4'-C4'-C5'-O5'
11	p	119	IAS	CA-CB-CG-OD1
1	2	527	G7M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
24	1	2503	2MA	O4'-C4'-C5'-O5'
12	q	89	D2T	SB-CB-CG-OD2
24	1	2069	G7M	C4'-C5'-O5'-P
24	1	746	PSU	O4'-C1'-C5-C6
1	2	1402	4OC	C4'-C5'-O5'-P
24	1	2069	G7M	O4'-C4'-C5'-O5'
1	2	1402	4OC	C3'-C4'-C5'-O5'
34	M	81	4D4	O-C-CA-CB
24	1	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

15 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	2030	6MZ	2	0
1	2	1518	MA6	2	0
24	1	2457	PSU	1	0
24	1	1917	PSU	1	0
1	2	1516	2MG	1	0
1	2	1402	4OC	1	0
24	1	2498	OMC	1	0
24	1	2552	OMU	1	0
24	1	2251	OMG	1	0
1	2	1207	2MG	1	0
1	2	1407	5MC	1	0
12	q	89	D2T	1	0
1	2	966	2MG	1	0
1	2	1498	UR3	1	0
1	2	1519	MA6	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 487 ligands modelled in this entry, 460 are monoatomic - leaving 27 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	$\# Z > 2$
60	PUT	1	3329	-	5,5,5	0.10	0	4,4,4	0.15	0
60	PUT	1	3335	-	5,5,5	0.10	0	4,4,4	0.18	0
58	SPD	1	3214	-	9,9,9	0.07	0	8,8,8	0.14	0
58	SPD	1	3207	-	9,9,9	0.08	0	8,8,8	0.19	0
58	SPD	1	3212	-	9,9,9	0.09	0	8,8,8	0.32	0
60	PUT	1	3337	-	5,5,5	0.11	0	4,4,4	0.17	0
60	PUT	1	3334	-	5,5,5	0.09	0	4,4,4	0.20	0
58	SPD	1	3208	-	9,9,9	0.13	0	8,8,8	0.10	0
61	SPM	1	3216	-	13,13,13	0.36	0	12,12,12	0.95	0
58	SPD	1	3215	-	9,9,9	0.09	0	8,8,8	0.14	0
60	PUT	1	3331	-	5,5,5	0.07	0	4,4,4	0.19	0
60	PUT	1	3330	-	5,5,5	0.12	0	4,4,4	0.17	0
60	PUT	1	3333	-	5,5,5	0.09	0	4,4,4	0.18	0
60	PUT	1	3336	-	5,5,5	0.15	0	4,4,4	0.15	0
58	SPD	1	3338	-	9,9,9	0.10	0	8,8,8	0.15	0
58	SPD	1	3210	-	9,9,9	0.11	0	8,8,8	0.16	0
58	SPD	1	3206	-	9,9,9	0.08	0	8,8,8	0.16	0
60	PUT	1	3328	-	5,5,5	0.07	0	4,4,4	0.20	0
58	SPD	1	3211	-	9,9,9	0.08	0	8,8,8	0.18	0
58	SPD	1	3209	-	9,9,9	0.10	0	8,8,8	0.14	0
58	SPD	2	1691	-	9,9,9	0.07	0	8,8,8	0.19	0
60	PUT	2	1731	-	5,5,5	0.13	0	4,4,4	0.16	0
58	SPD	2	1690	-	9,9,9	0.12	0	8,8,8	0.12	0
60	PUT	2	1732	-	5,5,5	0.15	0	4,4,4	0.16	0
60	PUT	1	3339	-	5,5,5	0.10	0	4,4,4	0.17	0
58	SPD	1	3213	-	9,9,9	0.07	0	8,8,8	0.17	0
60	PUT	1	3332	-	5,5,5	0.14	0	4,4,4	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PUT	1	3329	-	-	2/3/3/3	-
60	PUT	1	3335	-	-	3/3/3/3	-
58	SPD	1	3214	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SPD	1	3207	-	-	2/7/7/7	-
58	SPD	1	3212	-	-	5/7/7/7	-
60	PUT	1	3337	-	-	1/3/3/3	-
60	PUT	1	3334	-	-	1/3/3/3	-
58	SPD	1	3208	-	-	2/7/7/7	-
61	SPM	1	3216	-	-	8/11/11/11	-
58	SPD	1	3215	-	-	5/7/7/7	-
60	PUT	1	3331	-	-	1/3/3/3	-
60	PUT	1	3330	-	-	2/3/3/3	-
60	PUT	1	3333	-	-	0/3/3/3	-
60	PUT	1	3336	-	-	3/3/3/3	-
58	SPD	1	3338	-	-	3/7/7/7	-
58	SPD	1	3210	-	-	5/7/7/7	-
58	SPD	1	3206	-	-	1/7/7/7	-
60	PUT	1	3328	-	-	1/3/3/3	-
58	SPD	1	3211	-	-	1/7/7/7	-
58	SPD	1	3209	-	-	1/7/7/7	-
58	SPD	2	1691	-	-	5/7/7/7	-
60	PUT	2	1731	-	-	0/3/3/3	-
58	SPD	2	1690	-	-	2/7/7/7	-
60	PUT	2	1732	-	-	3/3/3/3	-
60	PUT	1	3339	-	-	3/3/3/3	-
58	SPD	1	3213	-	-	3/7/7/7	-
60	PUT	1	3332	-	-	1/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	2	1691	SPD	C7-C8-C9-N10
58	1	3211	SPD	N6-C7-C8-C9
60	1	3332	PUT	C1-C2-C3-C4
58	1	3212	SPD	C3-C4-C5-N6
58	2	1690	SPD	C4-C5-N6-C7
61	1	3216	SPM	C7-C8-C9-N10
58	1	3213	SPD	C3-C4-C5-N6

