



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:02 AM UTC

PDB ID : 8CRX / pdb_00008crx
EMDB ID : EMD-26959
Title : Cutibacterium acnes 70S ribosome with mRNA, P-site tRNA and Sarecycline bound
Authors : Lomakin, I.B.; Devarkar, S.C.; Bunick, C.G.
Deposited on : 2022-05-12
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

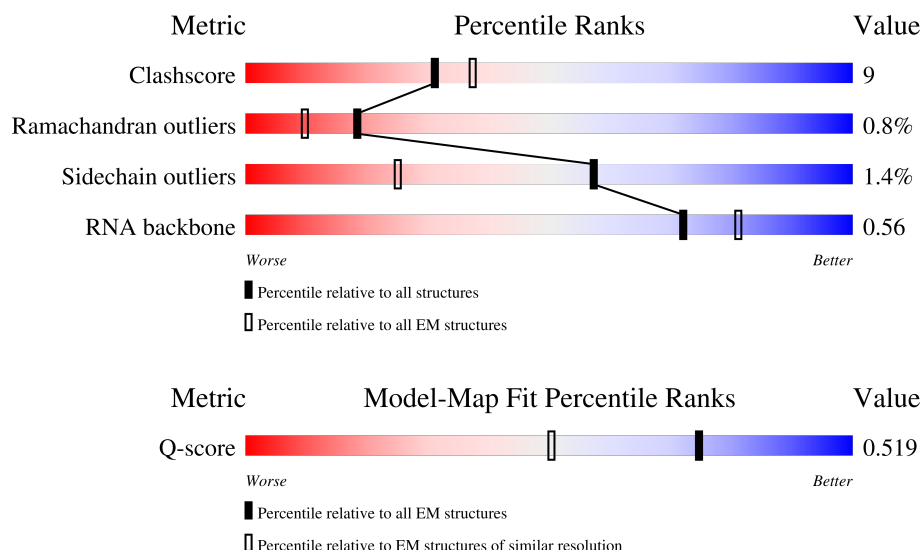
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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.



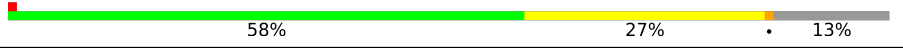
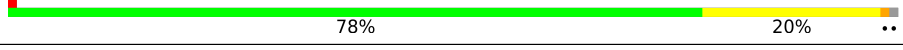
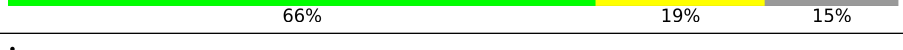
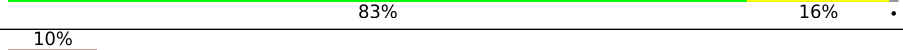
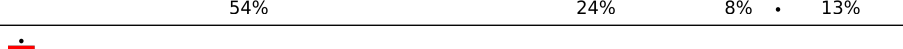
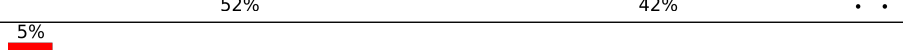
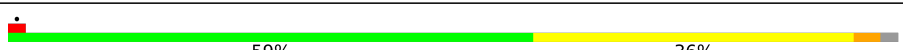
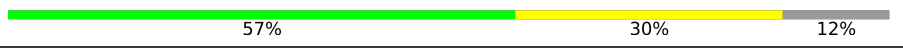
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10754 (2.28 - 3.28)

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

Mol	Chain	Length	Quality of chain
1	A	1537	
2	D	201	
3	E	215	

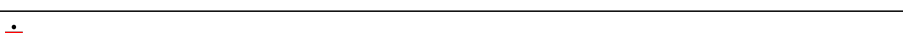
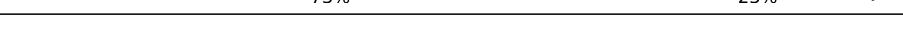
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Mol	Chain	Length	Quality of chain
4	F	96	
5	H	135	
6	K	135	
7	L	123	
8	O	87	
9	Q	90	
10	R	79	
11	T	88	
12	P	147	
13	X	33	
14	G	269	
15	I	156	
16	J	173	
17	M	103	
18	N	123	
19	S	61	
20	U	93	
21	B	283	
22	c	278	
23	d	223	
24	e	301	
25	f	210	
26	g	180	
27	i	147	
28	j	122	

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Mol	Chain	Length	Quality of chain
29	k	146	
30	l	139	
31	m	187	
32	n	127	
33	o	117	
34	p	123	
35	q	102	
36	r	153	
37	s	102	
38	t	122	
39	u	205	
40	v	89	
41	w	61	
42	x	77	
43	y	60	
44	z	63	
45	0	56	
46	1	44	
47	2	68	
48	4	69	
49	a	3086	
50	b	120	
51	V	24	
52	Y	22	
53	C	77	

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Mol	Chain	Length	Quality of chain
54	3	37	24% 65% 35%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 144606 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 RNA (1537-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1505	Total	C	N	O	P	0	0
			32340	14408	5893	10534	1505		

- Molecule 2 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	200	Total	C	N	O	S	0	0
			1632	1021	313	297	1		

- Molecule 3 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	179	Total	C	N	O	S	0	0
			1309	816	244	245	4		

- Molecule 4 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	96	Total	C	N	O	S	0	0
			785	496	134	149	6		

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	134	Total	C	N	O	S	0	0
			1021	642	182	194	3		

- Molecule 6 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	117	Total	C	N	O	S	0	0
			858	532	168	154	4		

- Molecule 7 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	122	Total	C	N	O	S	0	0
			948	587	195	164	2		

- Molecule 8 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	87	Total	C	N	O	S	0	0
			708	440	140	125	3		

- Molecule 9 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	90	Total	C	N	O	S	0	0
			728	446	142	134	6		

- Molecule 10 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	67	Total	C	N	O	0	0
			527	334	103	90		

- Molecule 11 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	T	87	Total	C	N	O	0	0
			673	408	144	121		

- Molecule 12 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	128	Total	C	N	O	S	0	0
			994	621	185	187	1		

- Molecule 13 is a protein called 30S ribosomal protein bS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	X	32	Total	C	N	O	S	0	0
			277	170	71	35	1		

- Molecule 14 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	206	Total	C	N	O	S	0	0
			1613	1010	305	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	155	Total	C	N	O	S	0	0
			1225	764	235	220	6		

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	134	Total	C	N	O	S	0	0
			1012	629	204	177	2		

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	98	Total	C	N	O	S	0	0
			786	496	146	141	3		

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	122	Total	C	N	O		0	0
			976	598	205	173			

- Molecule 19 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	60	Total	C	N	O	S	0	0
			474	298	98	73	5		

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	84	Total	C	N	O	S	0	0
			658	416	126	113	3		

- Molecule 21 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	233	Total	C	N	O	S	0	0
			1836	1163	326	338	9		

- Molecule 22 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	274	Total	C	N	O	S	0	0
			2091	1289	425	372	5		

- Molecule 23 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	214	Total	C	N	O	S	0	0
			1586	984	304	291	7		

- Molecule 24 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	210	Total	C	N	O	S	0	0
			1577	979	301	295	2		

- Molecule 25 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	184	Total	C	N	O	S	0	0
			1468	924	269	266	9		

- Molecule 26 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	177	Total	C	N	O	S	0	0
			1376	867	250	258	1		

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	146	Total	C	N	O	S	0	0
			1139	718	213	205	3		

- Molecule 28 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	122	Total	C	N	O	S	0	0
			946	596	177	169	4		

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	k	144	Total	C	N	O	S	0	0
			1072	675	196	199	2		

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	136	Total	C	N	O	S	0	0
			1082	685	210	181	6		

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	m	120	Total	C	N	O	S	0	0
			936	583	188	163	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	102	ILE	ASN	conflict	UNP A0A085AZY3

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	126	Total	C	N	O	S	0	0
			952	583	190	176	3		

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	114	Total	C	N	O	S	0	0
			896	559	174	162	1		

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	p	119	Total	C	N	O	S	0	0
			958	589	196	171	2		

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q	102	Total	C	N	O	S	0	0
			778	487	140	150	1		

- Molecule 36 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	r	132	Total	C	N	O	S	0	0
			1017	624	204	182	7		

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	95	Total	C	N	O	S	0	0
			751	474	138	138	1		

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	107	Total	C	N	O	S	0	0
			833	516	163	153	1		

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	179	Total	C	N	O	S	0	0
			1376	865	240	268	3		

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	v	78	Total	C	N	O	0	0
			591	355	127	109		

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	60	Total	C	N	O	S	0	0
			474	290	102	77	5		

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	x	69	Total	C	N	O		0	0
			564	348	108	108			

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	58	Total	C	N	O	S	0	0
			467	290	91	83	3		

- Molecule 44 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	62	Total	C	N	O	S	0	0
			477	287	102	83	5		

- Molecule 45 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	0	50	Total	C	N	O	S	0	0
			423	253	91	73	6		

- Molecule 46 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	44	Total	C	N	O	S	0	0
			362	213	91	56	2		

- Molecule 47 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	67	Total	C	N	O	S	0	0
			513	315	110	87	1		

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	66	Total	C	N	O	S	0	0
			512	313	97	97	5		

- Molecule 49 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	a	2903	Total	C	N	O	P	6	0
			62531	27850	11406	20366	2909		

- Molecule 50 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	b	120	Total	C	N	O	P	0	0
			2567	1145	466	836	120		

- Molecule 51 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	V	23	Total	C	N	O	0	0
			183	106	50	27		

- Molecule 52 is a RNA chain called 32MF mRNA.

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

- Molecule 53 is a RNA chain called P-site initiator tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	C	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	37	Total	C	N	O	S	0	0
			302	184	66	47	5		

- Molecule 55 is Sarecycline (CCD ID: V7A) (formula: C₂₄H₂₉N₃O₈).



Mol	Chain	Residues	Atoms				AltConf
55	A	1	Total 35	C 24	N 3	O 8	0
55	a	1	Total 35	C 24	N 3	O 8	0

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

Mol	Chain	Residues	Atoms	AltConf
56	A	82	Total Mg 82 82	0
56	c	3	Total Mg 3 3	0
56	d	1	Total Mg 1 1	0
56	k	2	Total Mg 2 2	0
56	1	1	Total Mg 1 1	0
56	a	294	Total Mg 294 294	0
56	b	2	Total Mg 2 2	0
56	C	1	Total Mg 1 1	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	S	1	Total 1	Zn 1	0
57	w	1	Total 1	Zn 1	0
57	z	1	Total 1	Zn 1	0
57	0	1	Total 1	Zn 1	0
57	4	1	Total 1	Zn 1	0

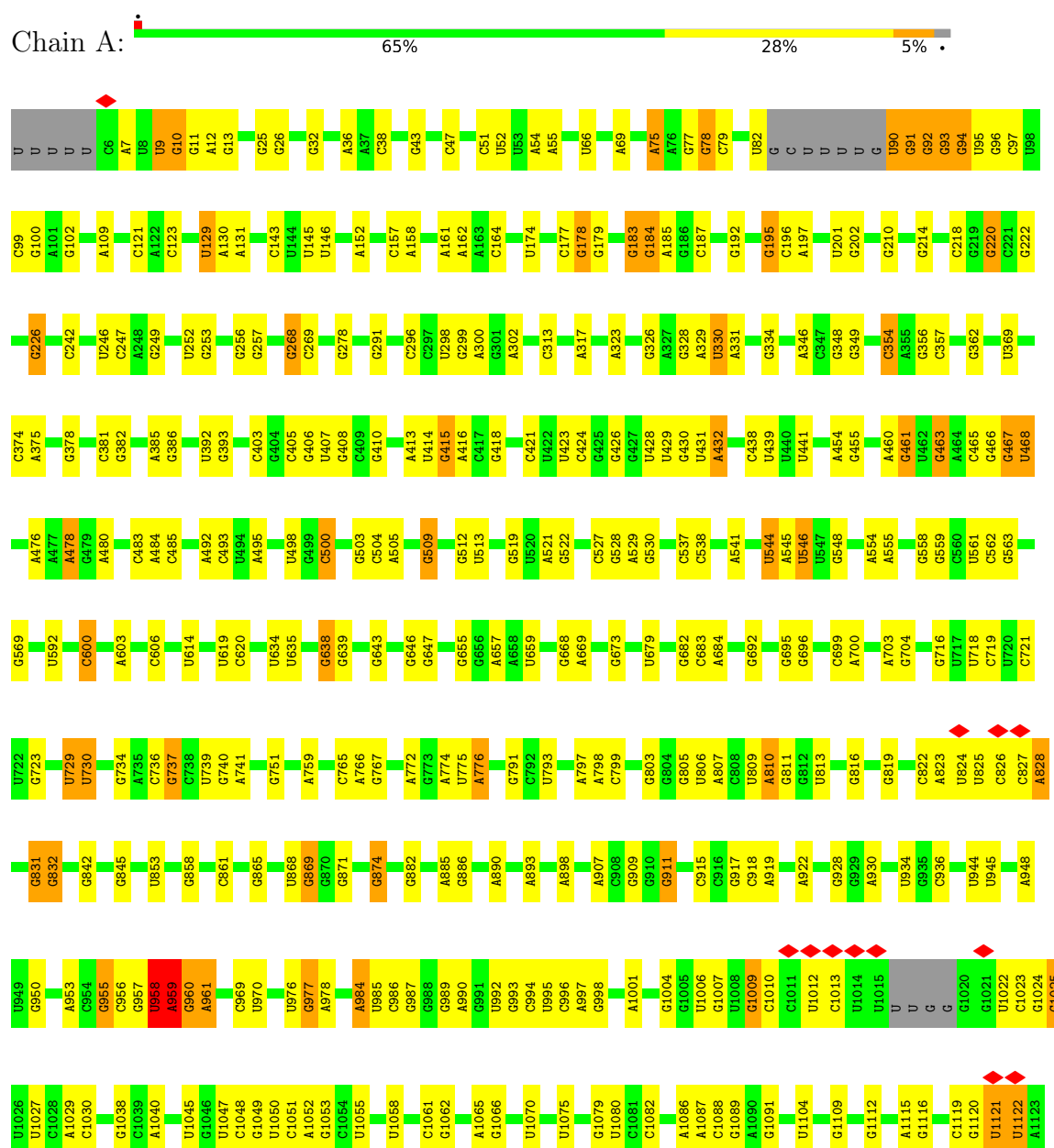
- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	A	1	Total 1	O 1	0
58	d	1	Total 1	O 1	0
58	s	1	Total 1	O 1	0
58	a	123	Total 123	O 123	0
58	b	3	Total 3	O 3	0

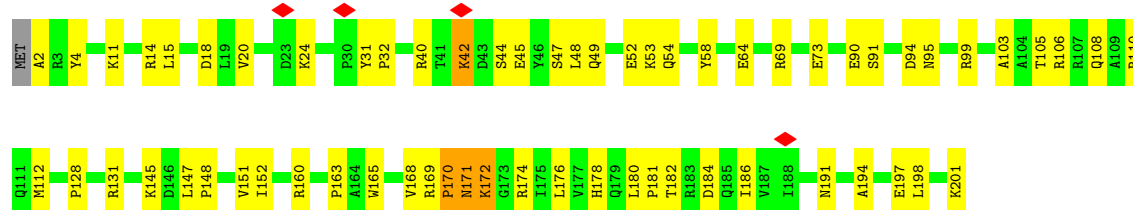
3 Residue-property plots

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

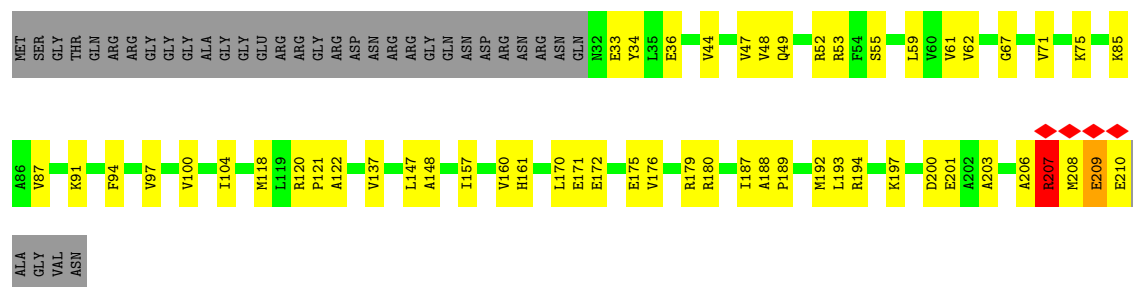
• Molecule 1: RNA (1537-MER)



- Molecule 2: 30S ribosomal protein S4



- Molecule 3: 30S ribosomal protein S5



- Molecule 4: 30S ribosomal protein S6



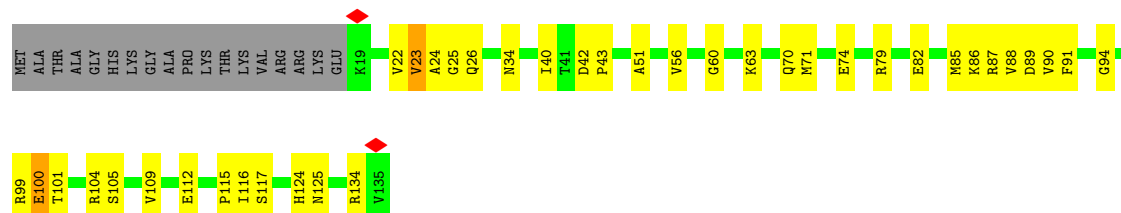
- Molecule 5: 30S ribosomal protein S8

Chain H:  80% 19% ..



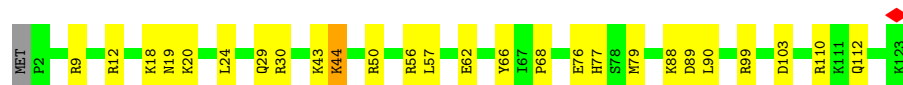
- Molecule 6: 30S ribosomal protein S11

Chain K:  58% 27% 13%



- Molecule 7: 30S ribosomal protein S12

Chain L:  78% 20% ..



- Molecule 8: 30S ribosomal protein S15

Chain O:  71% 29%



- Molecule 9: 30S ribosomal protein S17

Chain Q:  6% 68% 27% ..