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Mol	Chain	Res	Type	Atoms
58	1	3215	SPD	C3-C4-C5-N6
61	1	3216	SPM	C3-C4-N5-C6
58	2	1691	SPD	N6-C7-C8-C9
58	1	3206	SPD	C8-C7-N6-C5
58	1	3212	SPD	C4-C5-N6-C7
58	1	3210	SPD	C3-C4-C5-N6
58	1	3215	SPD	C4-C5-N6-C7
60	1	3331	PUT	C1-C2-C3-C4
58	1	3215	SPD	C7-C8-C9-N10
58	1	3213	SPD	C2-C3-C4-C5
60	1	3337	PUT	N1-C1-C2-C3
60	1	3339	PUT	C2-C3-C4-N2
60	1	3336	PUT	C1-C2-C3-C4
58	1	3210	SPD	C2-C3-C4-C5
60	1	3335	PUT	C1-C2-C3-C4
58	1	3207	SPD	C2-C3-C4-C5
58	2	1691	SPD	C2-C3-C4-C5
58	2	1691	SPD	N1-C2-C3-C4
60	1	3330	PUT	N1-C1-C2-C3
60	1	3339	PUT	C1-C2-C3-C4
60	1	3329	PUT	C1-C2-C3-C4
58	1	3210	SPD	N6-C7-C8-C9
60	2	1732	PUT	C2-C3-C4-N2
60	1	3328	PUT	N1-C1-C2-C3
60	1	3329	PUT	N1-C1-C2-C3
60	1	3336	PUT	C2-C3-C4-N2
60	1	3339	PUT	N1-C1-C2-C3
61	1	3216	SPM	C11-C12-C13-N14
58	1	3208	SPD	C8-C7-N6-C5
58	1	3210	SPD	C4-C5-N6-C7
58	1	3338	SPD	C4-C5-N6-C7
58	1	3338	SPD	C8-C7-N6-C5
60	1	3335	PUT	C2-C3-C4-N2
58	1	3212	SPD	N6-C7-C8-C9
61	1	3216	SPM	C6-C7-C8-C9
58	1	3207	SPD	C3-C4-C5-N6
58	2	1691	SPD	C4-C5-N6-C7
60	1	3336	PUT	N1-C1-C2-C3
58	1	3338	SPD	C3-C4-C5-N6
58	1	3215	SPD	C8-C7-N6-C5
61	1	3216	SPM	C8-C9-N10-C11
60	2	1732	PUT	N1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
60	1	3330	PUT	C2-C3-C4-N2
58	1	3212	SPD	C2-C3-C4-C5
60	1	3335	PUT	N1-C1-C2-C3
58	1	3210	SPD	C8-C7-N6-C5
58	1	3215	SPD	N1-C2-C3-C4
58	1	3213	SPD	C8-C7-N6-C5
61	1	3216	SPM	C7-C6-N5-C4
61	1	3216	SPM	N1-C2-C3-C4
58	1	3208	SPD	C4-C5-N6-C7
58	1	3212	SPD	N1-C2-C3-C4
58	1	3209	SPD	C4-C5-N6-C7
61	1	3216	SPM	C12-C11-N10-C9
60	2	1732	PUT	C1-C2-C3-C4
58	2	1690	SPD	C2-C3-C4-C5
60	1	3334	PUT	C1-C2-C3-C4

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1	3212	SPD	1	0
60	1	3334	PUT	1	0
60	1	3330	PUT	1	0
60	1	3333	PUT	1	0
60	1	3336	PUT	1	0
58	2	1691	SPD	1	0
60	2	1731	PUT	1	0
58	2	1690	SPD	2	0
60	2	1732	PUT	1	0
60	1	3332	PUT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

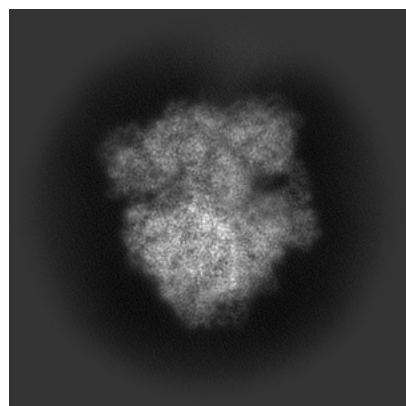
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17346. These allow visual inspection of the internal detail of the map and identification of artifacts.

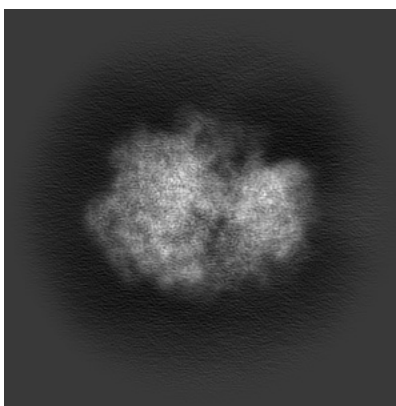
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

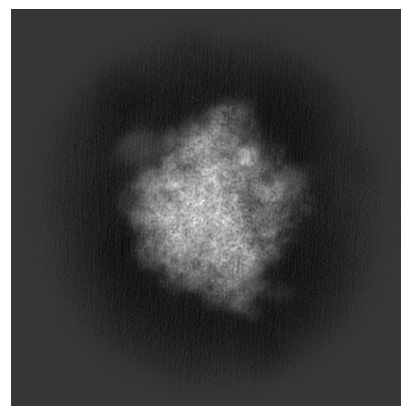
6.1.1 Primary map



X

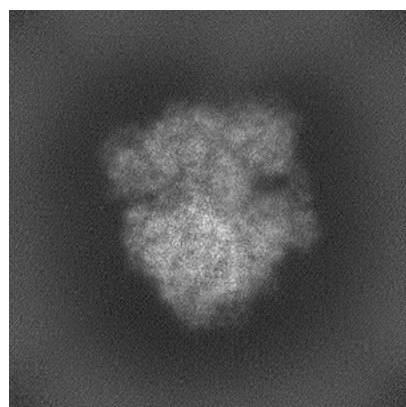


Y

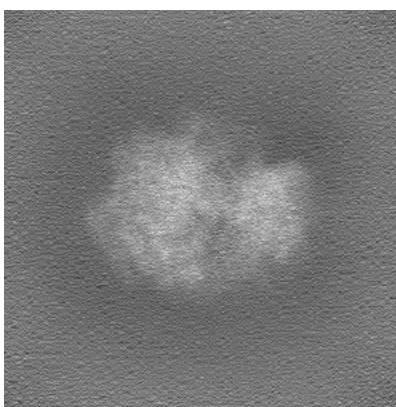


Z

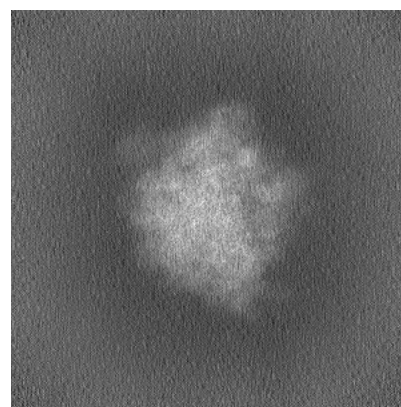
6.1.2 Raw map



X



Y

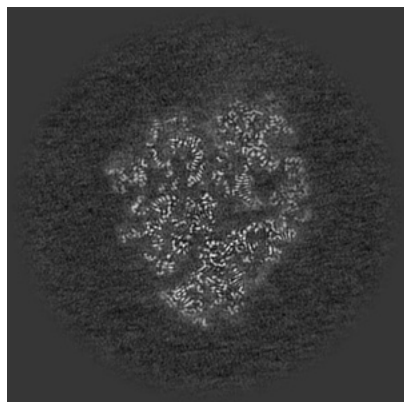


Z

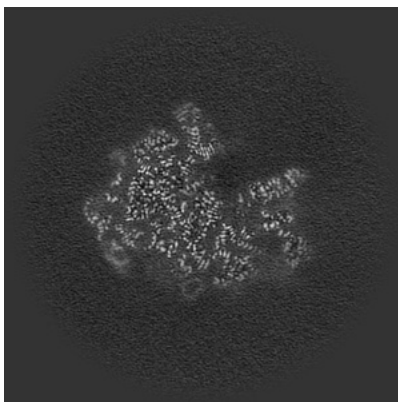
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

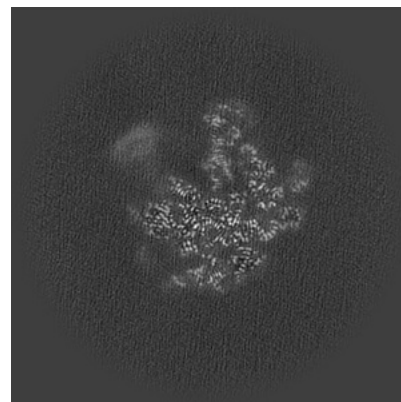
6.2.1 Primary map



X Index: 260

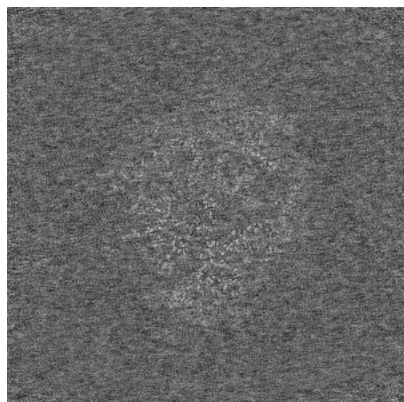


Y Index: 260

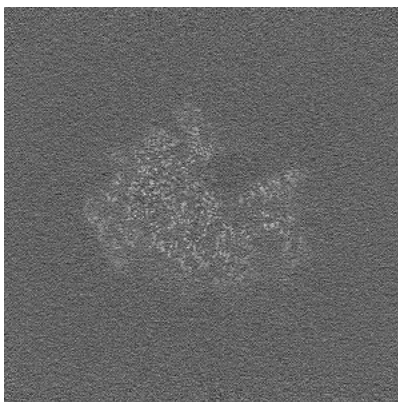


Z Index: 260

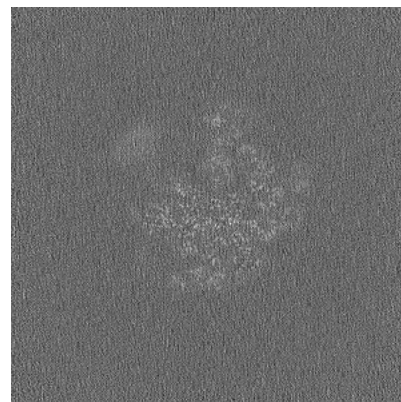
6.2.2 Raw map



X Index: 260



Y Index: 260

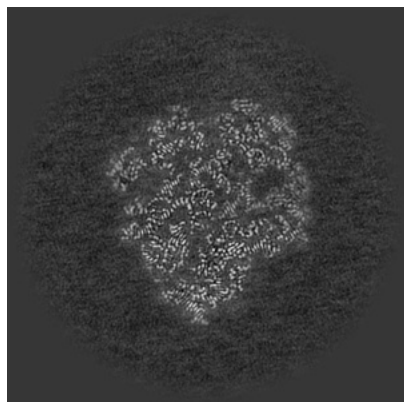


Z Index: 260

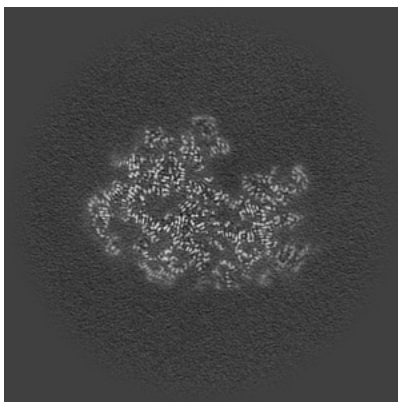
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