- Molecule 10: 30S ribosomal protein S18

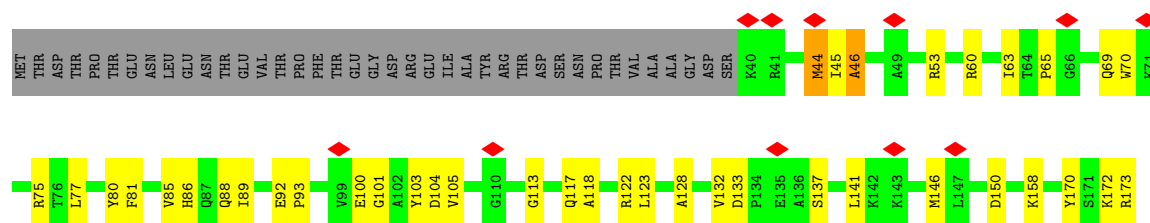
Chain R:  6% 66% 19% 15%



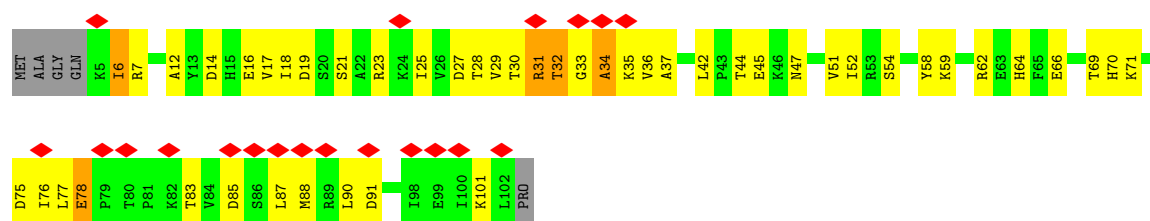
- Molecule 11: 30S ribosomal protein S20

Chain T:  83% 16%

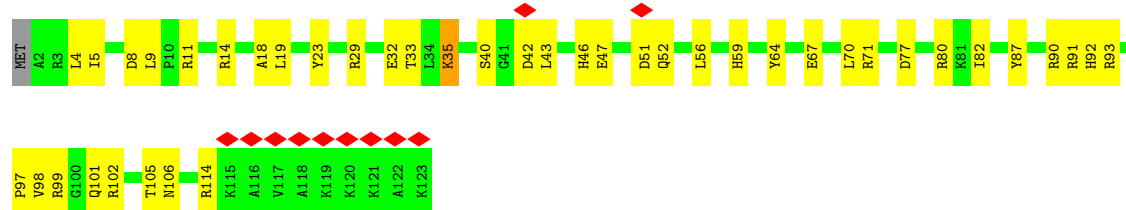




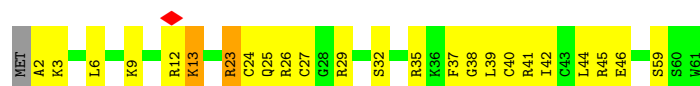
• Molecule 17: 30S ribosomal protein S10



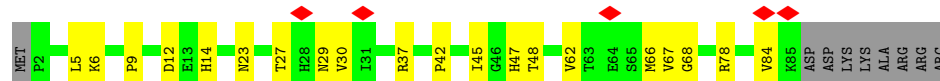
• Molecule 18: 30S ribosomal protein S13



• Molecule 19: 30S ribosomal protein S14 type Z

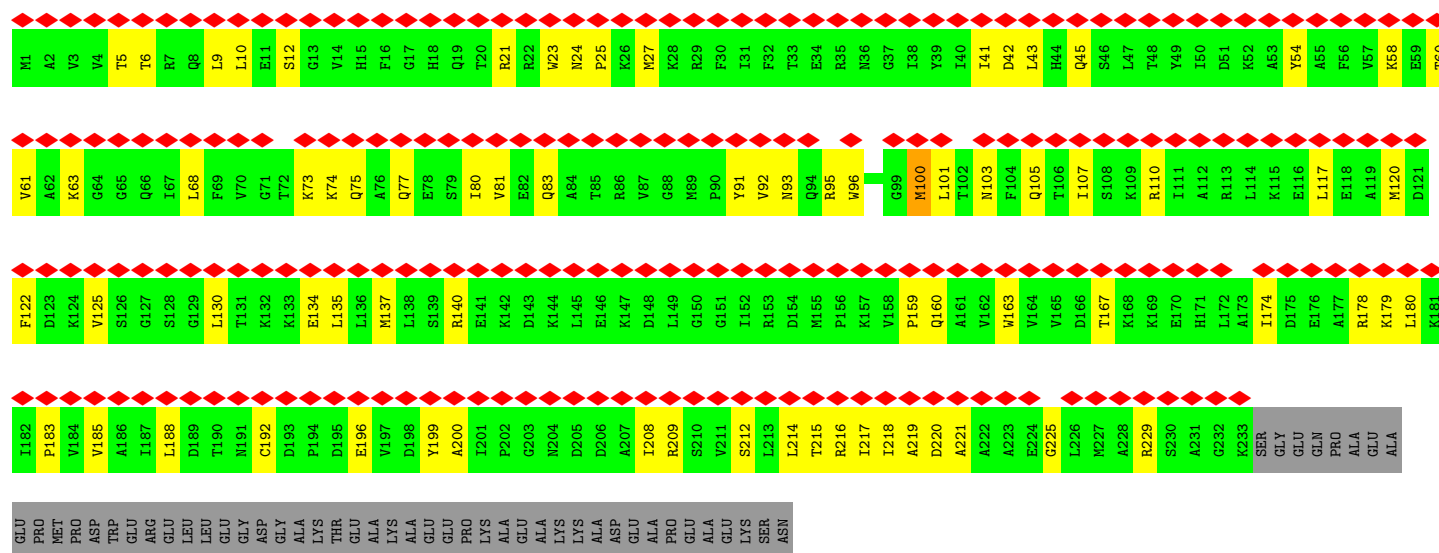


• Molecule 20: 30S ribosomal protein S19



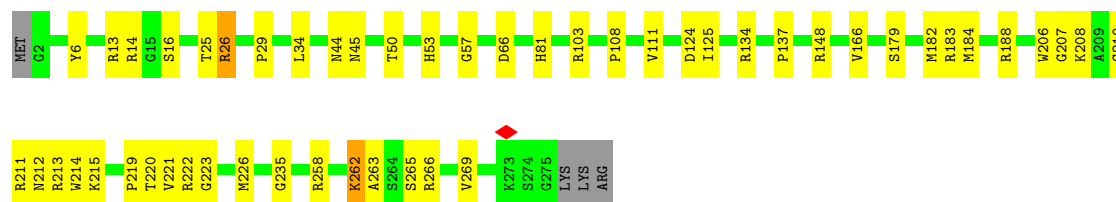
• Molecule 21: 30S ribosomal protein S2





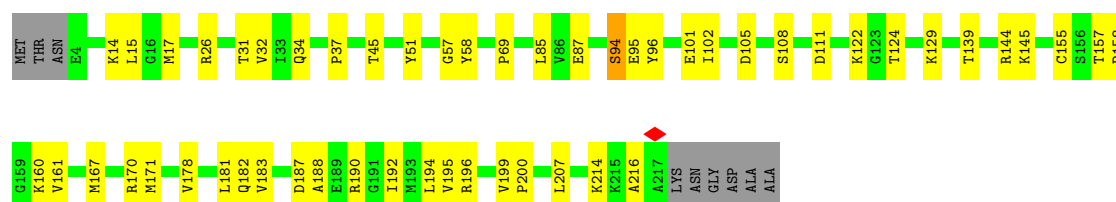
• Molecule 22: 50S ribosomal protein L2

Chain c: 80% 18% ..



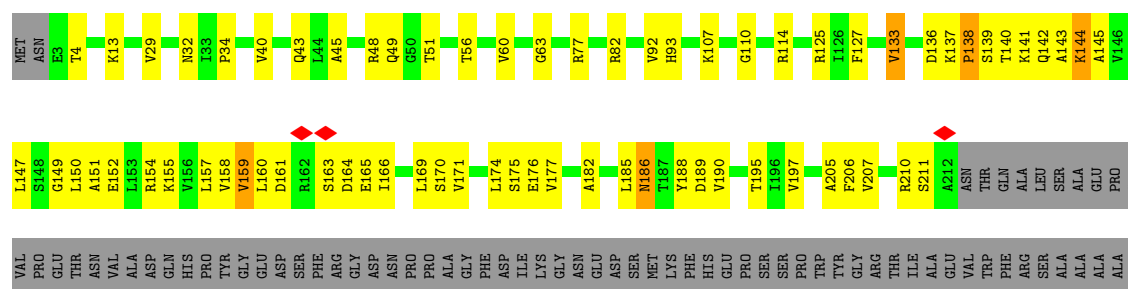
• Molecule 23: 50S ribosomal protein L3

Chain d: 72% 23% .



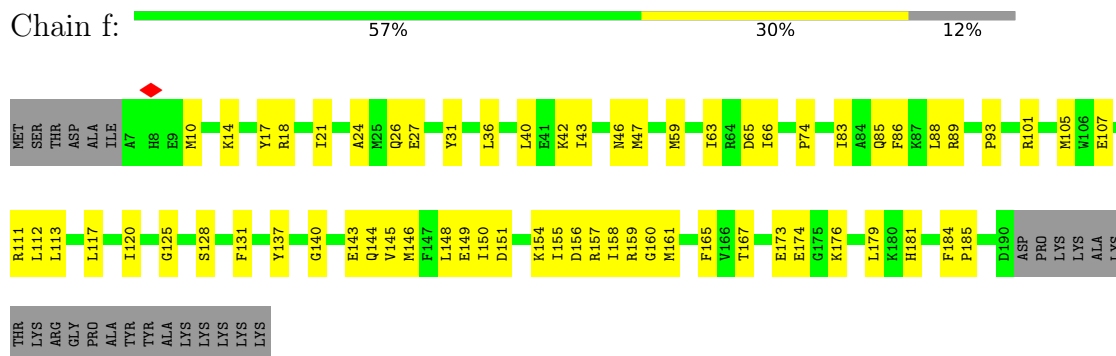
• Molecule 24: 50S ribosomal protein L4

Chain e: 47% 22% 30%

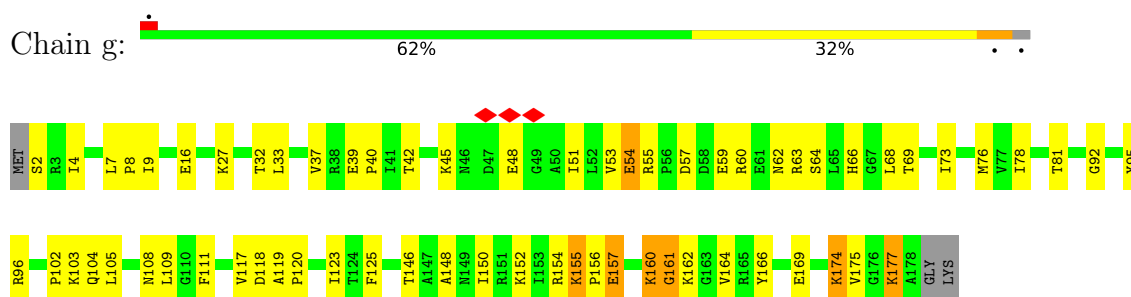


GLU
ALA
ALA
GLY
ASP
PHE
VAL
ASN
ALA
VAL
LYS
SER
SER
SER
GLU
LYS
GLU
ASP
ALA
LYS

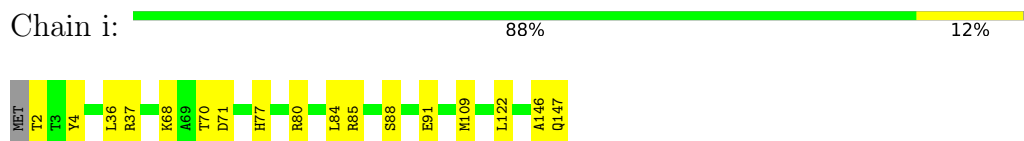
• Molecule 25: 50S ribosomal protein L5



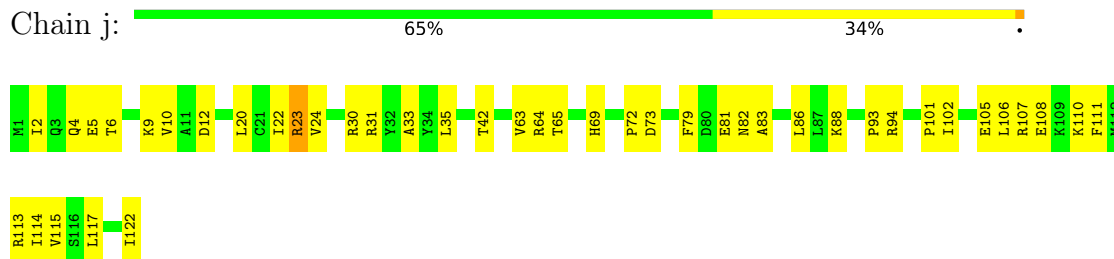
• Molecule 26: 50S ribosomal protein L6



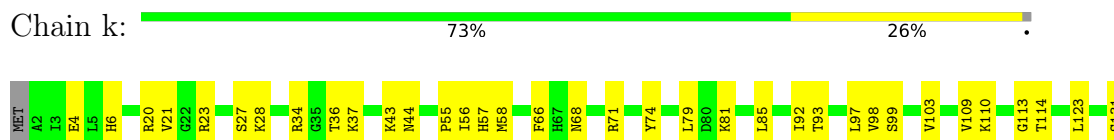
• Molecule 27: 50S ribosomal protein L13



• Molecule 28: 50S ribosomal protein L14



• Molecule 29: 50S ribosomal protein L15





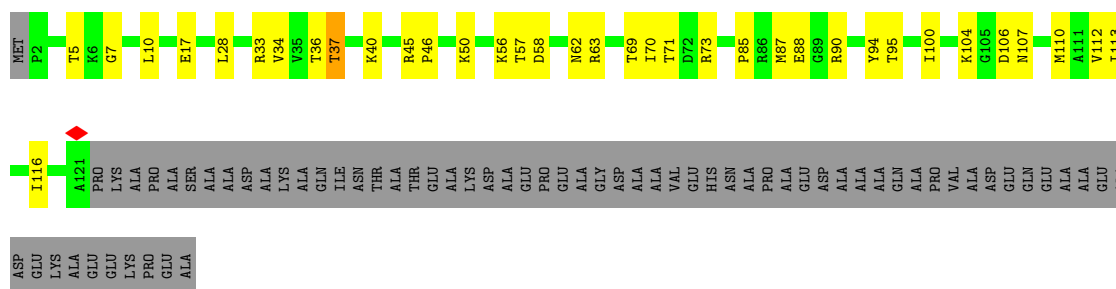
- Molecule 30: 50S ribosomal protein L16

Chain l: 80% 18%



- Molecule 31: 50S ribosomal protein L17

Chain m: 45% 19% 36%



- Molecule 32: 50S ribosomal protein L18

Chain n: 73% 26%



- Molecule 33: 50S ribosomal protein L19

Chain o: 76% 21%



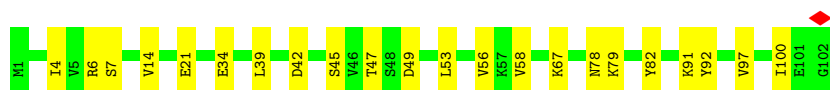
- Molecule 34: 50S ribosomal protein L20

Chain p: 81% 15%

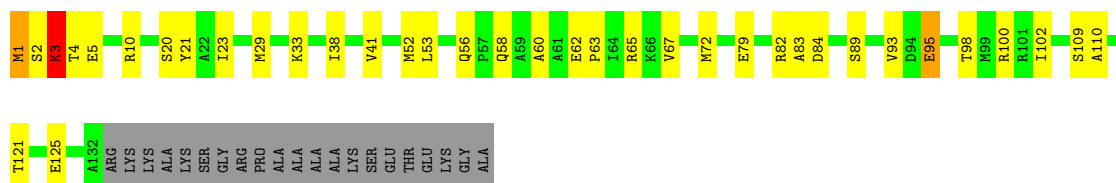


- Molecule 35: 50S ribosomal protein L21

Chain q: 78% 22%



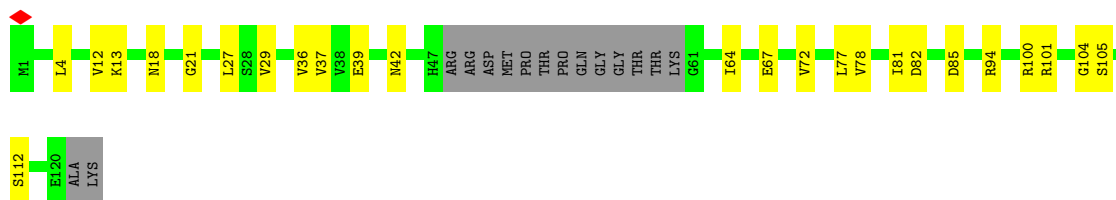
- Molecule 36: 50S ribosomal protein L22



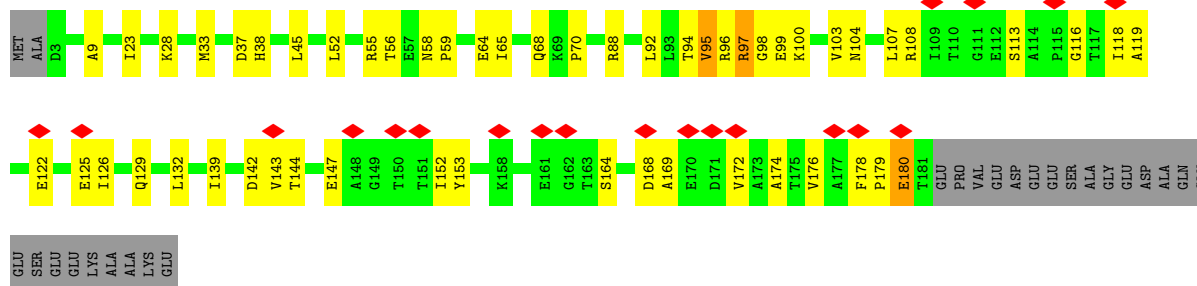
- Molecule 37: 50S ribosomal protein L23



- Molecule 38: 50S ribosomal protein L24



- Molecule 39: 50S ribosomal protein L25

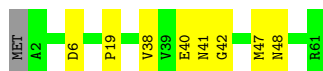
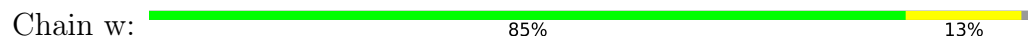


- Molecule 40: 50S ribosomal protein L27

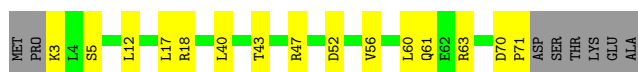




- Molecule 41: 50S ribosomal protein L28



- Molecule 42: 50S ribosomal protein L29



- Molecule 43: 50S ribosomal protein L30



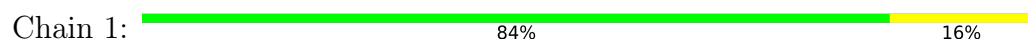
- Molecule 44: 50S ribosomal protein L32



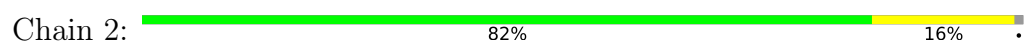
- Molecule 45: 50S ribosomal protein L33

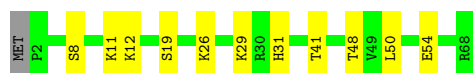


- Molecule 46: 50S ribosomal protein L34



- Molecule 47: 50S ribosomal protein L35

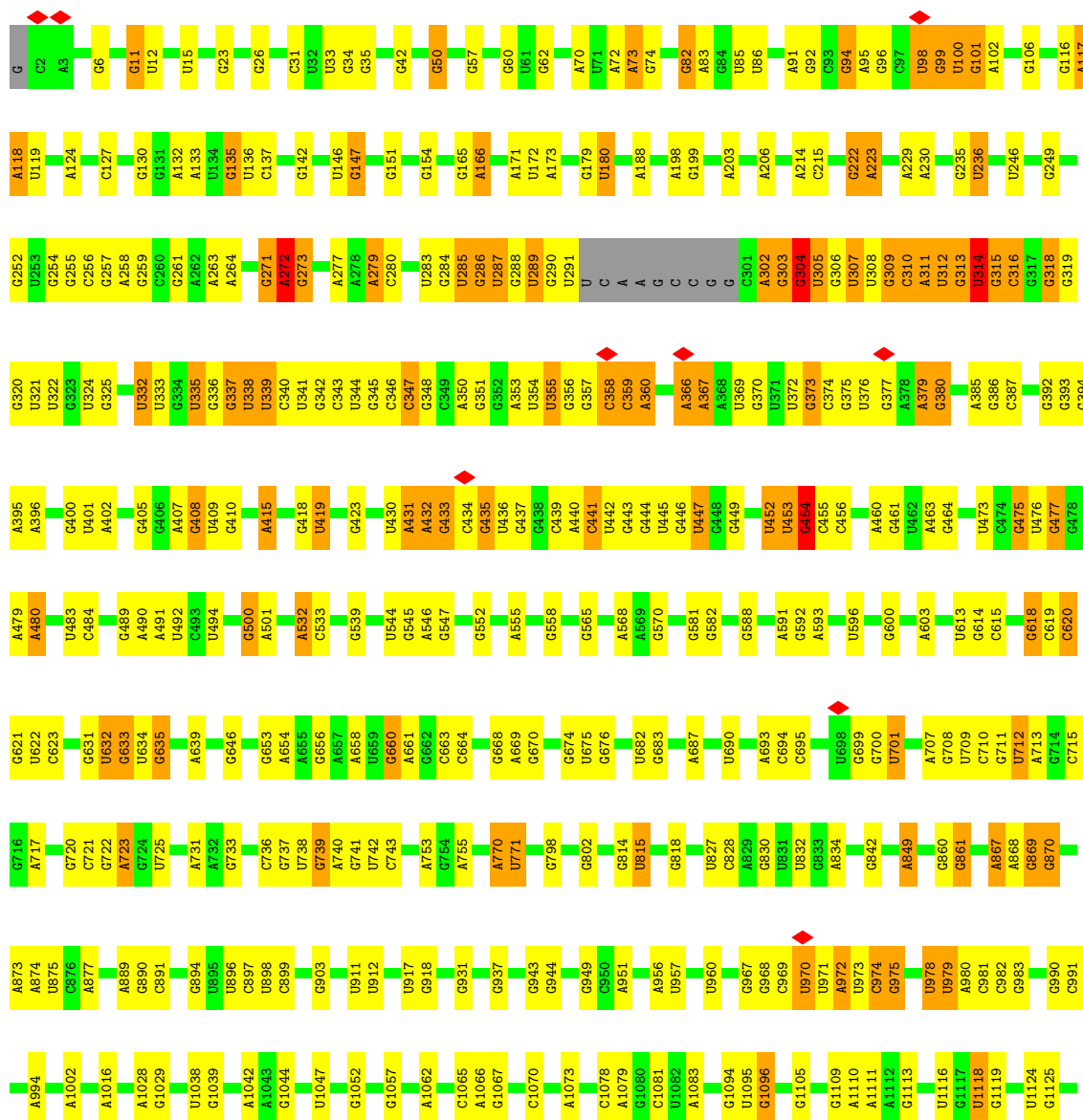




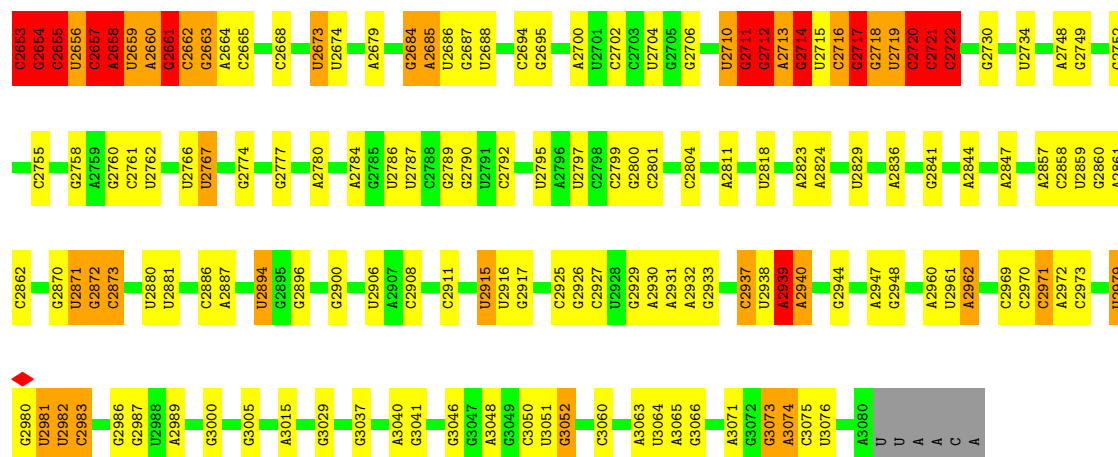
- Molecule 48: 50S ribosomal protein L31



- Molecule 49: 23S ribosomal RNA



G2533	U2433	G	U281	A2149	A2036	G1903	G1723	G1612	G	U	G1329	A1194	U128
A2536	G2432	U	G2282	C2150	G2040	U1904	G1724	U1613	U	A1471	A1330	G1195	A1129
G2544	G2433	C	G2283	A2153	G2041	G1905	G1725	U1726	U	U1472	U1331	G1196	G1130
U2545	A2449	U	A2284	G2155	A2042	A1907	U1726	U1726	U	C1474	G1332	U1199	G1137
G2546	A2450	U	A2285	G2155	A2043	G1910	G1727	A1623	U	U1488	G1333	U1200	G1138
A2548	A2455	G	G2287	U2174	G2048	G1911	A1728	U1625	U	C1489	G1343	G1139	A1140
A2555	G2459	G	G2288	G2175	A2049	U1912	U1730	C1626	A	A1490	U1344	U1215	G1141
A2560	A2460	U	U2289	U2176	G2050	G1913	G1731	G1627	U	C1491	A1345	U1216	G1142
G2561	G2461	A	U2291	C2183	U2051	C1914	A1743	C1629	G	C1492	G1347	U1217	U1143
U2562	G2464	U	G	G2186	G2052	G1915	G1749	G1630	U	U1493	G1348	U1218	U1144
G2563	G2465	U	U	G2192	U2053	U1916	A1752	G1633	C	C	G1349	G1222	G1145
G2564	G2466	U	U	G2192	A2054	U1917	G1761	U1638	G	U	G1350	U1224	G1146
G2565	G2467	C	U	G2195	U2055	G1918	G1768	U1639	G	U	U1351	U1225	C1147
G2566	A2468	C	G	A2198	G2056	G1921	A1769	G1640	U	U	G1355	U1226	U1148
U2567	A2469	U	G	A2198	G2057	G1929	G1770	U1641	U	C	G1359	A1227	U1149
A2574	U2473	U	A	G2201	U2059	G1933	G1771	G1642	G	U	G1360	U1230	G1150
G2582	G2486	G	G	C2202	G2066	U1937	U1772	G1647	G	A	G1361	A1231	G1151
G2583	U2487	U	U	A2203	A2068	A1938	G1773	C1648	U	U	U1364	U1232	A1152
G2584	G2490	C	G	U2204	A2072	G1939	C1774	G1686	G	U	G1365	C1233	A1153
G2585	U2491	U	U	U2205	A2073	G1947	G1777	G1689	A	G	U1376	C1251	G1154
G2586	A2492	C	A	A2206	G2089	G1956	G1777	G1663	U	U	U1377	C1252	G1155
U2587	G2493	G	U	G2210	G2090	A1961	A1792	U1673	G	U	G1385	U1253	A1156
U2588	U2494	C	G	A2213	U2091	U1962	A1798	A1674	U	U	U1385	G1254	G1157
U2589	G2495	U	U	A2214	U2094	U1965	G1815	U1677	U	U	C1390	U1255	C1158
U2590	G2496	U	U	A2215	A2095	C1966	U1818	G1689	A	C	G1393	U1256	C1159
G2606	U2497	C	U	A2216	A2096	A1968	A1830	A1691	U	U	G1394	U1257	A1160
A2607	U2499	U	G	G2222	G2097	A1969	U1831	G1692	C	A	U1403	G1264	U1161
G2611	G2500	A	A	C2226	U2100	C1970	G1833	G1696	A	U	G1400	U1265	C1162
A2612	G2501	C	G	U2106	U2106	C1971	G1837	A1697	U	U	U1403	G1276	C1163
U2613	U2502	C	U	A2110	A2110	C1972	A1838	G1698	U	U	C1411	U1280	U1164
A2617	G2503	U	U	G2112	G2112	C1973	U1843	G1706	U	U	U1416	G1281	G1165
C2623	A2504	C	C	G2113	G2113	A1974	U1843	G1707	U	U	G1417	A1282	G1166
G2626	G2505	C	U	A2119	A2119	G1982	G1851	G1708	U	A	U1428	G1283	A1167
G2627	G2506	U	U	A2120	A2120	C1983	G1851	G1709	G	C	U1428	G1288	A1168
A2630	U2507	C	A	A2121	A2121	A1985	G1858	A1710	U	U	C1433	A1289	G1170
U2631	G2510	C	U	A2135	A2135	C1989	G1879	G1711	A	U	G1434	G1297	A1171
G2636	G2511	U	U	U2138	U2138	U1999	U1894	G1712	U	U	A1441	G1305	G1172
U2639	G2512	C	G	G2141	G2141	G2011	G1895	G1713	C	C	G1306	G1174	U1173
G2649	G2513	U	U	G2142	G2142	A2012	G1896	U1715	U	U	C1307	G1175	G1174
G2650	U2427	C	U	C2145	C2145	C2020	G1897	G1716	U	U	A1443	G1176	C1175
A2651	A2429	G	U	U2146	U2146	G2020	C1898	G1717	G	G	G1447	U1177	G1176
G2652	C2430	A	A	U2280	U2280	A2031	U1901	U1719	U	A	U1455	G1318	A1177
							G1607	U1720	G	G	G1327	A1328	A1179
							C1608	G1721	U	U	A1460		A1181
								U1722					G1182
													C1183
													U1184
													C1185
													A1186
													C1187
													U1188
													G1189
													G1190
													A1193



- Molecule 50: 5S ribosomal RNA

Chain b: 72% 27%



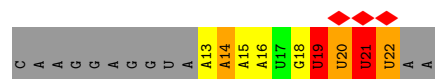
- Molecule 51: 50S ribosomal protein bL37

Chain V: 83% 12%



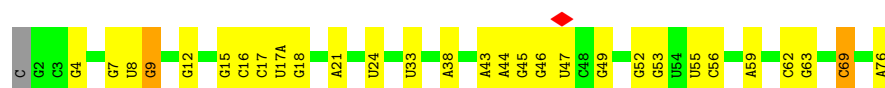
- Molecule 52: 32MF mRNA

Chain Y: 5% 14% 18% 14% 9% 55%



- Molecule 53: P-site initiator tRNA

Chain C: 61% 35%



- Molecule 54: 50S ribosomal protein L36

Chain 3: 24% 65% 35%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.56	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.518	Depositor
Minimum map value	-0.551	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	363.12, 363.12, 363.12	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: V7A, PSU, 4SU, 5MU, OMC, 2MA, MG, 5MC, G7M, OMU, OMG, 3TD, MA6, H2U, 2MG, UR3, ZN, 4OC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	2/35898 (0.0%)	0.27	11/56012 (0.0%)
2	D	0.30	0/1662	0.48	0/2239
3	E	0.29	0/1325	0.47	0/1789
4	F	0.18	0/794	0.41	0/1069
5	H	0.26	0/1036	0.42	0/1395
6	K	0.20	0/874	0.50	0/1177
7	L	0.29	0/960	0.43	0/1283
8	O	0.19	0/718	0.37	0/959
9	Q	0.35	0/734	0.50	0/978
10	R	0.19	0/532	0.37	0/713
11	T	0.21	0/676	0.25	0/897
12	P	0.49	0/1013	0.77	3/1370 (0.2%)
13	X	0.21	0/277	0.41	0/355
14	G	0.22	0/1638	0.39	0/2201
15	I	0.18	0/1246	0.42	0/1679
16	J	0.21	0/1027	0.42	0/1376
17	M	0.36	0/800	0.67	0/1080
18	N	0.20	0/985	0.43	0/1317
19	S	0.32	0/484	0.49	0/644
20	U	0.22	0/675	0.42	0/908
21	B	0.13	0/1864	0.36	0/2509
22	c	0.23	0/2132	0.38	0/2871
23	d	0.32	0/1611	0.46	0/2172
24	e	0.34	0/1600	0.61	0/2165
25	f	0.18	0/1493	0.41	0/2001
26	g	0.34	0/1398	0.53	0/1884
27	i	0.24	0/1164	0.30	0/1574
28	j	0.25	0/957	0.41	0/1282
29	k	0.30	0/1090	0.54	0/1465
30	l	0.23	0/1108	0.31	0/1488
31	m	0.24	0/949	0.39	0/1277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	n	0.17	0/959	0.32	0/1281
33	o	0.19	0/909	0.30	0/1216
34	p	0.23	0/969	0.31	0/1292
35	q	0.22	0/785	0.38	0/1050
36	r	0.31	0/1028	0.42	0/1379
37	s	0.22	0/759	0.34	0/1022
38	t	0.17	0/840	0.33	0/1123
39	u	0.24	0/1396	0.42	0/1896
40	v	0.25	0/598	0.35	0/800
41	w	0.24	0/483	0.32	0/648
42	x	0.18	0/567	0.31	0/759
43	y	0.21	0/471	0.32	0/627
44	z	0.33	0/487	0.46	0/654
45	0	0.40	0/429	0.63	0/569
46	1	0.22	0/365	0.26	0/478
47	2	0.23	0/519	0.35	0/682
48	4	0.38	0/521	0.65	1/700 (0.1%)
49	a	0.26	1/69579 (0.0%)	0.35	67/108567 (0.1%)
50	b	0.19	0/2871	0.19	0/4475
51	V	0.23	0/184	0.32	0/236
52	Y	0.46	0/235	0.91	4/363 (1.1%)
53	C	0.14	0/1725	0.17	0/2689
54	3	0.18	0/305	0.31	0/401
All	All	0.25	3/155704 (0.0%)	0.36	86/233036 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	L	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1153	U	C1'-N1	6.06	1.57	1.48
1	A	1154	C	C1'-N1	6.03	1.57	1.48
49	a	445	U	C1'-N1	5.90	1.57	1.48

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	a	1349	U	P-O3'-C3'	-9.86	105.41	120.20
49	a	315	G	P-O3'-C3'	-9.85	105.42	120.20
49	a	2711	G	P-O3'-C3'	-9.61	105.78	120.20
49	a	2661	G	P-O3'-C3'	-9.50	105.95	120.20
49	a	2653	C	P-O3'-C3'	-9.34	106.19	120.20
49	a	2940	A	P-O3'-C3'	-9.18	106.43	120.20
49	a	660	G	P-O3'-C3'	-8.94	106.79	120.20
1	A	853	U	P-O3'-C3'	-8.74	107.09	120.20
49	a	2052	G	P-O3'-C3'	-8.51	107.44	120.20
49	a	2249	C	P-O3'-C3'	-8.46	107.50	120.20
49	a	441	C	P-O3'-C3'	-8.34	107.70	120.20
49	a	314	U	P-O3'-C3'	-8.30	107.75	120.20
49	a	2652	G	P-O3'-C3'	-8.16	107.96	120.20
49	a	1189	G	P-O3'-C3'	-8.05	108.12	120.20
49	a	1118	U	P-O3'-C3'	-8.04	108.14	120.20
49	a	2657	C	P-O3'-C3'	-8.03	108.15	120.20
49	a	2051	U	P-O3'-C3'	-8.03	108.16	120.20
1	A	810	A	P-O3'-C3'	-7.94	108.29	120.20
49	a	2050	G	P-O3'-C3'	-7.93	108.30	120.20
1	A	432	A	P-O3'-C3'	-7.92	108.32	120.20
12	P	118	GLU	N-CA-C	-7.90	103.53	113.01
49	a	2937	C	P-O3'-C3'	7.90	132.05	120.20
49	a	2939	A	P-O3'-C3'	-7.89	108.36	120.20
49	a	2654	G	P-O3'-C3'	-7.81	108.49	120.20
49	a	2719	U	P-O3'-C3'	-7.79	108.51	120.20
49	a	712	U	P-O3'-C3'	-7.75	108.58	120.20
49	a	2588	U	P-O3'-C3'	-7.74	108.59	120.20
52	Y	18	G	P-O3'-C3'	-7.67	108.70	120.20
49	a	2714	G	P-O3'-C3'	-7.61	108.78	120.20
52	Y	19	U	P-O3'-C3'	-7.59	108.81	120.20
49	a	990	G	P-O3'-C3'	-7.56	108.86	120.20
48	4	46	THR	N-CA-C	-7.56	103.16	112.38
49	a	2053	U	P-O3'-C3'	-7.54	108.89	120.20
1	A	195	G	P-O3'-C3'	-7.52	108.92	120.20
49	a	2722	C	P-O3'-C3'	-7.50	108.95	120.20
49	a	2721	C	P-O3'-C3'	-7.47	108.99	120.20
49	a	911	U	P-O3'-C3'	-7.46	109.01	120.20
1	A	958	U	P-O3'-C3'	-7.38	109.13	120.20
49	a	2710	U	P-O3'-C3'	-7.28	109.28	120.20
49	a	2887	A	P-O3'-C3'	-7.25	109.32	120.20
49	a	2662	C	P-O3'-C3'	-7.22	109.36	120.20
49	a	2655	C	P-O3'-C3'	-7.20	109.40	120.20
49	a	711	G	P-O3'-C3'	-7.10	109.55	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	a	2886	C	P-O3'-C3'	-7.00	109.71	120.20
49	a	2894	U	P-O3'-C3'	-6.98	109.74	120.20
49	a	304	G	P-O3'-C3'	-6.96	109.75	120.20
49	a	2153	A	P-O3'-C3'	-6.92	109.83	120.20
49	a	2525	U	P-O3'-C3'	-6.91	109.83	120.20
1	A	196	C	P-O3'-C3'	-6.89	109.87	120.20
49	a	2055	U	P-O3'-C3'	-6.88	109.88	120.20
1	A	1343	A	P-O3'-C3'	-6.87	109.89	120.20
1	A	129	U	P-O3'-C3'	-6.83	109.95	120.20
49	a	2717	G	P-O3'-C3'	-6.82	109.98	120.20
49	a	1637	G	P-O3'-C3'	-6.81	109.98	120.20
49	a	1832	C	P-O3'-C3'	-6.79	110.02	120.20
49	a	2651	A	P-O3'-C3'	-6.78	110.04	120.20
49	a	2658	A	P-O3'-C3'	-6.75	110.08	120.20
52	Y	20	U	P-O3'-C3'	-6.73	110.11	120.20
1	A	959	A	P-O3'-C3'	-6.72	110.11	120.20
49	a	2054	A	P-O3'-C3'	-6.64	110.24	120.20
49	a	2720	C	P-O3'-C3'	-6.62	110.26	120.20
49	a	303	G	P-O3'-C3'	-6.61	110.28	120.20
49	a	2056	G	P-O3'-C3'	-6.59	110.31	120.20
49	a	454	G	P-O3'-C3'	-6.56	110.36	120.20
49	a	2718	G	P-O3'-C3'	-6.51	110.43	120.20
1	A	809	U	P-O3'-C3'	-6.44	110.53	120.20
49	a	272	A	P-O3'-C3'	-6.30	110.75	120.20
49	a	2587	U	P-O3'-C3'	-6.30	110.75	120.20
52	Y	21	U	P-O3'-C3'	-6.22	110.87	120.20
49	a	2712	G	P-O3'-C3'	-6.21	110.89	120.20
49	a	2250	G	P-O3'-C3'	-6.11	111.04	120.20
49	a	1348	G	P-O3'-C3'	-6.09	111.06	120.20
49	a	2612	A	P-O3'-C3'	-6.09	111.07	120.20
49	a	271	G	C2'-C3'-O3'	6.04	122.76	113.70
49	a	2049	A	P-O3'-C3'	-5.97	111.25	120.20
1	A	1344	U	P-O3'-C3'	-5.84	111.44	120.20
49	a	1638	U	P-O3'-C3'	-5.77	111.55	120.20
12	P	123	LYS	N-CA-C	-5.76	104.92	111.14
49	a	1833	G	P-O3'-C3'	-5.69	111.67	120.20
49	a	452	U	P-O3'-C3'	-5.59	111.82	120.20
49	a	738	U	P-O3'-C3'	-5.55	111.87	120.20
49	a	302	A	P-O3'-C3'	-5.45	112.03	120.20
12	P	46	PRO	N-CA-CB	-5.34	97.64	103.25
49	a	272	A	C1'-O4'-C4'	-5.24	104.66	109.90
49	a	271	G	C4'-C3'-C2'	-5.22	97.38	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	a	2715	U	P-O3'-C3'	-5.04	112.64	120.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	L	44	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32340	0	16267	299	0
2	D	1632	0	1663	71	0
3	E	1309	0	1349	47	0
4	F	785	0	818	34	0
5	H	1021	0	1059	19	0
6	K	858	0	884	31	0
7	L	948	0	1031	20	0
8	O	708	0	737	20	0
9	Q	728	0	772	28	0
10	R	527	0	580	10	0
11	T	673	0	726	13	0
12	P	994	0	1008	84	0
13	X	277	0	338	11	0
14	G	1613	0	1626	39	0
15	I	1225	0	1275	28	0
16	J	1012	0	1069	35	0
17	M	786	0	823	40	0
18	N	976	0	1031	35	0
19	S	474	0	499	27	0
20	U	658	0	671	16	0
21	B	1836	0	1902	56	0
22	c	2091	0	2150	46	0
23	d	1586	0	1634	39	0
24	e	1577	0	1619	60	0
25	f	1468	0	1487	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	g	1376	0	1421	56	0
27	i	1139	0	1163	13	0
28	j	946	0	1011	32	0
29	k	1072	0	1106	30	0
30	l	1082	0	1117	20	0
31	m	936	0	997	25	0
32	n	952	0	995	21	0
33	o	896	0	928	19	0
34	p	958	0	986	19	0
35	q	778	0	824	15	0
36	r	1017	0	1070	28	0
37	s	751	0	803	11	0
38	t	833	0	883	15	0
39	u	1376	0	1397	35	0
40	v	591	0	581	10	0
41	w	474	0	487	4	0
42	x	564	0	582	11	0
43	y	467	0	504	11	0
44	z	477	0	479	13	0
45	0	423	0	429	17	0
46	1	362	0	387	5	0
47	2	513	0	565	8	0
48	4	512	0	497	41	0
49	a	62531	0	31359	612	0
50	b	2567	0	1297	21	0
51	V	183	0	202	4	0
52	Y	211	0	106	8	0
53	C	1625	0	829	15	0
54	3	302	0	333	9	0
55	A	35	0	0	0	0
55	a	35	0	0	1	0
56	1	1	0	0	0	0
56	A	82	0	0	0	0
56	C	1	0	0	0	0
56	a	294	0	0	0	0
56	b	2	0	0	0	0
56	c	3	0	0	0	0
56	d	1	0	0	0	0
56	k	2	0	0	0	0
57	0	1	0	0	0	0
57	4	1	0	0	0	0
57	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	w	1	0	0	0	0
57	z	1	0	0	0	0
58	A	1	0	0	0	0
58	a	123	0	0	5	0
58	b	3	0	0	0	0
58	d	1	0	0	0	0
58	s	1	0	0	0	0
All	All	144606	0	96356	1953	0