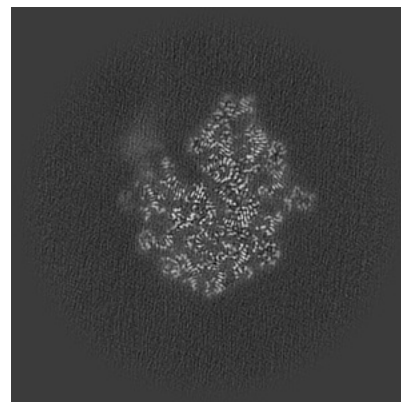
6.3.1 Primary map



X Index: 266

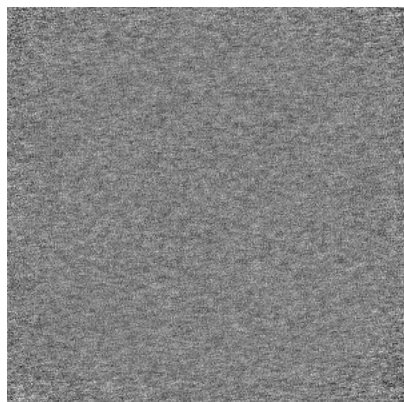


Y Index: 246

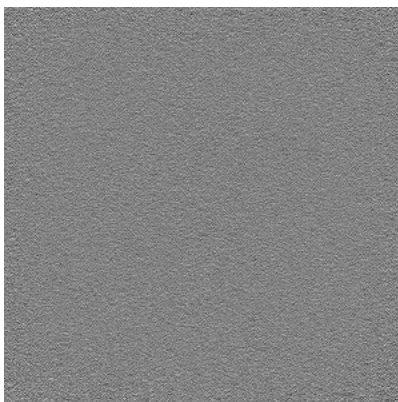


Z Index: 231

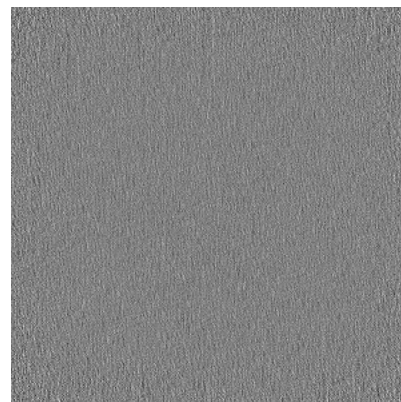
6.3.2 Raw map



X Index: 0



Y Index: 0

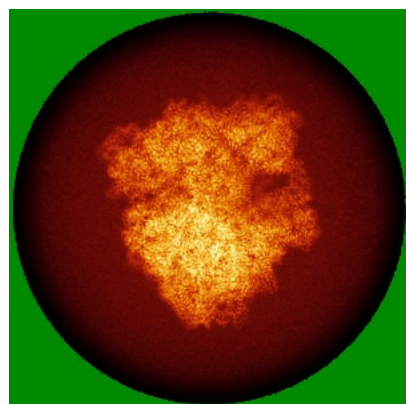


Z Index: 0

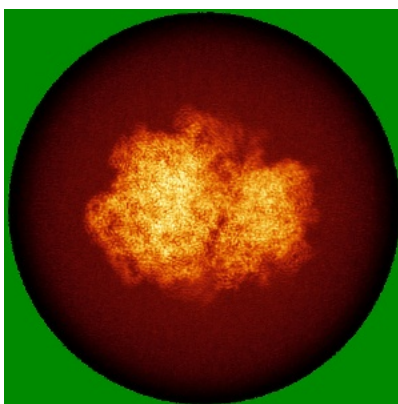
The images above show the largest variance slices of the map in three orthogonal directions.

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

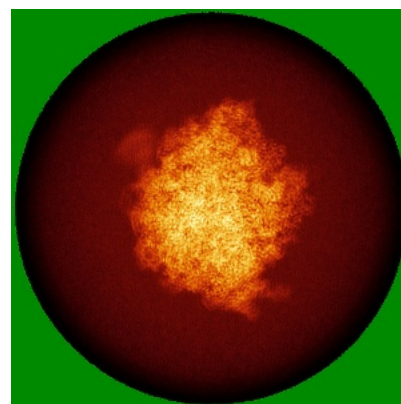
6.4.1 Primary map



X

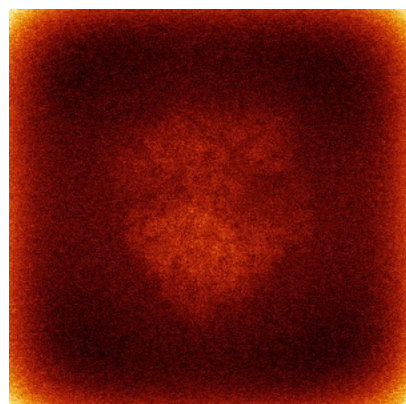


Y

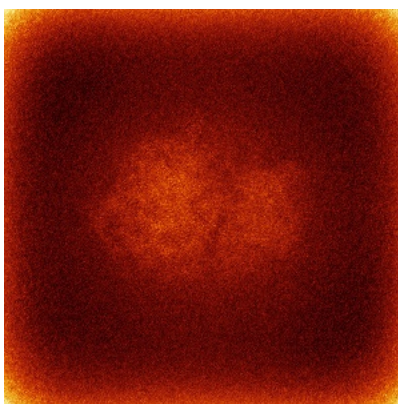


Z

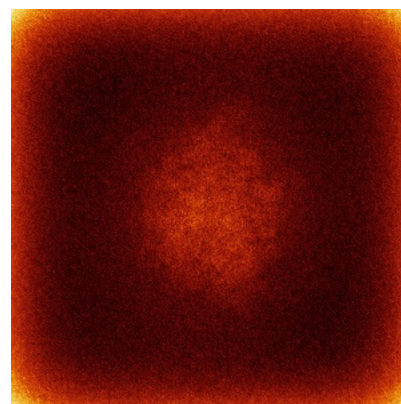
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