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

All (1953) 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:e:142:GLN:HE21	24:e:174:LEU:HD21	1.14	1.10
12:P:114:GLU:HA	12:P:117:ARG:HB2	1.30	1.08
2:D:171:ASN:HB2	12:P:119:ALA:C	1.86	1.01
12:P:45:ASP:HB2	12:P:46:PRO:HD2	1.48	0.94
1:A:1480:A:H4'	52:Y:19:U:H1'	1.52	0.91
45:0:8:VAL:HA	45:0:30:ARG:HH21	1.35	0.88
24:e:160:LEU:HB3	24:e:164:ASP:HB2	1.54	0.88
37:s:69:ARG:HH21	49:a:1411:C:H5''	1.38	0.87
25:f:43:ILE:HG12	25:f:105:MET:HG3	1.56	0.85
49:a:1912:U:H5'	49:a:1914:C:H5'	1.57	0.85
2:D:171:ASN:CB	12:P:119:ALA:HB1	2.06	0.85
49:a:367:A:H61	49:a:444:G:H21	1.26	0.84
25:f:21:ILE:HD12	25:f:181:HIS:HB3	1.60	0.83
49:a:2654:G:H3'	49:a:2657:C:H42	1.44	0.82
1:A:1392:G:H4'	13:X:12:MET:HE2	1.60	0.82
29:k:20:ARG:NH2	49:a:1327:G:N7	2.26	0.82
17:M:51:VAL:HG13	19:S:41:ARG:HG2	1.60	0.82
49:a:669:A:H62	49:a:1328:A:H2	1.27	0.82
49:a:1831:U:H5'	49:a:1832:C:H5'	1.62	0.81
12:P:108:ALA:HA	12:P:111:GLU:HB2	1.61	0.81
24:e:138:PRO:HG2	24:e:141:LYS:HB2	1.62	0.81
9:Q:7:GLU:C	9:Q:9:THR:H	1.89	0.81
33:o:94:ARG:HH21	49:a:1937:C:H5	1.29	0.81
48:4:16:CYS:SG	48:4:38:CYS:HB3	2.21	0.80
29:k:36:THR:HG22	29:k:37:LYS:HG2	1.64	0.79
1:A:183:G:H21	1:A:226:G:H4'	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:142:GLN:HG3	24:e:171:VAL:HG12	1.65	0.79
49:a:3073:G:H4'	49:a:3074:A:H5'	1.64	0.79
49:a:2053:U:H3'	49:a:2054:A:H8	1.46	0.79
22:c:262:LYS:HG3	22:c:263:ALA:H	1.47	0.78
49:a:1281:C:H5	49:a:1318:G:H1	1.31	0.78
48:4:14:VAL:HG12	48:4:33:LEU:HB2	1.65	0.78
48:4:20:ASN:ND2	48:4:38:CYS:SG	2.57	0.78
49:a:2053:U:H3'	49:a:2054:A:C8	2.19	0.77
1:A:824:U:H3	1:A:828:A:H61	1.31	0.77
24:e:142:GLN:NE2	24:e:174:LEU:HD21	1.97	0.77
49:a:2279:A:H61	49:a:2374:U:H3	1.32	0.77
12:P:45:ASP:O	12:P:46:PRO:C	2.28	0.76
49:a:302:A:H3'	49:a:303:G:H8	1.51	0.76
49:a:332:U:H3	49:a:449:G:H1	1.34	0.76
30:l:63:LYS:HG3	39:u:180:GLU:HG2	1.67	0.76
1:A:646:G:H22	1:A:723:G:H1	1.30	0.76
3:E:59:LEU:HD11	3:E:157:ILE:HG13	1.67	0.76
1:A:917:G:N7	15:I:3:ARG:NH1	2.33	0.76
1:A:1272:G:H2'	1:A:1273:A:H4'	1.67	0.76
16:J:100:GLU:HG3	16:J:101:GLY:H	1.49	0.75
32:n:2:ALA:N	50:b:9:G:N7	2.34	0.75
24:e:152:GLU:HB3	24:e:176:GLU:HG3	1.66	0.75
49:a:142:G:H22	49:a:147:G:H22	1.33	0.75
48:4:16:CYS:SG	48:4:38:CYS:CB	2.75	0.75
12:P:122:LYS:HA	12:P:125:GLU:HB2	1.68	0.75
2:D:49:GLN:HB3	2:D:198:LEU:HB2	1.69	0.74
22:c:222:ARG:NH1	49:a:1972:A:OP2	2.20	0.74
29:k:43:LYS:NZ	49:a:889:A:OP1	2.21	0.74
49:a:1716:U:O2'	49:a:1721:G:N2	2.21	0.74
31:m:10:LEU:HB2	31:m:17:GLU:HG3	1.70	0.74
49:a:970:U:H3	49:a:975:G:H1	1.35	0.74
49:a:1698:G:H1	49:a:1915:G:H22	1.35	0.74
12:P:112:ALA:O	12:P:115:ALA:N	2.20	0.73
49:a:1904:U:H5	49:a:1921:G:H21	1.32	0.73
3:E:171:GLU:HG3	3:E:176:VAL:HG22	1.70	0.73
21:B:23:TRP:HE1	21:B:27:MET:HB2	1.53	0.73
49:a:85:U:H3	49:a:95:A:H61	1.36	0.73
27:i:85:ARG:NH1	49:a:2823:A:OP1	2.21	0.73
34:p:31:LEU:HD22	49:a:664:C:H5'	1.69	0.73
49:a:1623:C:H5	49:a:1731:G:H1	1.36	0.73
12:P:117:ARG:O	12:P:121:THR:HG23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:G:HO2'	5:H:2:THR:N	1.87	0.72
49:a:60:G:H22	49:a:92:G:H1	1.37	0.72
4:F:15:GLU:O	4:F:17:ARG:NH1	2.22	0.72
26:g:9:ILE:HB	26:g:51:ILE:HB	1.70	0.72
12:P:116:PRO:HA	12:P:119:ALA:HB3	1.71	0.72
18:N:19:LEU:HD21	18:N:56:LEU:HD21	1.72	0.72
26:g:104:GLN:NE2	26:g:118:ASP:OD1	2.21	0.72
24:e:133:VAL:HA	24:e:141:LYS:HE2	1.71	0.72
1:A:11:G:N7	3:E:120:ARG:NH1	2.38	0.71
12:P:116:PRO:HA	12:P:119:ALA:CB	2.21	0.71
49:a:360:A:H2	49:a:444:G:H22	1.35	0.71
48:4:18:CYS:CB	48:4:41:CYS:SG	2.78	0.71
2:D:178:HIS:CE1	12:P:109:LEU:HD11	2.25	0.71
17:M:34:ALA:HA	17:M:78:GLU:HB2	1.73	0.70
49:a:2706:G:H22	49:a:2721:C:H5	1.38	0.70
1:A:700:A:C8	6:K:124:HIS:HD2	2.09	0.70
49:a:2052:G:H21	49:a:2055:U:H5	1.37	0.70
49:a:82:G:N2	49:a:102:A:OP2	2.23	0.70
1:A:984:A:N6	1:A:1025:G:O6	2.25	0.70
39:u:52:LEU:HD22	39:u:55:ARG:HH12	1.57	0.70
49:a:2284:G:H1	49:a:2369:U:H3	1.38	0.70
2:D:171:ASN:C	12:P:119:ALA:HB1	2.17	0.70
20:U:12:ASP:OD2	20:U:14:HIS:NE2	2.25	0.70
23:d:178:VAL:HG12	23:d:181:LEU:HD11	1.72	0.70
29:k:55:PRO:HG2	29:k:58:MET:HG3	1.74	0.70
49:a:2584:G:N2	49:a:2584:G:OP2	2.25	0.70
22:c:53:HIS:CE1	22:c:220:THR:HA	2.27	0.69
3:E:179:ARG:HG2	5:H:76:SER:HA	1.74	0.69
12:P:115:ALA:HB3	12:P:116:PRO:CD	2.20	0.69
49:a:106:G:H4'	49:a:379:A:H5''	1.74	0.69
1:A:476:A:H2'	1:A:478:A:H8	1.57	0.69
26:g:37:VAL:HG13	26:g:69:THR:HG21	1.74	0.69
49:a:86:U:H3	49:a:94:G:H1	1.40	0.69
6:K:94:GLY:O	6:K:99:ARG:NH2	2.23	0.69
9:Q:9:THR:O	9:Q:10:THR:C	2.36	0.69
12:P:116:PRO:O	12:P:119:ALA:HB3	1.91	0.69
39:u:64:GLU:HG3	39:u:70:PRO:HB3	1.74	0.69
16:J:85:VAL:O	16:J:88:GLN:NE2	2.22	0.69
25:f:143:GLU:OE2	25:f:145:VAL:HG12	1.93	0.69
49:a:6:G:H1	49:a:3076:U:H3	1.38	0.69
14:G:110:THR:HG22	14:G:203:LYS:HE2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:2042:A:H61	49:a:2066:G:H1	1.40	0.69
32:n:76:ASP:OD1	32:n:77:LYS:N	2.25	0.68
31:m:37:THR:HA	31:m:110:MET:HA	1.74	0.68
25:f:46:ASN:ND2	49:a:2495:C:O4'	2.26	0.68
1:A:512:G:C2	52:Y:22:U:H5''	2.27	0.68
3:E:179:ARG:NH2	5:H:135:TRP:OXT	2.26	0.68
12:P:116:PRO:C	12:P:119:ALA:HB3	2.18	0.68
1:A:961:A:N6	1:A:1210:U:OP1	2.25	0.68
2:D:171:ASN:CG	12:P:119:ALA:HB1	2.19	0.68
29:k:114:THR:HB	49:a:723:A:H5''	1.76	0.68
49:a:712:U:H4'	49:a:739:G:N7	2.09	0.68
6:K:70:GLN:NE2	6:K:74:GLU:OE1	2.27	0.68
24:e:77:ARG:NH1	49:a:2627:2MG:OP1	2.24	0.68
1:A:1304:A:H1'	20:U:37:ARG:HD2	1.76	0.68
24:e:158:VAL:O	24:e:160:LEU:N	2.24	0.68
31:m:33:ARG:NH2	44:z:60:VAL:O	2.27	0.68
49:a:372:U:H3	49:a:439:C:H42	1.40	0.68
21:B:117:LEU:HA	21:B:120:MET:HG3	1.75	0.67
49:a:2684:G:H5''	49:a:2685:2MA:H5''	1.75	0.67
1:A:1247:A:N6	1:A:1260:G:O2'	2.26	0.67
12:P:114:GLU:CA	12:P:117:ARG:HB2	2.18	0.67
49:a:2673:U:H5'	49:a:2752:G:H5''	1.76	0.67
1:A:1058:U:O2'	21:B:105:GLN:NE2	2.27	0.67
39:u:107:LEU:O	39:u:108:ARG:NH1	2.28	0.67
49:a:2870:G:O2'	49:a:2872:G:N2	2.28	0.67
50:b:87:G:H21	50:b:90:A:H2	1.41	0.67
14:G:141:MET:HE2	14:G:148:ILE:HG22	1.75	0.67
49:a:1490:A:H2	49:a:1772:G:H22	1.41	0.67
16:J:92:GLU:OE1	16:J:122:ARG:NH1	2.27	0.67
23:d:182:GLN:OE1	23:d:196:ARG:NH1	2.20	0.67
34:p:92:ARG:NH2	49:a:1081:C:OP2	2.28	0.67
1:A:1246:G:H8	1:A:1261:A:H62	1.42	0.67
49:a:2660:A:H8	49:a:2660:A:H5''	1.60	0.67
1:A:348:G:OP1	33:o:39:ARG:NH1	2.28	0.66
1:A:1062:G:N2	1:A:1065:A:OP2	2.27	0.66
15:I:138:ARG:NH2	15:I:139:GLU:OE2	2.28	0.66
35:q:67:LYS:HG2	35:q:91:LYS:HG3	1.76	0.66
14:G:21:ARG:NH2	14:G:57:GLU:OE2	2.28	0.66
12:P:111:GLU:O	12:P:112:ALA:C	2.37	0.66
15:I:70:LYS:NZ	15:I:97:THR:OG1	2.29	0.66
26:g:2:SER:OG	26:g:66:HIS:ND1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:j:10:VAL:HG12	28:j:12:ASP:H	1.59	0.66
8:O:45:LYS:O	8:O:51:ARG:NH2	2.29	0.66
1:A:1363:U:O4	15:I:10:ARG:NH1	2.29	0.66
3:E:71:VAL:HG21	3:E:160:VAL:HG11	1.78	0.66
46:l:24:THR:HG23	46:l:27:GLY:H	1.59	0.66
3:E:61:VAL:HG11	3:E:137:VAL:HA	1.77	0.66
31:m:87:MET:HE3	31:m:94:TYR:HB3	1.78	0.66
26:g:152:LYS:NZ	49:a:2925:C:O2	2.29	0.65
39:u:178:PHE:HB3	39:u:179:PRO:HD2	1.79	0.65
1:A:1450:C:OP1	33:o:109:LYS:NZ	2.26	0.65
12:P:125:GLU:O	12:P:129:ALA:N	2.27	0.65
29:k:103:VAL:HG21	29:k:109:VAL:HG13	1.79	0.65
49:a:379:A:O2'	49:a:380:G:O4'	2.14	0.65
22:c:66:ASP:OD1	22:c:103:ARG:NH1	2.30	0.65
49:a:1143:U:H4'	49:a:1144:U:H5'	1.78	0.65
6:K:25:GLY:HA2	6:K:43:PRO:HD3	1.78	0.65
49:a:2766:U:H2'	49:a:2767:U:H2'	1.77	0.65
1:A:1138:U:OP1	17:M:70:HIS:ND1	2.30	0.65
2:D:171:ASN:HB2	12:P:119:ALA:O	1.96	0.65
2:D:171:ASN:HB2	12:P:119:ALA:HB1	1.77	0.65
28:j:107:ARG:HD3	28:j:115:VAL:HG11	1.77	0.65
24:e:43:GLN:HG3	49:a:701:U:H1'	1.79	0.65
25:f:101:ARG:NH1	50:b:43:C:O2	2.30	0.65
49:a:552:G:N2	49:a:555:A:OP2	2.28	0.65
12:P:124:SER:O	12:P:127:ALA:HB3	1.98	0.64
43:y:5:LEU:HD11	43:y:45:ARG:HD2	1.79	0.64
4:F:16:GLU:O	4:F:18:GLN:N	2.30	0.64
12:P:112:ALA:O	12:P:113:ASP:C	2.40	0.64
49:a:85:U:O2	49:a:96:G:N2	2.31	0.64
49:a:1600:C:O2'	49:a:2393:G:N1	2.30	0.64
29:k:99:SER:HA	29:k:103:VAL:HG12	1.79	0.64
3:E:207:ARG:O	3:E:210:GLU:HB2	1.97	0.64
9:Q:7:GLU:C	9:Q:9:THR:N	2.55	0.64
48:4:16:CYS:SG	48:4:16:CYS:O	2.55	0.64
1:A:657:A:H1'	6:K:124:HIS:ND1	2.12	0.64
49:a:3037:G:N2	49:a:3040:A:OP2	2.26	0.64
21:B:100:MET:HA	21:B:107:ILE:HG13	1.80	0.64
32:n:42:ARG:HB2	32:n:113:ILE:HD11	1.80	0.64
2:D:171:ASN:HB2	12:P:119:ALA:CA	2.28	0.64
1:A:1386:C:H4'	1:A:1387:5MC:H3'	1.80	0.64
3:E:157:ILE:HG22	3:E:161:HIS:CE1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:g:177:LYS:HG3	49:a:2713:A:C8	2.33	0.64
49:a:1698:G:H22	49:a:1915:G:N2	1.94	0.64
8:O:34:ILE:HG23	8:O:54:LEU:HD11	1.80	0.63
12:P:111:GLU:OE2	12:P:114:GLU:HG3	1.97	0.63
1:A:179:G:OP1	11:T:56:ARG:NH2	2.30	0.63
1:A:1500:A:OP2	13:X:18:ARG:NH2	2.30	0.63
11:T:15:GLU:OE2	11:T:19:GLN:NE2	2.31	0.63
26:g:92:GLY:HA3	26:g:162:LYS:HG2	1.79	0.63
31:m:107:ASN:O	31:m:107:ASN:ND2	2.31	0.63
49:a:2287:G:H1	49:a:2366:U:H3	1.47	0.63
1:A:959:A:H5'	1:A:959:A:H8	1.64	0.63
12:P:112:ALA:O	12:P:116:PRO:HD2	1.99	0.63
24:e:43:GLN:HE22	24:e:186:ASN:HB2	1.64	0.63
1:A:177:C:H2'	1:A:178:G:H5''	1.80	0.63
1:A:793:U:O2'	1:A:885:A:N1	2.30	0.63
14:G:129:PHE:O	14:G:133:MET:HG3	1.98	0.63
15:I:118:GLU:HB2	15:I:121:MET:HE3	1.80	0.63
24:e:154:ARG:HB2	24:e:177:VAL:HG22	1.81	0.63
32:n:46:HIS:ND1	32:n:65:THR:OG1	2.28	0.63
49:a:1139:G:H22	49:a:1185:C:H3'	1.63	0.63
2:D:103:ALA:O	2:D:160:ARG:NH1	2.32	0.63
14:G:131:ARG:HG2	14:G:134:ARG:HH21	1.64	0.63
19:S:24:CYS:HB2	19:S:40:CYS:HB3	1.80	0.63
49:a:127:C:C4	49:a:127:C:C2	2.87	0.63
1:A:192:G:H21	9:Q:1:MET:H3	1.47	0.63
2:D:171:ASN:HB2	12:P:119:ALA:CB	2.29	0.62
3:E:209:GLU:O	3:E:210:GLU:C	2.41	0.62
16:J:81:PHE:CD2	16:J:86:HIS:CE1	2.87	0.62
43:y:3:SER:H	43:y:40:ASP:HB2	1.63	0.62
1:A:1302:G:N1	1:A:1305:A:OP2	2.31	0.62
26:g:166:TYR:HB2	26:g:169:GLU:HB2	1.80	0.62
2:D:169:ARG:NH1	12:P:112:ALA:HA	2.14	0.62
49:a:1962:U:OP2	49:a:1967:A:N6	2.23	0.62
1:A:1082:C:OP1	21:B:140:ARG:NH1	2.32	0.62
30:l:124:LYS:NZ	49:a:2665:C:N3	2.46	0.62
46:l:15:ASN:ND2	49:a:770:A:OP1	2.32	0.62
49:a:1974:A:N6	49:a:2011:G:O2'	2.32	0.62
40:v:38:VAL:HG12	40:v:59:LEU:HB2	1.80	0.62
44:z:45:CYS:HB3	44:z:48:CYS:SG	2.39	0.62
1:A:1429:G:N2	33:o:114:GLY:O	2.33	0.62
4:F:27:LEU:HD11	4:F:40:VAL:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:188:LEU:HB2	21:B:192:CYS:HB2	1.81	0.62
30:l:128:LYS:NZ	49:a:1113:G:OP2	2.33	0.62
1:A:1045:U:OP1	19:S:45:ARG:NH2	2.30	0.62
33:o:103:ARG:NH2	49:a:1937:C:O3'	2.33	0.62
1:A:1061:C:OP2	21:B:179:LYS:NZ	2.33	0.62
2:D:171:ASN:OD1	12:P:119:ALA:HB1	1.99	0.62
23:d:51:TYR:HH	49:a:2818:U:HO2'	1.48	0.62
49:a:50:G:O2'	49:a:117:A:N6	2.33	0.62
49:a:2049:A:C5	49:a:2050:G:H1'	2.35	0.62
21:B:125:VAL:HG23	21:B:135:LEU:HD21	1.80	0.61
1:A:930:A:O2'	1:A:1319:A:N3	2.30	0.61
2:D:168:VAL:O	2:D:170:PRO:HD3	2.00	0.61
4:F:68:GLU:HB2	4:F:71:THR:HG23	1.82	0.61
1:A:47:C:OP1	12:P:14:ARG:NH2	2.33	0.61
26:g:103:LYS:HB3	26:g:119:ALA:HB3	1.83	0.61
3:E:193:LEU:HB3	3:E:197:LYS:NZ	2.16	0.61
6:K:40:ILE:HG21	6:K:85:MET:HE2	1.83	0.61
24:e:127:PHE:HB2	24:e:197:VAL:HG12	1.83	0.61
42:x:17:LEU:HB3	42:x:60:LEU:HD21	1.81	0.61
45:0:45:ARG:NH2	49:a:2582:G:O2'	2.33	0.61
1:A:75:A:N1	1:A:99:C:O2'	2.31	0.61
1:A:1023:C:H2'	1:A:1024:G:H8	1.66	0.61
3:E:172:GLU:O	3:E:175:GLU:HG2	2.00	0.61
48:4:29:GLN:O	48:4:30:SER:C	2.44	0.61
49:a:373:G:H22	49:a:437:G:H1	1.49	0.61
1:A:1300:C:OP1	20:U:6:LYS:NZ	2.34	0.61
1:A:1428:G:H8	1:A:1447:A:H62	1.47	0.61
1:A:439:U:H5''	2:D:147:LEU:HD22	1.82	0.61
18:N:91:ARG:HB2	18:N:98:VAL:HG12	1.83	0.61
4:F:11:ASP:OD1	4:F:55:LYS:NZ	2.34	0.61
7:L:24:LEU:O	7:L:30:ARG:NH2	2.33	0.61
25:f:144:GLN:HG2	25:f:159:ARG:HG3	1.83	0.61
49:a:1255:U:O3'	49:a:1256:G:N2	2.34	0.61
49:a:2042:A:N6	49:a:2066:G:H1	1.99	0.61
49:a:350:A:H2'	49:a:351:G:H8	1.65	0.61
1:A:1040:A:O2'	14:G:155:ARG:NH1	2.28	0.60
16:J:81:PHE:HD2	16:J:86:HIS:CE1	2.18	0.60
25:f:156:ASP:OD1	25:f:157:ARG:N	2.31	0.60
48:4:10:ARG:HH22	48:4:30:SER:N	1.99	0.60
49:a:454:G:C2	49:a:455:C:H1'	2.36	0.60
29:k:34:ARG:HD2	49:a:670:G:H1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:358:C:H41	49:a:446:G:H21	1.48	0.60
15:I:40:GLN:HE21	16:J:85:VAL:HG22	1.67	0.60
17:M:59:LYS:HG2	17:M:62:ARG:HH21	1.66	0.60
15:I:27:VAL:HG21	15:I:40:GLN:HB3	1.83	0.60
22:c:166:VAL:HG21	22:c:182:MET:HE1	1.83	0.60
23:d:170:ARG:NH1	49:a:3005:G:O6	2.34	0.60
24:e:143:ALA:O	24:e:147:LEU:HD23	2.02	0.60
49:a:2872:G:H8	49:a:3052:G:C8	2.19	0.60
1:A:406:G:OP2	2:D:110:ARG:NH2	2.34	0.60
49:a:198:A:H2'	49:a:199:G:C8	2.36	0.60
26:g:53:VAL:O	26:g:66:HIS:NE2	2.30	0.60
1:A:977:G:O2'	1:A:978:A:N7	2.35	0.60
3:E:104:ILE:HD12	3:E:170:LEU:HD11	1.84	0.60
36:r:3:LYS:HA	36:r:3:LYS:HZ2	1.65	0.60
1:A:959:A:H5'	1:A:959:A:C8	2.36	0.60
1:A:992:U:H2'	1:A:993:G:H8	1.67	0.60
46:l:7:PRO:HB2	49:a:1385:G:H4'	1.83	0.60
49:a:302:A:H3'	49:a:303:G:C8	2.33	0.60
8:O:24:ASP:OD2	8:O:75:HIS:NE2	2.34	0.59
22:c:25:THR:O	22:c:26:ARG:HB2	2.01	0.59
38:t:100:ARG:NH2	49:a:100:U:O4'	2.35	0.59
36:r:1:MET:HE1	49:a:1288:G:H2'	1.83	0.59
16:J:173:ARG:NH2	53:C:33:U:OP2	2.26	0.59
26:g:109:LEU:HB3	26:g:154:ARG:HD2	1.84	0.59
29:k:81:LYS:HG3	29:k:85:LEU:HD13	1.84	0.59
38:t:13:LYS:HE2	38:t:21:GLY:HA2	1.84	0.59
29:k:68:ASN:HB3	29:k:71:ARG:HB2	1.84	0.59
42:x:47:ARG:NH2	49:a:73:A:OP1	2.32	0.59
24:e:142:GLN:OE1	24:e:170:SER:HB3	2.02	0.59
25:f:179:LEU:HD12	25:f:184:PHE:CZ	2.37	0.59
26:g:95:TYR:HE2	26:g:162:LYS:HB3	1.66	0.59
49:a:83:A:H62	49:a:101:G:H8	1.49	0.59
21:B:185:VAL:HG12	21:B:199:TYR:HB2	1.85	0.59
27:i:147:GLN:HG3	34:p:78:ARG:HG3	1.84	0.59
49:a:2925:C:OP1	54:3:33:LYS:NZ	2.30	0.59
18:N:14:ARG:HE	18:N:42:ASP:HA	1.67	0.59
48:4:47:GLY:CA	48:4:50:LYS:HZ3	2.16	0.59
1:A:1240:A:OP1	17:M:47:ASN:ND2	2.35	0.58
49:a:279:A:N7	49:a:319:G:N2	2.51	0.58
49:a:480:A:H1'	49:a:500:G:O4'	2.03	0.58
49:a:1447:G:N7	58:a:3413:HOH:O	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:37:PHE:HZ	19:S:44:LEU:HD22	1.68	0.58
34:p:58:ARG:NH2	34:p:92:ARG:HH21	2.00	0.58
38:t:12:VAL:HG12	38:t:77:LEU:HD23	1.84	0.58
49:a:2052:G:H3'	49:a:2053:U:C5'	2.33	0.58
1:A:659:U:H3	1:A:695:G:H22	1.50	0.58
2:D:172:LYS:HB2	12:P:119:ALA:HB2	1.85	0.58
37:s:36:LYS:NZ	37:s:38:THR:OG1	2.36	0.58
17:M:45:GLU:HB3	17:M:69:THR:HB	1.85	0.58
49:a:1709:G:N2	49:a:1729:G:O6	2.35	0.58
1:A:326:G:N1	1:A:329:A:OP2	2.36	0.58
2:D:182:THR:O	2:D:186:ILE:HD12	2.03	0.58
12:P:120:ILE:HA	12:P:123:LYS:HB3	1.85	0.58
21:B:188:LEU:HD21	21:B:200:ALA:HB1	1.86	0.58
26:g:102:PRO:O	26:g:125:PHE:N	2.33	0.58
36:r:56:GLN:HE21	44:z:25:THR:H	1.51	0.58
49:a:2291:U:O2'	49:a:2362:U:O4	2.21	0.58
1:A:192:G:H1'	9:Q:1:MET:SD	2.44	0.58
2:D:105:THR:HG23	2:D:108:GLN:H	1.67	0.58
14:G:34:GLU:HG3	14:G:58:ARG:HH22	1.69	0.58
21:B:24:ASN:ND2	21:B:192:CYS:O	2.36	0.58
25:f:140:GLY:HA3	49:a:2487:U:H5''	1.86	0.58
8:O:21:GLY:O	8:O:26:GLN:NE2	2.36	0.58
12:P:116:PRO:CA	12:P:119:ALA:HB3	2.33	0.58
24:e:133:VAL:HG11	24:e:137:LYS:HA	1.85	0.58
38:t:81:ILE:HG13	38:t:82:ASP:H	1.69	0.58
49:a:631:G:O2'	49:a:633:G:O4'	2.22	0.58
49:a:712:U:H4'	49:a:739:G:C8	2.38	0.58
53:C:4:G:H1	53:C:69:C:H42	1.50	0.58
1:A:1153:U:C5	1:A:1154:C:C4	2.91	0.58
1:A:210:G:OP1	11:T:56:ARG:NH1	2.37	0.58
23:d:57:GLY:HA2	23:d:85:LEU:HD23	1.84	0.58
49:a:289:U:HO2'	49:a:306:G:HO2'	1.49	0.58
21:B:80:ILE:O	21:B:83:GLN:NE2	2.36	0.57
30:l:87:LYS:NZ	49:a:1039:G:OP2	2.37	0.57
36:r:38:ILE:HG13	36:r:93:VAL:HG23	1.86	0.57
1:A:9:U:O2'	1:A:10:G:O5'	2.20	0.57
14:G:179:ALA:HB1	14:G:202:TYR:HE1	1.69	0.57
39:u:126:ILE:HD11	39:u:139:ILE:HG21	1.86	0.57
17:M:7:ARG:HB2	17:M:101:LYS:HB3	1.85	0.57
22:c:57:GLY:HA2	22:c:214:TRP:HA	1.85	0.57
31:m:87:MET:HE1	31:m:116:ILE:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:306:G:H4'	49:a:307:U:O5'	2.04	0.57
33:o:27:LYS:NZ	33:o:87:ASP:OD1	2.37	0.57
1:A:563:G:OP1	8:O:63:ARG:NH1	2.35	0.57
1:A:1152:G:O2'	1:A:1155:A:N6	2.37	0.57
1:A:1380:U:HO2'	1:A:1488:C:HO2'	1.52	0.57
4:F:9:ILE:HG22	4:F:86:MET:HE3	1.85	0.57
49:a:461:G:N2	49:a:490:A:OP2	2.34	0.57
49:a:2052:G:N1	49:a:2054:A:H5''	2.19	0.57
49:a:2841:G:N2	49:a:2844:A:OP2	2.38	0.57
30:l:54:MET:HG3	30:l:121:ALA:HB2	1.85	0.57
8:O:14:ALA:HB1	8:O:19:ASP:HB3	1.87	0.57
21:B:101:LEU:HB3	21:B:180:LEU:HD21	1.87	0.57
24:e:142:GLN:HE21	24:e:174:LEU:CD2	2.04	0.57
49:a:1253:U:H2'	49:a:1254:G:C8	2.39	0.57
49:a:2145:5MC:H4'	49:a:2146:U:OP1	2.03	0.57
49:a:2718:G:O2'	49:a:2719:U:H5''	2.04	0.57
45:O:36:ARG:NH2	45:O:53:ARG:HE	2.03	0.57
49:a:2040:G:N2	49:a:2067:A:O2'	2.28	0.57
1:A:634:U:O4	1:A:734:G:O2'	2.22	0.57
24:e:139:SER:HA	24:e:142:GLN:HE22	1.70	0.57
26:g:16:GLU:HB2	26:g:27:LYS:HB2	1.86	0.57
49:a:1289:A:N3	49:a:1315:G:O2'	2.37	0.57
4:F:26:TYR:OH	4:F:82:ASP:OD2	2.23	0.56
14:G:21:ARG:NH1	14:G:55:GLU:OE2	2.28	0.56
32:n:65:THR:HA	32:n:70:LEU:HD22	1.87	0.56
49:a:357:G:N2	49:a:446:G:O6	2.37	0.56
4:F:47:ARG:HA	4:F:57:GLU:HG2	1.88	0.56
1:A:299:G:N2	1:A:302:A:OP2	2.36	0.56
8:O:87:ARG:NH2	49:a:798:G:OP2	2.38	0.56
16:J:44:MET:HE2	16:J:133:ASP:HA	1.87	0.56
20:U:42:PRO:HA	20:U:45:ILE:HG13	1.87	0.56
26:g:59:GLU:HG2	26:g:62:ASN:HB2	1.86	0.56
29:k:109:VAL:O	29:k:109:VAL:HG12	2.05	0.56
31:m:36:THR:O	31:m:37:THR:HG22	2.06	0.56
32:n:48:PHE:HD1	32:n:64:SER:HB3	1.69	0.56
35:q:82:TYR:CE1	49:a:1264:G:H5''	2.41	0.56
49:a:392:G:N1	49:a:395:A:OP2	2.34	0.56
1:A:202:G:H1'	9:Q:1:MET:HG2	1.87	0.56
1:A:1188:U:O2'	19:S:27:CYS:SG	2.51	0.56
1:A:10:G:H2'	3:E:147:LEU:HD21	1.87	0.56
1:A:772:A:OP1	53:C:38:A:O2'	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1479:A:H4'	1:A:1480:A:C6	2.41	0.56
23:d:87:GLU:OE2	49:a:2818:U:H4'	2.06	0.56
39:u:104:ASN:HB3	39:u:125:GLU:HB3	1.87	0.56
49:a:967:G:H1	49:a:978:U:H3	1.53	0.56
1:A:1129:G:H2'	1:A:1130:G:H8	1.69	0.56
25:f:46:ASN:OD1	25:f:47:MET:N	2.38	0.56
25:f:128:SER:O	25:f:176:LYS:NZ	2.39	0.56
26:g:57:ASP:HB3	26:g:62:ASN:OD1	2.05	0.56
40:v:25:ARG:NE	40:v:35:GLU:OE1	2.38	0.56
21:B:61:VAL:HG11	21:B:225:GLY:HA3	1.87	0.56
49:a:1698:G:H22	49:a:1915:G:H22	1.51	0.56
9:Q:16:GLU:OE2	9:Q:67:ARG:NH2	2.39	0.56
49:a:974:C:H3'	49:a:975:G:H8	1.71	0.56
1:A:12:A:N6	2:D:197:GLU:O	2.38	0.56
1:A:268:G:H3'	9:Q:76:ALA:HB2	1.88	0.56
25:f:111:ARG:NH1	48:4:25:ARG:O	2.39	0.56
49:a:949:G:H21	49:a:951:A:H62	1.54	0.56
1:A:257:G:OP1	9:Q:78:LYS:NZ	2.35	0.56
19:S:37:PHE:CD2	19:S:39:LEU:HD12	2.40	0.56
24:e:150:LEU:O	24:e:154:ARG:NH1	2.39	0.56
27:i:68:LYS:NZ	49:a:1224:U:OP2	2.38	0.56
30:l:43:THR:HG22	30:l:94:ILE:HG22	1.87	0.56
44:z:61:VAL:HG12	44:z:63:ALA:H	1.69	0.56
49:a:1139:G:N2	49:a:1186:A:OP2	2.35	0.56
1:A:544:U:H1'	7:L:12:ARG:HB3	1.88	0.55
24:e:32:ASN:OD1	24:e:34:PRO:HD2	2.06	0.55
35:q:14:VAL:HB	35:q:97:VAL:HG21	1.87	0.55
49:a:442:U:H3'	49:a:443:G:C8	2.41	0.55
53:C:7:G:O2'	53:C:49:G:OP2	2.21	0.55
1:A:959:A:H4'	1:A:960:G:H5''	1.87	0.55
1:A:1506:MA6:H5'	13:X:12:MET:HE1	1.89	0.55
12:P:100:ASN:OD1	12:P:101:LYS:N	2.40	0.55
21:B:209:ARG:HA	21:B:212:SER:HB2	1.87	0.55
49:a:430:U:H4'	49:a:431:A:H8	1.70	0.55
49:a:1489:C:H2'	49:a:1490:A:C8	2.41	0.55
49:a:2706:G:N2	49:a:2721:C:H5	2.04	0.55
1:A:990:A:OP2	1:A:1009:G:N2	2.36	0.55
24:e:139:SER:HA	24:e:142:GLN:OE1	2.07	0.55
39:u:95:VAL:HB	39:u:132:LEU:HD21	1.89	0.55
49:a:179:G:N2	49:a:180:U:O4	2.37	0.55
49:a:1151:G:O2'	49:a:1179:A:O2'	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:35:ASP:OD1	14:G:58:ARG:NH2	2.25	0.55
49:a:2971:C:H1'	49:a:3071:A:H2	1.71	0.55
49:a:1727:G:H2'	49:a:1728:A:C8	2.42	0.55
2:D:171:ASN:CA	12:P:119:ALA:HB1	2.37	0.55
14:G:75:VAL:HG11	14:G:102:ILE:HG12	1.89	0.55
17:M:54:SER:HB3	17:M:58:TYR:HB2	1.88	0.55
18:N:32:GLU:HG2	18:N:35:LYS:HZ2	1.72	0.55
25:f:113:LEU:HD13	25:f:117:LEU:HD21	1.88	0.55
49:a:433:G:H2'	49:a:435:G:O4'	2.07	0.55
49:a:1912:U:H3'	49:a:1913:G:H3'	1.88	0.55
49:a:2052:G:N2	49:a:2055:U:H5	2.03	0.55
52:Y:21:U:H2'	52:Y:22:U:H4'	1.88	0.55
1:A:505:A:N6	7:L:89:ASP:OD1	2.28	0.55
1:A:751:G:H4'	1:A:1500:A:H4'	1.88	0.55
1:A:1298:G:H5'	20:U:5:LEU:HD11	1.88	0.55
21:B:92:VAL:HG11	21:B:96:TRP:HD1	1.70	0.55
49:a:379:A:N6	49:a:431:A:N7	2.54	0.55
49:a:631:G:O2'	49:a:633:G:OP1	2.23	0.55
49:a:1140:A:N6	49:a:1170:G:OP2	2.40	0.55
49:a:2872:G:O2'	49:a:2873:C:H6	1.90	0.55
27:i:80:ARG:HD2	49:a:2824:A:H5''	1.89	0.55
49:a:1130:G:H21	49:a:1194:A:H62	1.54	0.55
49:a:2872:G:O2'	49:a:2873:C:O5'	2.21	0.55
6:K:91:PHE:HA	6:K:117:SER:HB2	1.89	0.55
10:R:21:VAL:HG21	10:R:54:LYS:HB3	1.88	0.55
10:R:42:ARG:HA	10:R:45:THR:HG22	1.89	0.55
36:r:38:ILE:HA	36:r:41:VAL:HG12	1.88	0.55
39:u:96:ARG:O	39:u:97:ARG:C	2.49	0.55
17:M:59:LYS:HE2	17:M:62:ARG:NH2	2.23	0.55
37:s:72:ARG:O	37:s:73:THR:OG1	2.18	0.55
39:u:113:SER:HB2	39:u:147:GLU:HG3	1.88	0.55