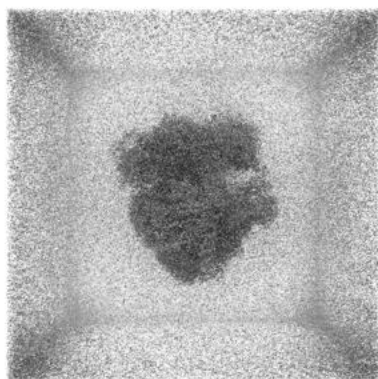
Y



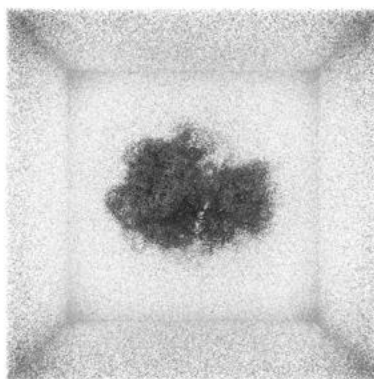
Z

The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

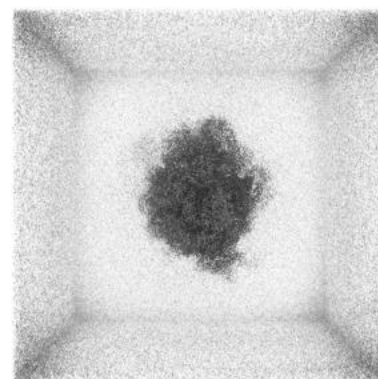
6.5.2 Raw map



X



Y



Z

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

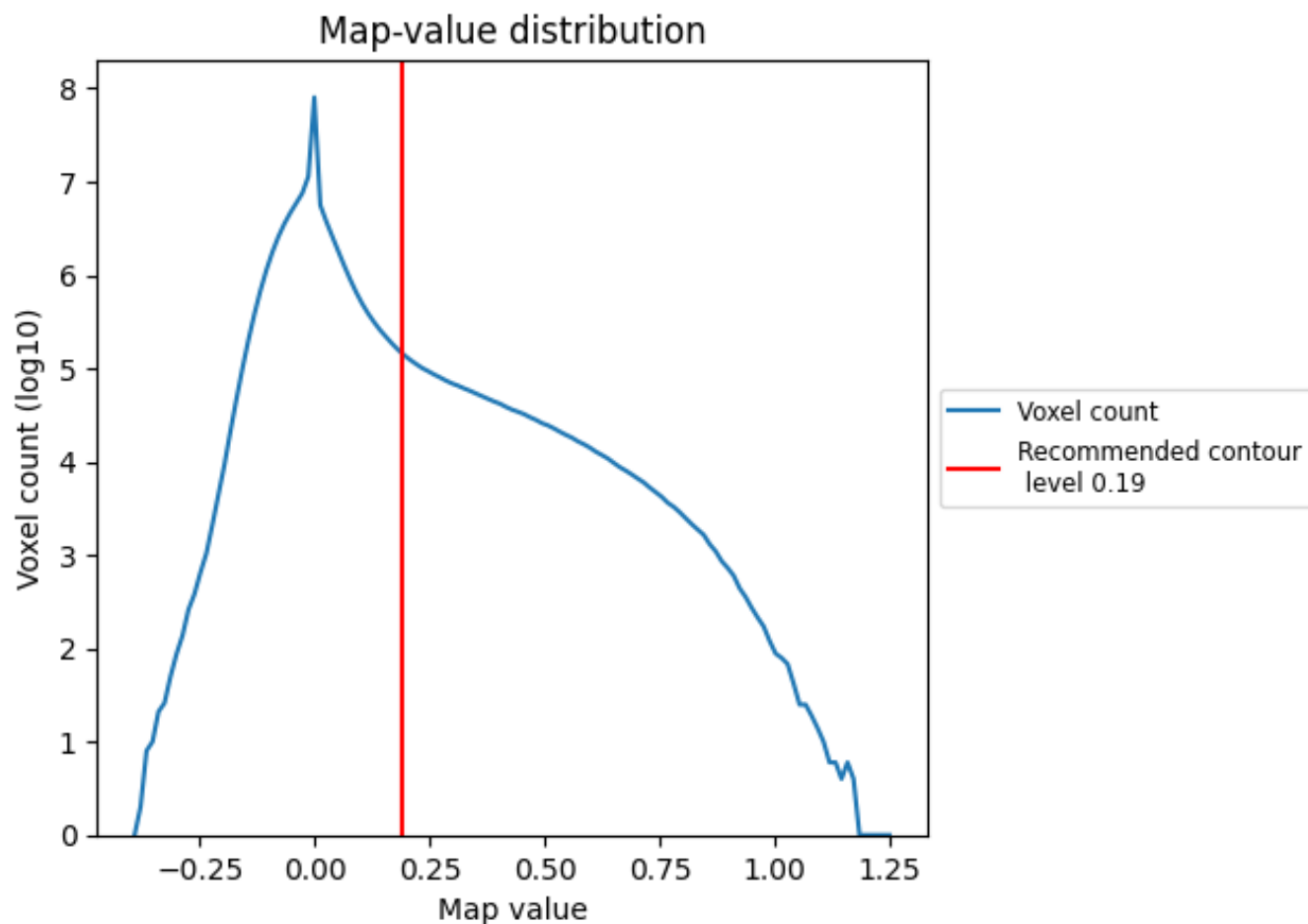
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

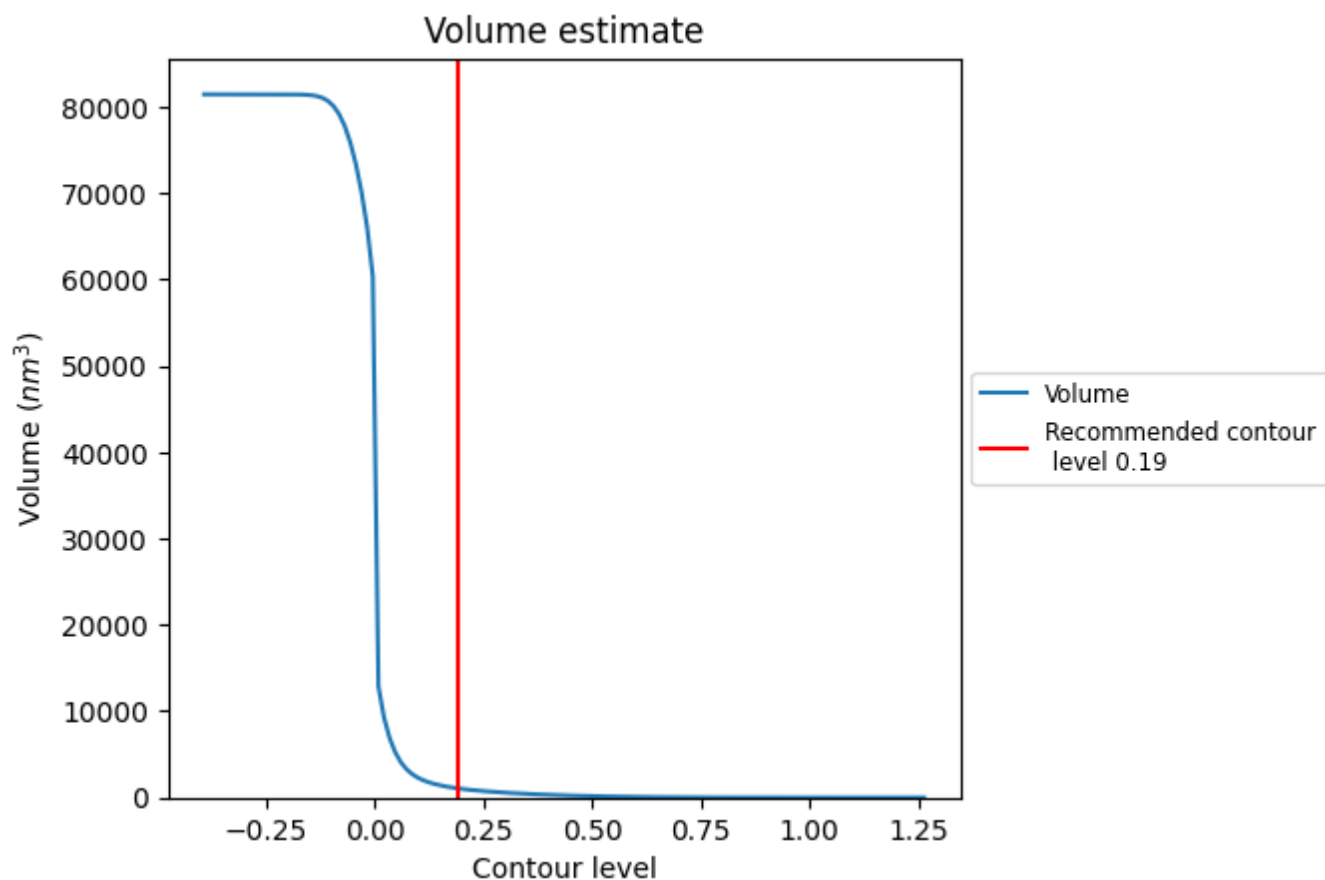
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