47:2:8:SER:HA	47:2:11:LYS:HE2	1.89	0.55
49:a:2979:U:OP1	49:a:2982:U:N3	2.40	0.55
1:A:958:U:OP1	1:A:958:U:H6	1.91	0.54
17:M:6:ILE:HB	17:M:76:ILE:HB	1.88	0.54
25:f:17:TYR:HA	25:f:21:ILE:HG12	1.88	0.54
25:f:26:GLN:NE2	25:f:26:GLN:O	2.40	0.54
25:f:43:ILE:HD12	25:f:165:PHE:CD1	2.42	0.54
49:a:60:G:H22	49:a:92:G:H22	1.56	0.54
1:A:668:G:N2	1:A:668:G:OP2	2.39	0.54
11:T:32:VAL:HG22	11:T:79:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:30:VAL:HA	20:U:48:THR:HG23	1.88	0.54
36:r:62:GLU:OE1	36:r:65:ARG:NH1	2.37	0.54
49:a:452:U:C2	49:a:453:U:H5	2.25	0.54
49:a:1169:A:O2'	49:a:1186:A:N1	2.36	0.54
1:A:1088:C:OP1	21:B:95:ARG:NH2	2.39	0.54
1:A:1481:G:HO2'	49:a:2095:A:HO2'	1.55	0.54
9:Q:24:MET:HG3	9:Q:27:THR:HB	1.88	0.54
22:c:266:ARG:NH2	49:a:2405:G:O5'	2.40	0.54
25:f:125:GLY:HA2	25:f:185:PRO:HB2	1.89	0.54
26:g:59:GLU:O	26:g:63:ARG:NE	2.35	0.54
31:m:69:THR:HG22	31:m:70:ILE:H	1.72	0.54
49:a:2658:A:H3'	49:a:2659:U:C6	2.43	0.54
12:P:103:ASP:OD1	12:P:104:LEU:N	2.39	0.54
12:P:110:ALA:O	12:P:111:GLU:C	2.50	0.54
1:A:54:A:O2'	1:A:362:G:N2	2.40	0.54
1:A:94:G:N2	1:A:97:C:OP2	2.40	0.54
2:D:18:ASP:OD1	2:D:24:LYS:NZ	2.27	0.54
12:P:115:ALA:HB3	12:P:116:PRO:HD2	1.88	0.54
21:B:75:GLN:HG3	21:B:208:ILE:HG13	1.89	0.54
21:B:134:GLU:HG2	21:B:137:MET:HE2	1.89	0.54
31:m:69:THR:O	31:m:71:THR:N	2.40	0.54
39:u:23:ILE:HG23	39:u:28:LYS:HB2	1.90	0.54
40:v:75:ARG:NH2	49:a:2515:A:OP1	2.30	0.54
49:a:1647:G:H5''	49:a:1648:C:H5'	1.88	0.54
1:A:334:G:H4'	11:T:7:GLN:HG2	1.89	0.54
15:I:40:GLN:NE2	16:J:85:VAL:HG22	2.22	0.54
31:m:90:ARG:NH1	49:a:3060:C:O3'	2.41	0.54
32:n:4:THR:O	32:n:6:THR:N	2.40	0.54
49:a:490:A:H2'	49:a:491:A:C8	2.42	0.54
49:a:1111:A:N3	49:a:2668:C:O2'	2.34	0.54
5:H:7:ILE:HD11	5:H:32:ILE:HD13	1.88	0.54
33:o:21:ARG:NH1	49:a:3029:G:O6	2.38	0.54
49:a:2777:G:N2	49:a:2780:A:OP2	2.33	0.54
19:S:25:GLN:HG2	19:S:39:LEU:H	1.72	0.54
23:d:129:LYS:NZ	49:a:2906:U:OP1	2.40	0.54
28:j:22:ILE:HD11	28:j:42:THR:HB	1.90	0.54
49:a:818:G:N7	58:a:3415:HOH:O	2.33	0.54
49:a:1628:C:O2'	49:a:1727:G:N3	2.31	0.54
17:M:19:ASP:HB3	17:M:23:ARG:HH12	1.73	0.54
49:a:372:U:H2'	49:a:373:G:H8	1.73	0.54
1:A:810:A:H61	1:A:842:G:H1'	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:108:PRO:HD2	22:c:111:VAL:HG21	1.89	0.54
25:f:185:PRO:HB3	48:4:44:PHE:CE2	2.43	0.54
31:m:58:ASP:OD2	31:m:63:ARG:NH1	2.41	0.54
33:o:74:PHE:HB3	33:o:81:ILE:HD11	1.89	0.54
49:a:565:G:N1	49:a:568:A:OP2	2.38	0.54
2:D:73:GLU:OE2	2:D:131:ARG:NH2	2.35	0.53
11:T:33:ARG:HG2	11:T:33:ARG:HH11	1.73	0.53
43:y:10:ILE:HG13	43:y:11:LYS:HG2	1.89	0.53
1:A:845:G:HO2'	1:A:858:G:HO2'	1.55	0.53
1:A:1271:G:H5'	1:A:1272:G:C4	2.43	0.53
3:E:171:GLU:OE2	3:E:175:GLU:HG3	2.07	0.53
12:P:81:GLN:OE1	12:P:81:GLN:N	2.41	0.53
16:J:88:GLN:HG2	16:J:89:ILE:N	2.23	0.53
16:J:150:ASP:OD2	16:J:150:ASP:N	2.42	0.53
49:a:442:U:H2'	49:a:443:G:O4'	2.08	0.53
49:a:715:C:O2	49:a:725:U:O2'	2.25	0.53
49:a:2706:G:H1	49:a:2721:C:H5	1.55	0.53
1:A:874:G:OP2	13:X:10:LYS:NZ	2.41	0.53
1:A:1480:A:C4'	52:Y:19:U:H1'	2.33	0.53
2:D:178:HIS:HE1	12:P:109:LEU:HD11	1.70	0.53
24:e:125:ARG:HH22	24:e:150:LEU:HD22	1.73	0.53
31:m:34:VAL:HG23	49:a:1354:C:O3'	2.09	0.53
49:a:452:U:H2'	49:a:453:U:H6	1.72	0.53
49:a:2938:U:H4'	49:a:2939:A:OP1	2.09	0.53
24:e:182:ALA:HB1	24:e:206:PHE:HB2	1.90	0.53
54:3:14:CYS:SG	54:3:27:CYS:SG	3.04	0.53
7:L:30:ARG:HB3	7:L:57:LEU:HD23	1.90	0.53
14:G:137:GLN:HG3	14:G:148:ILE:HG21	1.89	0.53
25:f:143:GLU:HG2	25:f:158:ILE:HG23	1.91	0.53
49:a:2020:C:O2'	49:a:2110:A:N3	2.34	0.53
49:a:2051:U:H3'	49:a:2052:G:H8	1.73	0.53
49:a:2658:A:H3'	49:a:2659:U:H6	1.73	0.53
1:A:638:G:H4'	8:O:60:GLN:HE22	1.73	0.53
17:M:87:LEU:HA	17:M:90:LEU:HD22	1.91	0.53
39:u:65:ILE:HB	39:u:68:GLN:HB2	1.91	0.53
39:u:88:ARG:HH21	50:b:77:U:H5''	1.72	0.53
49:a:318:G:OP1	49:a:366:A:N6	2.42	0.53
49:a:1070:C:O2'	49:a:1083:A:N3	2.40	0.53
1:A:483:C:H2'	1:A:484:A:C8	2.44	0.53
1:A:643:G:O2'	1:A:819:G:OP1	2.26	0.53
1:A:824:U:H3	1:A:828:A:N6	2.03	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:LEU:HD12	2:D:181:PRO:HD2	1.89	0.53
29:k:131:SER:OG	49:a:723:A:OP1	2.25	0.53
48:4:13:THR:O	48:4:32:THR:HB	2.08	0.53
49:a:50:G:O2'	49:a:118:A:N6	2.42	0.53
49:a:971:U:H2'	49:a:972:A:C8	2.44	0.53
3:E:157:ILE:HG22	3:E:161:HIS:HE1	1.72	0.53
8:O:37:LEU:HB3	8:O:54:LEU:HD13	1.91	0.53
16:J:93:PRO:HA	16:J:146:MET:HE1	1.90	0.53
1:A:1384:C:OP2	3:E:52:ARG:NH2	2.41	0.53
31:m:57:THR:HG23	31:m:62:ASN:ND2	2.24	0.53
48:4:48:LYS:C	48:4:49:GLN:HG3	2.33	0.53
49:a:709:U:H2'	49:a:710:C:C6	2.44	0.53
49:a:1151:G:HO2'	49:a:1179:A:HO2'	1.56	0.53
49:a:2711:G:H5'	49:a:2711:G:C8	2.44	0.53
13:X:3:SER:C	13:X:5:ILE:H	2.17	0.53
18:N:5:ILE:H	18:N:5:ILE:HD12	1.74	0.53
21:B:77:GLN:NE2	21:B:93:ASN:OD1	2.42	0.53
24:e:49:GLN:HG2	24:e:51:THR:HG23	1.90	0.53
49:a:2248:C:H2'	49:a:2249:C:C6	2.44	0.53
52:Y:13:A:O2'	52:Y:14:A:H8	1.92	0.53
1:A:10:G:H4'	1:A:300:A:H4'	1.90	0.52
6:K:70:GLN:HG2	6:K:105:SER:OG	2.09	0.52
7:L:50:ARG:NH1	7:L:89:ASP:OD2	2.42	0.52
23:d:15:LEU:HD11	23:d:34:GLN:HB2	1.91	0.52
24:e:154:ARG:NH1	24:e:195:THR:OG1	2.42	0.52
29:k:56:ILE:HG13	29:k:57:HIS:N	2.25	0.52
48:4:27:THR:O	48:4:28:SER:C	2.53	0.52
49:a:418:G:O2'	49:a:419:U:OP1	2.25	0.52
49:a:1917:U:H2'	49:a:1918:G:C8	2.44	0.52
1:A:1189:C:OP1	19:S:2:ALA:N	2.41	0.52
1:A:1358:G:O3'	16:J:113:GLY:HA3	2.10	0.52
17:M:14:ASP:HB3	17:M:17:VAL:HG12	1.91	0.52
21:B:163:TRP:HE3	21:B:185:VAL:HG23	1.74	0.52
30:l:48:GLU:OE2	30:l:51:ARG:NH2	2.35	0.52
49:a:246:U:O2'	49:a:708:G:O2'	2.23	0.52
49:a:477:G:O2'	49:a:479:A:OP2	2.26	0.52
49:a:669:A:N1	49:a:894:G:O2'	2.37	0.52
49:a:2649:C:OP1	54:3:8:LYS:NZ	2.40	0.52
1:A:930:A:OP1	18:N:114:ARG:NH1	2.42	0.52
4:F:52:ILE:HD11	10:R:66:ALA:HB2	1.90	0.52
25:f:149:GLU:HG3	48:4:33:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:g:39:GLU:HG3	26:g:40:PRO:HD3	1.91	0.52
26:g:119:ALA:HB2	26:g:125:PHE:CE2	2.45	0.52
32:n:3:SER:O	50:b:11:C:N4	2.34	0.52
33:o:100:LEU:HD11	33:o:110:ILE:HD11	1.91	0.52
37:s:54:VAL:HG13	37:s:92:ASP:HB3	1.91	0.52
49:a:142:G:H21	49:a:147:G:H1	1.57	0.52
49:a:375:G:C2	49:a:376:U:H1'	2.44	0.52
1:A:683:C:OP1	1:A:684:A:O2'	2.20	0.52
1:A:893:A:OP1	7:L:18:LYS:NZ	2.42	0.52
1:A:1104:U:OP2	16:J:53:ARG:NH2	2.43	0.52
1:A:1422:G:H2'	1:A:1423:C:C6	2.44	0.52
28:j:108:GLU:HB2	28:j:110:LYS:NZ	2.24	0.52
30:l:62:GLY:O	39:u:180:GLU:HB2	2.09	0.52
49:a:660:G:H2'	49:a:661:A:C8	2.45	0.52
8:O:7:LYS:O	8:O:11:GLU:HG3	2.10	0.52
14:G:58:ARG:HG2	14:G:63:VAL:HG12	1.90	0.52
16:J:137:SER:O	16:J:141:LEU:HB2	2.09	0.52
22:c:184:MET:HE3	22:c:266:ARG:HA	1.92	0.52
26:g:96:ARG:HG2	26:g:108:ASN:HB2	1.91	0.52
45:0:38:GLU:OE2	45:0:53:ARG:NH1	2.37	0.52
49:a:130:G:H22	49:a:154:G:H1	1.57	0.52
49:a:2288:G:H22	49:a:2365:U:H3	1.57	0.52
49:a:2704:U:O2'	49:a:2829:U:OP1	2.20	0.52
9:Q:35:ARG:NH1	9:Q:46:THR:OG1	2.42	0.52
16:J:63:ILE:HD12	16:J:103:TYR:HE2	1.74	0.52
48:4:45:TYR:C	48:4:47:GLY:N	2.67	0.52
49:a:1647:G:H4'	49:a:1729:G:H21	1.74	0.52
1:A:1383:A:H2	3:E:47:VAL:HG11	1.75	0.52
14:G:82:GLU:HA	14:G:85:ARG:HG2	1.92	0.52
25:f:85:GLN:HE21	49:a:2492:A:H2	1.57	0.52
26:g:109:LEU:HD13	26:g:154:ARG:CB	2.39	0.52
35:q:58:VAL:HG22	35:q:100:ILE:HG23	1.91	0.52
49:a:374:C:H42	49:a:436:U:H3	1.57	0.52
49:a:2961:U:H5''	49:a:2962:A:H2'	1.92	0.52
1:A:392:U:H2'	1:A:393:G:C8	2.44	0.52
1:A:1169:U:O2'	1:A:1170:G:OP1	2.28	0.52
2:D:145:LYS:HD3	12:P:122:LYS:HG3	1.92	0.52
23:d:94:SER:C	23:d:96:TYR:H	2.17	0.52
25:f:47:MET:HE3	25:f:66:ILE:HD12	1.91	0.52
49:a:1130:G:N1	49:a:1193:A:N7	2.58	0.52
12:P:23:MET:HA	12:P:34:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:4:18:CYS:SG	48:4:20:ASN:ND2	2.82	0.52
49:a:868:A:H8	49:a:1961:U:HO2'	1.58	0.52
49:a:2938:U:H1'	49:a:2939:A:H5''	1.92	0.52
1:A:1346:A:OP2	19:S:35:ARG:NH2	2.43	0.52
22:c:223:GLY:HA2	22:c:226:MET:SD	2.50	0.52
23:d:122:LYS:HG3	23:d:171:MET:HE3	1.91	0.52
24:e:29:VAL:HG21	24:e:114:ARG:HB3	1.92	0.52
25:f:145:VAL:HA	25:f:150:ILE:HD11	1.92	0.52
39:u:116:GLY:O	39:u:179:PRO:HD3	2.09	0.52
49:a:60:G:N2	49:a:92:G:H1	2.04	0.52
49:a:532:A:H8	49:a:1277:G:H21	1.57	0.52
2:D:108:GLN:O	2:D:112:MET:HG3	2.10	0.51
6:K:99:ARG:HG3	6:K:100:GLU:H	1.73	0.51
22:c:44:ASN:ND2	49:a:1989:C:O2	2.43	0.51
1:A:957:G:H3'	1:A:958:U:H5''	1.92	0.51
22:c:258:ARG:NH1	49:a:1982:G:OP1	2.37	0.51
39:u:172:VAL:HG11	49:a:960:U:H4'	1.93	0.51
49:a:98:U:OP2	49:a:100:U:O2'	2.20	0.51
1:A:828:A:O3'	10:R:17:HIS:NE2	2.43	0.51
26:g:155:LYS:HG2	26:g:156:PRO:HD2	1.92	0.51
27:i:88:SER:OG	27:i:91:GLU:HG3	2.10	0.51
29:k:34:ARG:HH11	49:a:670:G:H1	1.58	0.51
1:A:12:A:C6	2:D:201:LYS:HB3	2.45	0.51
2:D:171:ASN:C	12:P:119:ALA:CB	2.82	0.51
17:M:34:ALA:HA	17:M:78:GLU:CB	2.38	0.51
22:c:25:THR:O	22:c:81:HIS:ND1	2.42	0.51
25:f:113:LEU:HD11	25:f:184:PHE:CD1	2.46	0.51
49:a:142:G:N2	49:a:147:G:H22	2.07	0.51
1:A:317:A:N7	1:A:330:U:H5	2.07	0.51
1:A:865:G:P	7:L:9:ARG:HH22	2.34	0.51
4:F:27:LEU:HD22	4:F:37:VAL:HG21	1.91	0.51
20:U:67:VAL:HG21	48:4:58:VAL:HG22	1.92	0.51
48:4:47:GLY:HA3	48:4:50:LYS:HZ3	1.74	0.51
49:a:130:G:N2	49:a:154:G:H22	2.09	0.51
1:A:1136:A:N6	1:A:1137:G:O6	2.44	0.51
2:D:40:ARG:HG3	2:D:42:LYS:NZ	2.25	0.51
13:X:26:ILE:O	13:X:30:ARG:HG2	2.10	0.51
24:e:159:VAL:O	24:e:161:ASP:N	2.44	0.51
1:A:600:C:O2	12:P:12:LYS:NZ	2.44	0.51
1:A:992:U:H2'	1:A:993:G:C8	2.46	0.51
49:a:286:G:N7	49:a:313:G:N2	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:917:U:H2'	49:a:918:G:C8	2.46	0.51
1:A:1230:U:H2'	1:A:1231:G:H8	1.74	0.51
11:T:33:ARG:O	11:T:37:ARG:HG3	2.10	0.51
42:x:17:LEU:HD22	42:x:56:VAL:HG13	1.92	0.51
49:a:374:C:H2'	49:a:375:G:C8	2.45	0.51
49:a:392:G:H21	49:a:415:A:H62	1.58	0.51
49:a:869:G:H5'	49:a:870:G:OP1	2.11	0.51
5:H:10:MET:HG3	5:H:27:MET:SD	2.51	0.51
14:G:41:TRP:CZ3	14:G:86:VAL:HG23	2.45	0.51
49:a:2915:U:H2'	49:a:2916:U:C6	2.46	0.51
53:C:52:G:H2'	53:C:53:G:H8	1.75	0.51
1:A:1087:A:H2	21:B:103:ASN:HD21	1.57	0.51
11:T:43:ASP:OD1	11:T:44:VAL:N	2.43	0.51
38:t:101:ARG:NH1	38:t:105:SER:OG	2.38	0.51
49:a:2040:G:H22	49:a:2067:A:HO2'	1.53	0.51
49:a:2284:G:H22	49:a:2369:U:H3	1.59	0.51
49:a:2503:G:O2'	49:a:2504:A:OP1	2.21	0.51
1:A:527:C:OP1	2:D:53:LYS:NZ	2.44	0.50
3:E:189:PRO:HG2	3:E:192:MET:HB3	1.92	0.50
4:F:79:LEU:HB3	4:F:88:THR:HG21	1.93	0.50
15:I:68:ASN:O	15:I:138:ARG:NH1	2.43	0.50