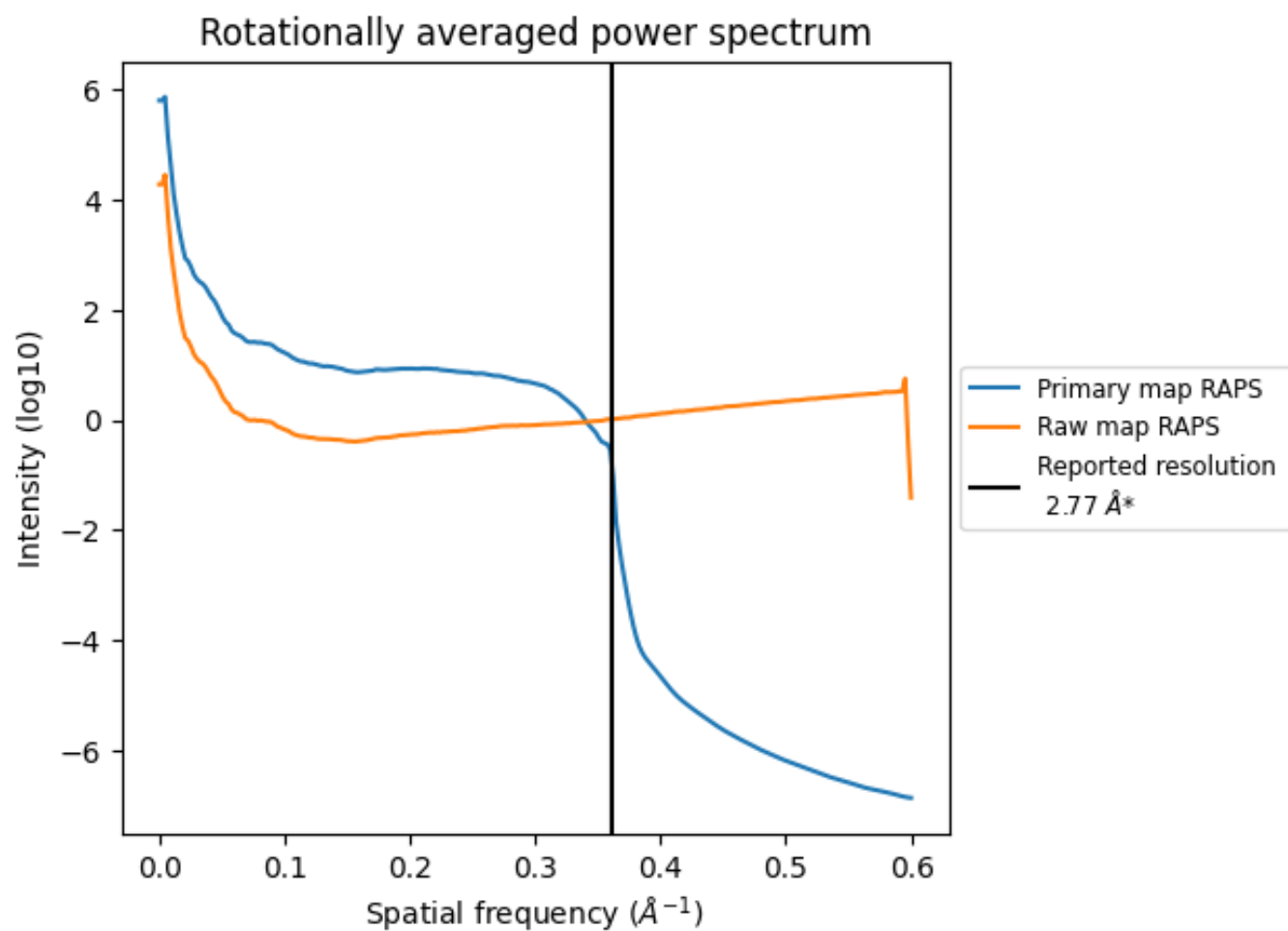
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1072 nm³; this corresponds to an approximate mass of 968 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 ⓘ

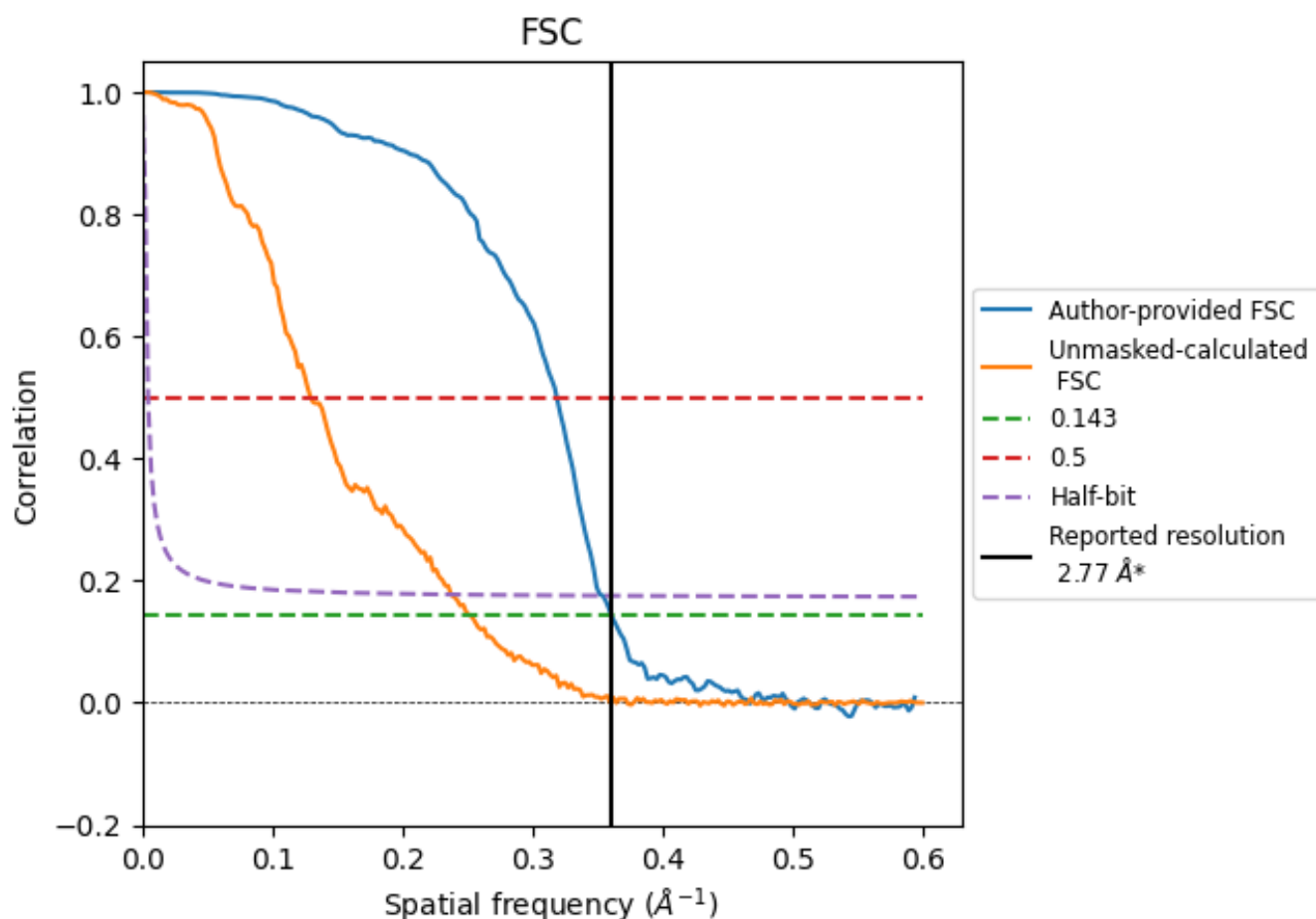


*Reported resolution corresponds to spatial frequency of 0.361 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.361 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

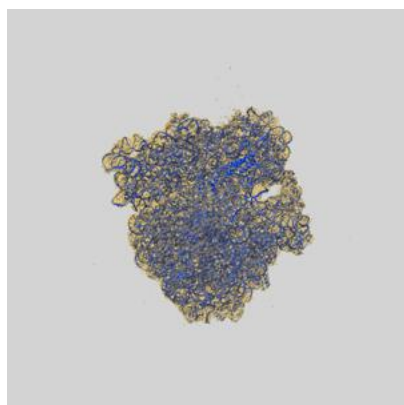
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.14	2.82
Unmasked-calculated*	3.97	7.72	4.21

*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 3.97 differs from the reported value 2.77 by more than 10 %

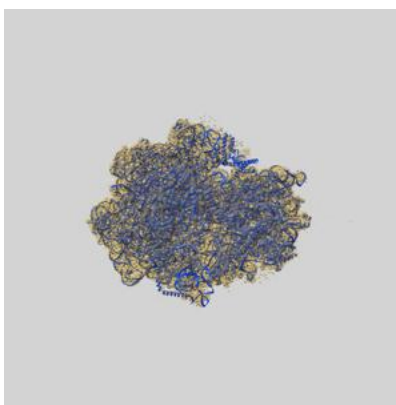
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17346 and PDB model 8P16. Per-residue inclusion information can be found in section 3 on page 18.

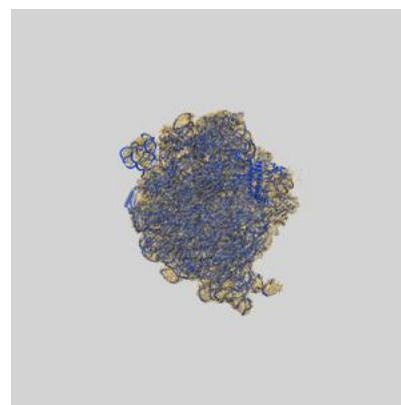
9.1 Map-model overlay [i](#)



X



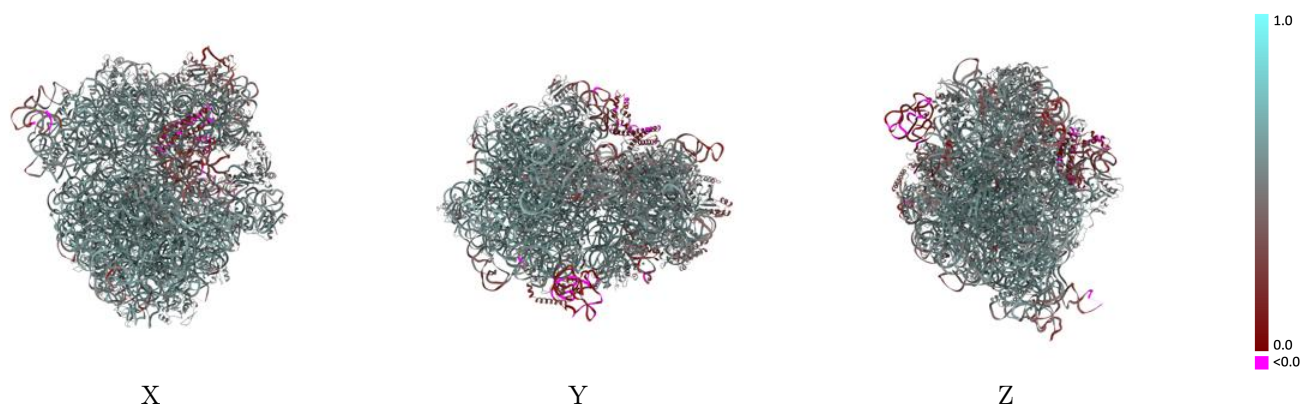
Y



Z

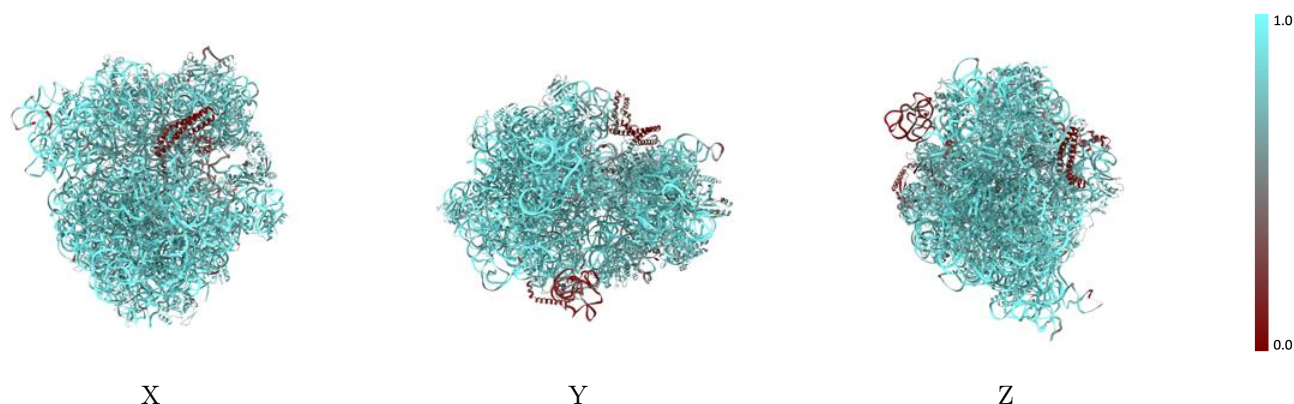
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