33:o:30:VAL:HG13	33:o:80:ILE:HD12	1.93	0.50
49:a:2048:G:N1	49:a:2059:U:OP2	2.34	0.50
49:a:2503:G:HO2'	49:a:2504:A:P	2.33	0.50
49:a:2660:A:H8	49:a:2660:A:C5'	2.23	0.50
1:A:657:A:H1'	6:K:124:HIS:CE1	2.46	0.50
9:Q:7:GLU:O	9:Q:9:THR:N	2.43	0.50
9:Q:8:ARG:O	9:Q:10:THR:N	2.44	0.50
11:T:15:GLU:O	11:T:19:GLN:HG2	2.12	0.50
17:M:37:ALA:HB3	17:M:75:ASP:HB2	1.93	0.50
18:N:67:GLU:OE1	18:N:71:ARG:NH2	2.44	0.50
45:0:36:ARG:NH1	45:0:54:GLU:O	2.45	0.50
49:a:653:G:H2'	49:a:2213:A:N7	2.25	0.50
1:A:655:G:H5''	4:F:87:ARG:NH1	2.26	0.50
2:D:44:SER:O	2:D:48:LEU:HG	2.11	0.50
2:D:172:LYS:N	12:P:119:ALA:HB1	2.26	0.50
4:F:33:GLU:HG2	4:F:33:GLU:O	2.11	0.50
12:P:40:TYR:CZ	12:P:42:PRO:HB3	2.47	0.50
12:P:59:TRP:HA	12:P:62:VAL:HG12	1.93	0.50
14:G:22:TRP:CG	14:G:58:ARG:HD2	2.45	0.50
17:M:85:ASP:HA	17:M:88:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:11:ARG:HG3	18:N:46:HIS:HB3	1.93	0.50
36:r:4:THR:O	36:r:5:GLU:C	2.54	0.50
49:a:1489:C:H2'	49:a:1490:A:H8	1.76	0.50
1:A:909:G:O2'	1:A:911:G:OP1	2.30	0.50
1:A:1204:C:H2'	1:A:1205:A:C8	2.46	0.50
22:c:6:TYR:CG	22:c:13:ARG:HD2	2.47	0.50
36:r:102:ILE:HG23	36:r:110:ALA:HB1	1.92	0.50
49:a:60:G:H1	49:a:92:G:H1	1.60	0.50
49:a:303:G:H2'	49:a:304:G:C8	2.46	0.50
1:A:187:C:O2'	11:T:84:ASN:ND2	2.38	0.50
17:M:32:THR:HB	17:M:83:THR:HG22	1.92	0.50
18:N:9:LEU:HG	18:N:18:ALA:HB1	1.93	0.50
28:j:63:VAL:HG22	28:j:106:LEU:HD21	1.94	0.50
35:q:4:ILE:HB	35:q:39:LEU:HB3	1.94	0.50
36:r:82:ARG:NH1	36:r:84:ASP:OD1	2.45	0.50
49:a:1896:A:N6	49:a:1929:G:O2'	2.44	0.50
1:A:721:C:O2'	8:O:40:HIS:ND1	2.35	0.50
18:N:33:THR:HG23	18:N:59:HIS:ND1	2.27	0.50
26:g:92:GLY:CA	26:g:162:LYS:HG2	2.40	0.50
48:4:10:ARG:NH2	48:4:30:SER:N	2.60	0.50
49:a:1656:G:O2'	49:a:1696:G:N1	2.40	0.50
1:A:1089:G:H5'	21:B:110:ARG:HH21	1.75	0.50
1:A:1109:G:O2'	1:A:1131:G:O6	2.26	0.50
17:M:32:THR:CB	17:M:83:THR:HG22	2.42	0.50
22:c:222:ARG:NH2	49:a:1971:C:OP1	2.44	0.50
24:e:149:GLY:O	24:e:150:LEU:HB2	2.12	0.50
45:0:30:ARG:HH22	45:0:31:ARG:NH2	2.10	0.50
49:a:130:G:H22	49:a:154:G:H22	1.60	0.50
49:a:660:G:O2'	49:a:1331:A:OP1	2.30	0.50
1:A:415:G:O2'	1:A:430:G:N2	2.44	0.50
1:A:467:G:H4'	1:A:468:U:O5'	2.12	0.50
1:A:956:C:O3'	17:M:59:LYS:HD2	2.12	0.50
15:I:86:GLN:NE2	15:I:148:ASN:OD1	2.45	0.50
24:e:160:LEU:HD23	24:e:163:SER:H	1.76	0.50
42:x:52:ASP:O	42:x:56:VAL:HG23	2.12	0.50
48:4:47:GLY:CA	48:4:50:LYS:NZ	2.75	0.50
49:a:286:G:N2	49:a:287:U:O4'	2.45	0.50
49:a:1399:A:N6	49:a:1400:G:O6	2.45	0.50
1:A:382:G:N2	1:A:385:A:OP2	2.36	0.50
1:A:639:G:H4'	8:O:26:GLN:HG2	1.94	0.50
1:A:936:C:H4'	1:A:948:A:N1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:GLU:OE1	2:D:95:ASN:ND2	2.38	0.50
2:D:148:PRO:O	2:D:152:ILE:HG12	2.12	0.50
4:F:48:LEU:HD13	4:F:52:ILE:HD12	1.94	0.50
49:a:2119:A:OP2	49:a:2145:5MC:N4	2.44	0.50
1:A:1399:C:H2'	1:A:1400:A:C8	2.47	0.49
6:K:89:ASP:OD1	6:K:115:PRO:HD2	2.12	0.49
6:K:101:THR:HG22	6:K:104:ARG:HH22	1.76	0.49
23:d:144:ARG:NH1	49:a:830:G:OP2	2.43	0.49
28:j:64:ARG:O	28:j:82:ASN:HA	2.12	0.49
31:m:56:LYS:NZ	31:m:90:ARG:O	2.45	0.49
39:u:58:ASN:ND2	39:u:103:VAL:HB	2.27	0.49
49:a:350:A:H2'	49:a:351:G:C8	2.45	0.49
49:a:2050:G:H2'	49:a:2051:U:O4'	2.12	0.49
49:a:2527:G:N3	49:a:2563:C:H2'	2.27	0.49
1:A:1115:A:H2'	1:A:1116:G:H8	1.77	0.49
1:A:1173:G:H5'	16:J:158:LYS:HE3	1.94	0.49
4:F:81:ILE:HD11	22:c:137:PRO:HG2	1.93	0.49
16:J:69:GLN:N	16:J:104:ASP:OD1	2.45	0.49
17:M:12:ALA:HB3	17:M:18:ILE:HG12	1.94	0.49
26:g:109:LEU:HD13	26:g:154:ARG:HB3	1.94	0.49
28:j:35:LEU:HD21	28:j:65:THR:H	1.77	0.49
37:s:3:GLU:HG2	49:a:151:G:H4'	1.93	0.49
41:w:38:VAL:HG21	41:w:47:MET:SD	2.52	0.49
49:a:338:U:O2'	49:a:339:U:O5'	2.29	0.49
49:a:2655:C:O2	49:a:2655:C:H2'	2.12	0.49
49:a:2721:C:O2	49:a:2721:C:H5''	2.12	0.49
49:a:2970:C:O2'	49:a:2989:A:N3	2.41	0.49
12:P:116:PRO:O	12:P:120:ILE:HG12	2.12	0.49
12:P:125:GLU:O	12:P:128:ALA:N	2.46	0.49
14:G:146:LEU:HB2	14:G:202:TYR:HD2	1.76	0.49
16:J:81:PHE:HE2	16:J:118:ALA:HB2	1.77	0.49
21:B:178:ARG:NH1	21:B:178:ARG:HB2	2.27	0.49
22:c:16:SER:HB3	22:c:207:GLY:HA3	1.94	0.49
24:e:142:GLN:O	24:e:143:ALA:C	2.55	0.49
25:f:10:MET:HG2	25:f:14:LYS:HD3	1.95	0.49
29:k:58:MET:CE	49:a:257:G:H4'	2.42	0.49
44:z:14:ARG:HB3	49:a:15:U:H5''	1.94	0.49
49:a:742:U:H2'	49:a:743:C:C6	2.48	0.49
49:a:2183:C:O2'	49:a:2871:U:OP2	2.29	0.49
1:A:1167:G:O2'	1:A:1168:G:N7	2.38	0.49
3:E:188:ALA:HB3	3:E:193:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:51:ASP:OD1	18:N:52:GLN:N	2.45	0.49
26:g:111:PHE:HE1	26:g:154:ARG:HH21	1.59	0.49
28:j:23:ARG:NH2	49:a:2730:G:H1'	2.27	0.49
37:s:4:LEU:HD22	42:x:61:GLN:HB2	1.95	0.49
48:4:18:CYS:HB3	48:4:41:CYS:SG	2.47	0.49
49:a:254:G:OP2	49:a:256:C:N4	2.44	0.49
49:a:1095:U:H5'	49:a:1096:G:H5''	1.95	0.49
1:A:1129:G:H2'	1:A:1130:G:C8	2.47	0.49
1:A:1295:G:N7	18:N:99:ARG:NH2	2.61	0.49
6:K:116:ILE:H	6:K:116:ILE:HD12	1.76	0.49
14:G:59:ARG:HG3	14:G:62:ARG:HH21	1.76	0.49
25:f:65:ASP:OD2	25:f:159:ARG:NH1	2.43	0.49
29:k:43:LYS:HG3	29:k:44:ASN:H	1.76	0.49
36:r:1:MET:CE	49:a:1288:G:H2'	2.43	0.49
43:y:3:SER:OG	43:y:40:ASP:OD1	2.26	0.49
49:a:1364:U:H5''	49:a:1365:C:OP2	2.12	0.49
49:a:2929:G:O6	49:a:2937:C:H5''	2.12	0.49
2:D:168:VAL:C	2:D:170:PRO:HD3	2.37	0.49
17:M:52:ILE:HB	19:S:41:ARG:HD2	1.93	0.49
20:U:12:ASP:OD1	20:U:37:ARG:NH2	2.31	0.49
26:g:60:ARG:CZ	49:a:1118:U:H5''	2.42	0.49
28:j:12:ASP:OD2	28:j:86:LEU:N	2.42	0.49
49:a:2106:U:OP1	53:C:24:U:O2'	2.25	0.49
50:b:5:C:OP1	50:b:61:C:O2'	2.29	0.49
1:A:1155:A:H2'	1:A:1156:A:C8	2.47	0.49
3:E:122:ALA:HB2	3:E:147:LEU:HD13	1.94	0.49
5:H:22:HIS:O	5:H:69:TYR:OH	2.26	0.49
22:c:134:ARG:HH21	22:c:188:ARG:HG3	1.77	0.49
23:d:190:ARG:HG3	23:d:192:ILE:HG12	1.94	0.49
33:o:89:HIS:HB3	33:o:113:ARG:HE	1.78	0.49
38:t:42:ASN:O	38:t:67:GLU:HA	2.11	0.49
46:l:16:HIS:HB2	46:l:44:ALA:HB3	1.93	0.49
49:a:235:G:H4'	49:a:236:U:C6	2.48	0.49
49:a:373:G:H2'	49:a:373:G:N3	2.27	0.49
49:a:1910:C:H4'	49:a:1911:G:C5	2.47	0.49
1:A:410:G:OP1	2:D:105:THR:HG21	2.13	0.49
2:D:15:LEU:HD11	2:D:54:GLN:HB2	1.95	0.49
2:D:171:ASN:CB	12:P:119:ALA:CB	2.83	0.49
18:N:29:ARG:HG3	18:N:64:TYR:CE2	2.48	0.49
21:B:74:LYS:HE2	21:B:77:GLN:HG3	1.93	0.49
36:r:72:MET:HE2	36:r:83:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:2660:A:C5'	49:a:2660:A:C8	2.95	0.49
3:E:48:VAL:HG22	3:E:49:GLN:H	1.77	0.49
49:a:891:C:O2	49:a:2626:G:O2'	2.30	0.49
49:a:2586:C:N4	49:a:2587:U:O4	2.46	0.49
49:a:2859:U:H2'	49:a:2860:G:C8	2.48	0.49
49:a:2894:U:OP1	49:a:2896:G:H4'	2.13	0.49
49:a:2971:C:H1'	49:a:3071:A:C2	2.48	0.49
49:a:3046:G:C2	49:a:3048:A:H1'	2.48	0.49
49:a:1065:C:N3	51:V:21:ARG:NH2	2.60	0.49
49:a:1815:G:N2	49:a:1818:U:OP2	2.34	0.49
54:3:16:VAL:HG22	54:3:25:VAL:HG22	1.95	0.49
1:A:1230:U:H2'	1:A:1231:G:C8	2.47	0.48
18:N:47:GLU:HG2	18:N:47:GLU:O	2.13	0.48
26:g:117:VAL:HG11	26:g:150:ILE:HD11	1.95	0.48
28:j:2:ILE:HB	28:j:33:ALA:HB3	1.94	0.48
39:u:9:ALA:HB2	39:u:45:LEU:HD23	1.95	0.48
49:a:433:G:H5'	49:a:435:G:O5'	2.11	0.48
49:a:1199:U:H2'	49:a:1200:U:C6	2.48	0.48
49:a:2716:C:C4	49:a:2717:G:C8	3.01	0.48
12:P:81:GLN:HE21	12:P:88:SER:HB3	1.77	0.48
19:S:6:LEU:HB3	19:S:23:ARG:NH2	2.28	0.48
20:U:29:ASN:OD1	20:U:30:VAL:N	2.45	0.48
26:g:78:ILE:HA	26:g:81:THR:HG22	1.95	0.48
31:m:36:THR:O	31:m:40:LYS:HB2	2.13	0.48
49:a:171:A:H2'	49:a:172:U:C6	2.48	0.48
49:a:1933:G:O2'	49:a:3040:A:N1	2.42	0.48
3:E:172:GLU:O	3:E:176:VAL:HG23	2.13	0.48
3:E:194:ARG:HA	3:E:197:LYS:HE2	1.94	0.48
17:M:27:ASP:OD1	17:M:28:THR:N	2.47	0.48
21:B:68:LEU:HD23	21:B:159:PRO:HB3	1.95	0.48
23:d:200:PRO:HA	49:a:2862:C:H5'	1.94	0.48
24:e:140:THR:O	24:e:144:LYS:HG2	2.13	0.48
29:k:79:LEU:HG	29:k:113:GLY:HA2	1.94	0.48
36:r:3:LYS:HD3	36:r:4:THR:HG23	1.93	0.48
37:s:64:ARG:NH2	49:a:1416:U:OP2	2.47	0.48
49:a:337:G:H22	49:a:355:U:H2'	1.78	0.48
49:a:1708:G:H22	49:a:1729:G:H1	1.60	0.48
49:a:2149:A:N3	49:a:2774:G:O2'	2.43	0.48
1:A:928:G:N1	1:A:1324:G:OP2	2.43	0.48
3:E:208:MET:O	3:E:209:GLU:C	2.55	0.48
6:K:105:SER:O	6:K:109:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:73:THR:OG1	10:R:74:ALA:N	2.46	0.48
15:I:42:ILE:HG23	15:I:117:ALA:HA	1.95	0.48
18:N:90:ARG:HA	18:N:93:ARG:HH12	1.78	0.48
19:S:37:PHE:HD2	19:S:39:LEU:HD12	1.77	0.48
24:e:43:GLN:NE2	24:e:186:ASN:HB2	2.27	0.48
39:u:153:TYR:HA	39:u:172:VAL:HA	1.95	0.48
49:a:943:G:N3	49:a:2450:A:H2'	2.28	0.48
49:a:2986:G:H2'	49:a:2987:G:C8	2.48	0.48
1:A:9:U:HO2'	1:A:10:G:P	2.36	0.48
3:E:157:ILE:CG2	3:E:161:HIS:HE1	2.25	0.48
21:B:41:ILE:HG22	21:B:43:LEU:H	1.78	0.48
37:s:69:ARG:NH1	37:s:71:THR:HG22	2.27	0.48
49:a:130:G:H22	49:a:154:G:N2	2.11	0.48
49:a:614:G:OP1	49:a:615:C:OP1	2.31	0.48
49:a:974:C:H3'	49:a:975:G:C8	2.49	0.48
49:a:1393:G:H2'	49:a:1394:G:H8	1.78	0.48
49:a:1901:U:H2'	49:a:1902:C:C6	2.49	0.48
1:A:183:G:H2'	1:A:184:G:H2'	1.94	0.48
1:A:438:C:H4'	2:D:148:PRO:HG2	1.96	0.48
2:D:90:GLU:HG3	2:D:186:ILE:HG12	1.95	0.48
15:I:93:PRO:HA	15:I:96:GLN:HG2	1.95	0.48
23:d:31:THR:HG21	23:d:199:VAL:HG22	1.94	0.48
24:e:139:SER:HA	24:e:142:GLN:NE2	2.28	0.48
24:e:139:SER:CA	24:e:142:GLN:HE22	2.26	0.48
26:g:95:TYR:CE2	26:g:162:LYS:HB3	2.46	0.48
30:l:18:THR:HG22	50:b:91:U:H5'	1.95	0.48
31:m:104:LYS:NZ	49:a:1361:G:O2'	2.34	0.48
49:a:2721:C:H3'	49:a:2722:C:H5''	1.95	0.48
1:A:32:G:O2'	1:A:298:U:OP1	2.22	0.48
1:A:822:C:H2'	1:A:823:A:C8	2.49	0.48
1:A:998:G:N2	1:A:1001:A:OP2	2.33	0.48
4:F:12:PRO:O	4:F:45:LYS:NZ	2.47	0.48
9:Q:6:ALA:C	9:Q:8:ARG:H	2.22	0.48
12:P:122:LYS:HE3	12:P:125:GLU:HG2	1.94	0.48
14:G:149:ARG:HG3	14:G:168:ARG:HB3	1.96	0.48
22:c:226:MET:HE2	49:a:867:A:N1	2.29	0.48
25:f:83:ILE:HG22	25:f:86:PHE:H	1.79	0.48
49:a:252:G:N2	49:a:473:U:O2'	2.33	0.48
49:a:2042:A:N6	49:a:2066:G:H22	2.11	0.48
49:a:2872:G:H8	49:a:3052:G:H8	1.59	0.48
49:a:2880:U:H2'	49:a:2881:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:U:H2'	1:A:202:G:H8	1.78	0.48
14:G:49:ALA:HA	14:G:74:ILE:HD13	1.95	0.48
30:l:118:MET:HG3	30:l:131:PHE:CD1	2.49	0.48
32:n:40:VAL:HG13	32:n:49:VAL:HG22	1.95	0.48
34:p:58:ARG:HH22	34:p:92:ARG:HH21	1.61	0.48
38:t:94:ARG:NH1	38:t:112:SER:OG	2.37	0.48
49:a:135:G:H2'	49:a:136:U:C6	2.49	0.48
1:A:1212:C:P	18:N:91:ARG:HH12	2.36	0.48
1:A:1391:5MC:O2	1:A:1506:MA6:O2'	2.32	0.48
8:O:74:GLU:O	8:O:78:GLU:HG3	2.14	0.48
16:J:53:ARG:H	16:J:123:LEU:HD23	1.79	0.48