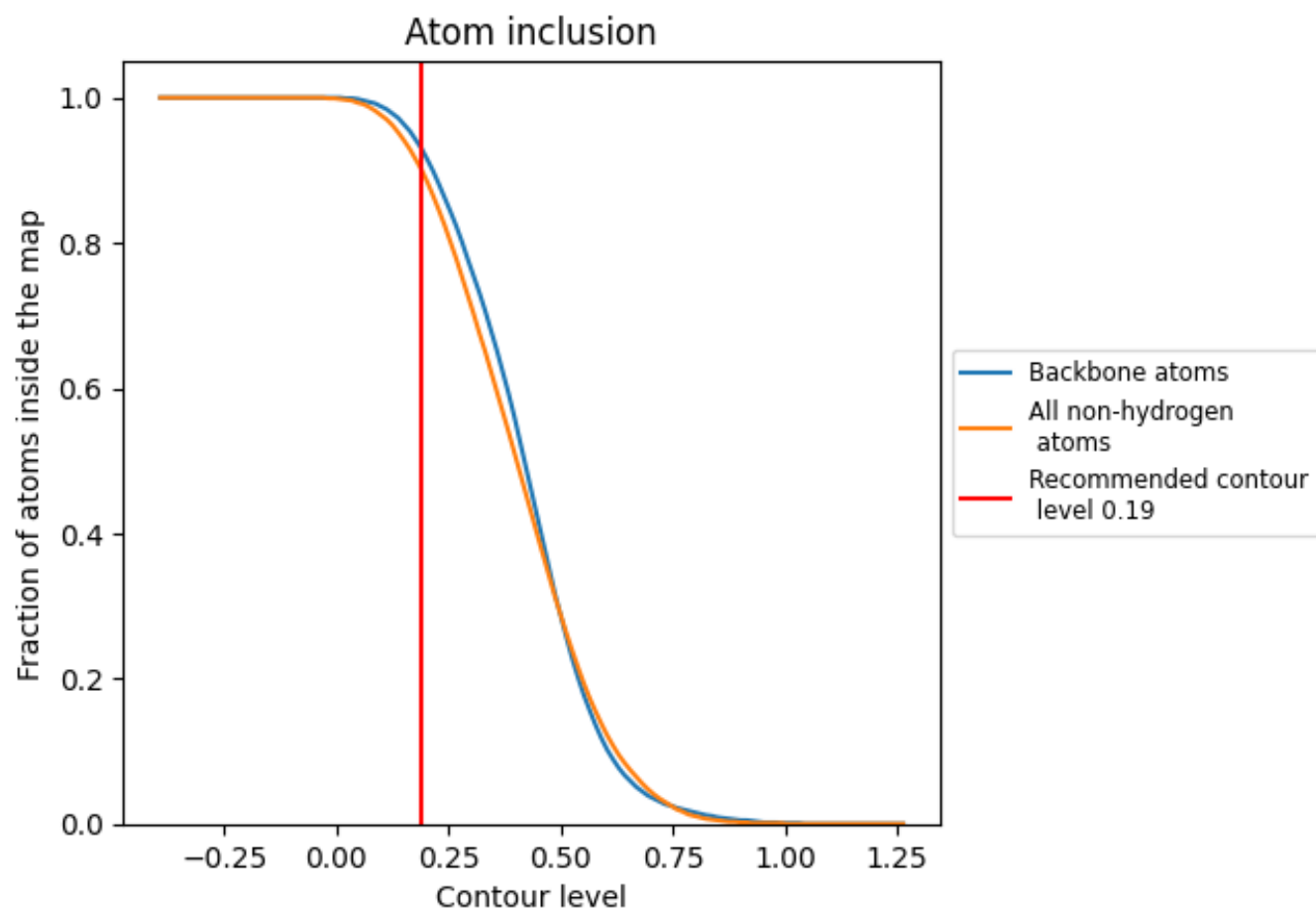
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.5430
1	 0.9440	 0.5610
2	 0.9510	 0.5480
3	 0.9540	 0.5490
4	 0.6390	 0.3320
5	 0.8970	 0.5380
6	 0.5370	 0.3920
B	 0.9160	 0.5940
C	 0.9070	 0.5840
D	 0.8680	 0.5560
E	 0.7640	 0.4860
F	 0.7380	 0.4700
G	 0.3150	 0.3670
I	 0.2240	 0.1340
J	 0.9170	 0.5820
K	 0.8550	 0.5750
L	 0.8910	 0.5720
M	 0.8820	 0.5730
N	 0.9450	 0.5950
O	 0.8460	 0.5310
P	 0.8450	 0.5680
Q	 0.9460	 0.5960
R	 0.8830	 0.5650
S	 0.8990	 0.5760
T	 0.8570	 0.5390
U	 0.8540	 0.5280
V	 0.8250	 0.5340
W	 0.8920	 0.5600
X	 0.8870	 0.5650
Y	 0.8020	 0.4980
Z	 0.8880	 0.5670
a	 0.6930	 0.4490
b	 0.8950	 0.5790
c	 0.8460	 0.5410
d	 0.9580	 0.6140



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Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.9490	 0.6080
f	 0.9210	 0.5720
g	 0.7060	 0.4530
h	 0.8280	 0.5030
i	 0.8430	 0.5200
j	 0.8850	 0.5590
k	 0.7950	 0.5160
l	 0.7580	 0.4810
m	 0.8710	 0.5540
n	 0.8260	 0.5050
o	 0.7620	 0.4480
p	 0.8340	 0.5420
q	 0.8560	 0.5650
r	 0.8060	 0.4960
s	 0.8440	 0.5170
t	 0.8250	 0.5330
u	 0.8780	 0.5450
v	 0.8050	 0.5100
w	 0.8360	 0.5180
x	 0.7700	 0.4930
y	 0.8550	 0.5160
z	 0.7100	 0.4420