18:N:8:ASP:OD1	18:N:8:ASP:N	2.43	0.48
22:c:148:ARG:NH2	49:a:2386:G:H5'	2.28	0.48
26:g:4:ILE:HG12	49:a:2933:G:H4'	1.94	0.48
35:q:91:LYS:H	35:q:91:LYS:HD2	1.79	0.48
49:a:618:G:O2'	49:a:620:C:C5	2.66	0.48
49:a:2533:G:H2'	49:a:2547:G:H22	1.79	0.48
51:V:21:ARG:HG3	51:V:22:PRO:HD2	1.96	0.48
1:A:96:G:H2'	1:A:97:C:C6	2.48	0.48
1:A:354:C:O2	1:A:357:C:N4	2.47	0.48
1:A:739:U:H2'	1:A:740:G:O4'	2.14	0.48
1:A:1505:MA6:H8	1:A:1505:MA6:O5'	2.13	0.48
2:D:172:LYS:N	12:P:119:ALA:CB	2.76	0.48
16:J:45:ILE:HG22	16:J:65:PRO:HG3	1.96	0.48
24:e:114:ARG:HH21	24:e:210:ARG:HG2	1.78	0.48
28:j:113:ARG:NH2	28:j:117:LEU:HD21	2.29	0.48
35:q:47:THR:HG22	35:q:53:LEU:HD22	1.96	0.48
44:z:53:PRO:O	44:z:54:ARG:C	2.57	0.48
49:a:358:C:H41	49:a:446:G:N2	2.11	0.48
49:a:1047:U:O2'	49:a:2455:A:N3	2.39	0.48
49:a:2660:A:H5''	49:a:2660:A:C8	2.47	0.48
54:3:10:ILE:HB	54:3:32:HIS:CD2	2.49	0.48
1:A:460:A:C5	1:A:461:G:H1'	2.49	0.47
1:A:521:A:H2'	1:A:522:G:C8	2.49	0.47
1:A:569:G:N1	1:A:736:C:OP2	2.47	0.47
14:G:24:ALA:HB1	14:G:27:GLN:CG	2.43	0.47
15:I:113:GLU:CD	15:I:114:LYS:N	2.72	0.47
23:d:187:ASP:OD2	23:d:190:ARG:HG2	2.14	0.47
38:t:27:LEU:HD21	38:t:39:GLU:HB3	1.96	0.47
42:x:40:LEU:HD21	42:x:43:THR:HA	1.96	0.47
49:a:50:G:H1'	49:a:117:A:H61	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:1156:A:O2'	49:a:2656:U:O3'	2.32	0.47
49:a:1612:G:H2'	49:a:1613:U:C6	2.48	0.47
49:a:1897:G:H1'	49:a:1898:C:H5'	1.96	0.47
53:C:52:G:H2'	53:C:53:G:C8	2.49	0.47
1:A:957:G:O3'	19:S:41:ARG:NH1	2.48	0.47
1:A:1112:G:H22	1:A:1131:G:H1	1.63	0.47
1:A:1137:G:H5''	17:M:44:THR:HG23	1.96	0.47
2:D:54:GLN:HE21	2:D:58:TYR:HE2	1.62	0.47
14:G:22:TRP:CD1	14:G:58:ARG:HD2	2.49	0.47
15:I:51:ARG:HB3	15:I:58:PRO:HD3	1.96	0.47
22:c:208:LYS:HD3	22:c:211:ARG:HG3	1.96	0.47
30:l:60:ARG:HD3	30:l:60:ARG:H	1.79	0.47
49:a:2215:G:OP1	49:a:2636:G:O2'	2.20	0.47
49:a:2510:A:H2'	49:a:2511:G:C8	2.49	0.47
1:A:955:G:N1	1:A:1350:A:OP2	2.41	0.47
1:A:1049:G:O2'	1:A:1176:G:N2	2.47	0.47
1:A:1479:A:H4'	1:A:1480:A:C5	2.49	0.47
6:K:79:ARG:HA	6:K:82:GLU:CD	2.39	0.47
19:S:24:CYS:HB3	19:S:29:ARG:H	1.79	0.47
23:d:94:SER:C	23:d:96:TYR:N	2.70	0.47
23:d:158:PRO:O	23:d:160:LYS:N	2.46	0.47
25:f:63:ILE:HD12	25:f:74:PRO:HG2	1.96	0.47
26:g:109:LEU:HD22	26:g:154:ARG:HD2	1.96	0.47
33:o:92:VAL:HG11	33:o:97:LEU:HD11	1.96	0.47
36:r:20:SER:OG	36:r:21:TYR:N	2.47	0.47
36:r:109:SER:O	49:a:1798:A:N6	2.40	0.47
49:a:116:G:OP2	49:a:118:A:O2'	2.26	0.47
49:a:603:A:HO2'	49:a:663:C:HO2'	1.62	0.47
3:E:193:LEU:HB3	3:E:197:LYS:HZ3	1.79	0.47
17:M:14:ASP:OD2	17:M:16:GLU:HB2	2.15	0.47
19:S:9:LYS:O	19:S:12:ARG:HG2	2.15	0.47
34:p:92:ARG:O	34:p:93:LYS:HB2	2.14	0.47
49:a:271:G:O2'	49:a:272:A:H5''	2.12	0.47
49:a:1488:U:H2'	49:a:1489:C:C6	2.50	0.47
49:a:1710:A:N6	49:a:1711:G:O6	2.47	0.47
49:a:1716:U:HO2'	49:a:1721:G:N2	2.12	0.47
49:a:2291:U:H1'	49:a:2361:C:H42	1.80	0.47
22:c:219:PRO:HG3	49:a:849:A:H2	1.79	0.47
29:k:123:LEU:HB2	29:k:143:VAL:HG12	1.96	0.47
49:a:2375:U:H2'	49:a:2376:A:C8	2.50	0.47
49:a:2714:G:H8	49:a:2714:G:O5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:2836:A:N1	49:a:2847:A:H5''	2.30	0.47
1:A:519:G:H5''	7:L:110:ARG:NH1	2.30	0.47
2:D:94:ASP:OD1	2:D:95:ASN:N	2.46	0.47
15:I:116:MET:HA	15:I:119:ARG:HE	1.79	0.47
21:B:9:LEU:HD13	21:B:43:LEU:HD22	1.95	0.47
25:f:113:LEU:HA	25:f:117:LEU:HD21	1.96	0.47
25:f:120:ILE:HD11	25:f:146:MET:HE3	1.95	0.47
29:k:21:VAL:HG13	29:k:28:LYS:HB2	1.96	0.47
47:2:12:LYS:NZ	49:a:254:G:O6	2.44	0.47
49:a:588:G:N1	49:a:591:A:OP2	2.47	0.47
49:a:1851:G:O2'	49:a:2174:U:O4	2.27	0.47
1:A:985:U:H2'	1:A:986:C:C6	2.50	0.47
1:A:1252:G:N2	1:A:1255:A:OP2	2.38	0.47
4:F:14:VAL:HG11	4:F:19:VAL:HB	1.96	0.47
4:F:74:GLU:HA	4:F:77:ARG:HG2	1.97	0.47
7:L:56:ARG:CZ	7:L:62:GLU:HB2	2.44	0.47
22:c:124:ASP:OD1	22:c:125:ILE:N	2.48	0.47
23:d:15:LEU:HD13	33:o:4:ILE:HG21	1.95	0.47
30:l:51:ARG:HG3	30:l:66:ILE:HD11	1.97	0.47
33:o:27:LYS:HG2	33:o:44:SER:OG	2.14	0.47
36:r:29:MET:HE1	36:r:60:ALA:HA	1.96	0.47
39:u:37:ASP:N	39:u:37:ASP:OD2	2.48	0.47
44:z:6:ARG:NH1	49:a:2202:C:H41	2.12	0.47
49:a:452:U:H2'	49:a:453:U:C6	2.49	0.47
49:a:1343:G:O2'	49:a:2195:G:O6	2.23	0.47
49:a:2525:U:H2'	49:a:2526:U:C6	2.50	0.47
49:a:2588:U:H2'	49:a:2588:U:OP2	2.15	0.47
49:a:2986:G:H2'	49:a:2987:G:H8	1.79	0.47
53:C:43:A:H2'	53:C:44:A:C8	2.50	0.47
53:C:62:C:H2'	53:C:63:G:H8	1.80	0.47
1:A:38:C:O4'	7:L:29:GLN:NE2	2.48	0.47
1:A:69:A:C2	1:A:220:G:H8	2.33	0.47
1:A:669:A:N1	1:A:682:G:O2'	2.41	0.47
2:D:171:ASN:OD1	12:P:119:ALA:CB	2.63	0.47
6:K:42:ASP:OD1	6:K:43:PRO:HD2	2.15	0.47
6:K:51:ALA:HB2	6:K:79:ARG:HH22	1.79	0.47
10:R:29:LEU:HD22	10:R:59:ILE:HG13	1.97	0.47
14:G:34:GLU:HG3	14:G:58:ARG:NH2	2.30	0.47
24:e:107:LYS:NZ	49:a:690:U:OP2	2.42	0.47
25:f:179:LEU:HD12	25:f:184:PHE:CE2	2.50	0.47
26:g:45:LYS:HB3	26:g:48:GLU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:314:U:H3'	49:a:315:G:H8	1.80	0.47
49:a:2517:A:O2'	49:a:2518:A:OP1	2.32	0.47
6:K:87:ARG:HB2	6:K:112:GLU:HB2	1.97	0.47
12:P:42:PRO:HA	12:P:47:SER:HB2	1.97	0.47
17:M:16:GLU:OE1	17:M:16:GLU:N	2.47	0.47
17:M:21:SER:O	17:M:25:ILE:HG12	2.15	0.47
18:N:82:ILE:HD11	18:N:92:HIS:HB3	1.97	0.47
21:B:5:THR:OG1	21:B:6:THR:N	2.48	0.47
26:g:59:GLU:HG3	26:g:62:ASN:H	1.79	0.47
38:t:81:ILE:HG13	38:t:82:ASP:N	2.30	0.47
49:a:834:A:H4'	49:a:1348:G:N3	2.29	0.47
1:A:699:C:H4'	6:K:125:ASN:OD1	2.15	0.47
1:A:865:G:OP2	7:L:9:ARG:NH2	2.48	0.47
19:S:42:ILE:H	19:S:42:ILE:HD12	1.79	0.47
24:e:63:GLY:HA3	24:e:82:ARG:HG2	1.97	0.47
48:4:10:ARG:HH22	48:4:30:SER:H	1.61	0.47
49:a:252:G:O2'	49:a:473:U:O2	2.21	0.47
49:a:376:U:H2'	49:a:377:G:C8	2.50	0.47
49:a:433:G:OP2	49:a:433:G:N2	2.25	0.47
49:a:898:U:H2'	49:a:899:C:C6	2.50	0.47
49:a:1433:C:H2'	49:a:1434:G:O4'	2.14	0.47
49:a:2141:C:H2'	49:a:2142:G:C8	2.50	0.47
1:A:561:U:H2'	1:A:562:C:C6	2.50	0.46
4:F:14:VAL:HG13	4:F:18:GLN:HG2	1.97	0.46
9:Q:12:ARG:HD3	9:Q:70:GLU:O	2.16	0.46
31:m:5:THR:O	31:m:7:GLY:N	2.47	0.46
31:m:28:LEU:HD13	31:m:34:VAL:HG12	1.97	0.46
36:r:3:LYS:HB3	36:r:4:THR:H	1.49	0.46
43:y:40:ASP:OD2	43:y:45:ARG:NH1	2.47	0.46
49:a:57:G:O2'	49:a:72:A:N1	2.45	0.46
49:a:254:G:H4'	49:a:475:G:C5	2.50	0.46
3:E:34:TYR:CE2	3:E:94:PHE:HE2	2.33	0.46
3:E:44:VAL:O	3:E:55:SER:N	2.42	0.46
4:F:9:ILE:HG12	4:F:60:TYR:CE1	2.50	0.46
22:c:53:HIS:HE1	22:c:220:THR:HA	1.76	0.46
23:d:94:SER:O	23:d:96:TYR:N	2.48	0.46
32:n:67:GLU:O	32:n:71:ARG:HG2	2.15	0.46
38:t:4:LEU:HD23	38:t:72:VAL:HG21	1.96	0.46
42:x:40:LEU:HD23	42:x:40:LEU:O	2.16	0.46
49:a:433:G:N3	49:a:433:G:H5''	2.29	0.46
49:a:1062:A:H2'	49:a:1065:C:H42	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:1137:A:N6	49:a:1189:G:C6	2.84	0.46
49:a:1716:U:HO2'	49:a:1721:G:H22	1.60	0.46
49:a:1771:U:H2'	49:a:1772:G:C8	2.50	0.46
1:A:463:G:O2'	1:A:465:C:N4	2.45	0.46
1:A:527:C:H5'	2:D:64:GLU:HB2	1.96	0.46
1:A:907:A:N6	1:A:1379:G:O6	2.48	0.46
4:F:9:ILE:HD11	10:R:65:LEU:HD12	1.97	0.46
25:f:59:MET:O	25:f:63:ILE:HG12	2.15	0.46
43:y:41:ARG:O	43:y:45:ARG:HG2	2.16	0.46
49:a:279:A:H5'	49:a:280:C:OP2	2.15	0.46
49:a:2415:U:H2'	49:a:2416:G:C8	2.50	0.46
49:a:2710:U:H2'	49:a:2712:G:H5''	1.96	0.46
1:A:721:C:P	4:F:2:ARG:HH22	2.38	0.46
1:A:798:A:OP1	1:A:1513:G:O2'	2.27	0.46
1:A:1354:U:H5'	17:M:62:ARG:NH1	2.30	0.46
2:D:40:ARG:HG3	2:D:42:LYS:HZ1	1.80	0.46
4:F:17:ARG:HG2	4:F:18:GLN:N	2.31	0.46
24:e:13:LYS:HA	24:e:13:LYS:HD2	1.75	0.46
27:i:77:HIS:HD2	27:i:84:LEU:HD13	1.79	0.46
49:a:2938:U:OP2	54:3:19:ARG:NE	2.44	0.46
1:A:157:C:H2'	1:A:158:A:H8	1.79	0.46
1:A:882:G:N2	1:A:885:A:OP2	2.44	0.46
25:f:144:GLN:NE2	25:f:155:ILE:HG21	2.30	0.46
27:i:2:THR:HG23	49:a:1078:C:H42	1.79	0.46
28:j:31:ARG:HH12	49:a:2857:A:H5''	1.81	0.46
34:p:6:ARG:NH1	49:a:668:G:N7	2.60	0.46
49:a:2718:G:O2'	49:a:2719:U:C6	2.69	0.46
14:G:31:LEU:HA	14:G:34:GLU:HG2	1.97	0.46
21:B:130:LEU:HD23	21:B:135:LEU:HB2	1.97	0.46
23:d:124:THR:O	49:a:1838:A:O2'	2.31	0.46
23:d:167:MET:HE1	49:a:2801:C:O2	2.16	0.46
28:j:22:ILE:HG23	49:a:2135:A:C2	2.51	0.46
39:u:97:ARG:O	39:u:132:LEU:HD22	2.15	0.46
49:a:1969:A:H1'	49:a:2121:A:N6	2.31	0.46
1:A:161:A:H1'	1:A:346:A:N7	2.31	0.46
1:A:774:A:O2'	1:A:776:A:N7	2.46	0.46
3:E:87:VAL:O	3:E:91:LYS:HG2	2.15	0.46
12:P:9:ARG:O	12:P:10:LEU:HD23	2.16	0.46
12:P:126:GLY:HA2	12:P:129:ALA:HB3	1.97	0.46
21:B:216:ARG:NH1	21:B:220:ASP:OD2	2.39	0.46
26:g:33:LEU:HD12	26:g:76:MET:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:g:150:ILE:HG22	26:g:164:VAL:HG11	1.96	0.46
45:0:12:ILE:HB	45:0:54:GLU:HG3	1.97	0.46
49:a:165:G:HO2'	49:a:166:A:P	2.38	0.46
49:a:305:U:O2'	49:a:307:U:H1'	2.16	0.46
49:a:453:U:H4'	49:a:454:G:O5'	2.16	0.46
49:a:1002:A:H5''	50:b:98:G:O2'	2.16	0.46
49:a:2248:C:H2'	49:a:2249:C:H6	1.80	0.46
49:a:2706:G:H1	49:a:2721:C:H41	1.64	0.46
1:A:129:U:H4'	1:A:131:A:OP1	2.15	0.46
1:A:378:G:H5''	12:P:6:ARG:HB2	1.97	0.46
1:A:454:A:O3'	12:P:76:ARG:NH2	2.48	0.46
1:A:765:C:H2'	1:A:766:A:C8	2.51	0.46
1:A:934:U:OP2	18:N:102:ARG:HD2	2.15	0.46
1:A:1307:U:O2'	20:U:78:ARG:NH2	2.48	0.46
2:D:163:PRO:HB2	2:D:165:TRP:CD1	2.51	0.46
2:D:171:ASN:CG	12:P:119:ALA:CB	2.88	0.46
4:F:39:ASN:OD1	4:F:40:VAL:N	2.49	0.46
12:P:117:ARG:HD3	12:P:117:ARG:HA	1.32	0.46
22:c:206:TRP:O	22:c:211:ARG:HD3	2.15	0.46
23:d:96:TYR:HE2	23:d:102:ILE:HD11	1.79	0.46
24:e:110:GLY:O	24:e:114:ARG:HD3	2.16	0.46
24:e:175:SER:HB3	49:a:408:G:O2'	2.15	0.46
28:j:64:ARG:HA	28:j:79:PHE:CD1	2.50	0.46
49:a:1492:C:H2'	49:a:1493:G:C8	2.51	0.46
49:a:2072:A:H2'	49:a:2073:A:C8	2.51	0.46
49:a:2496:A:H2'	49:a:2497:G:C8	2.51	0.46
1:A:1518:A:H2'	1:A:1519:U:C6	2.51	0.46
2:D:14:ARG:HA	2:D:32:PRO:HB3	1.97	0.46
3:E:187:ILE:HG13	3:E:188:ALA:N	2.30	0.46
17:M:29:VAL:HG11	17:M:76:ILE:HD12	1.98	0.46
18:N:32:GLU:O	18:N:35:LYS:HG3	2.16	0.46
18:N:87:TYR:O	18:N:91:ARG:HG2	2.15	0.46
24:e:155:LYS:HZ1	24:e:189:ASP:C	2.24	0.46
29:k:98:VAL:HG21	29:k:109:VAL:HG11	1.98	0.46
49:a:2052:G:H2'	49:a:2055:U:O4	2.16	0.46
1:A:296:C:OP1	1:A:592:U:O2'	2.24	0.46
1:A:606:C:O3'	12:P:11:GLY:HA2	2.16	0.46
24:e:137:LYS:HE3	24:e:169:LEU:CD1	2.46	0.46
28:j:9:LYS:NZ	28:j:81:GLU:HB2	2.31	0.46
36:r:23:ILE:HG12	36:r:121:THR:HG23	1.97	0.46
36:r:62:GLU:HB3	36:r:63:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:2051:U:C4	49:a:2052:G:C5	3.03	0.46
1:A:421:C:OP1	1:A:495:A:O2'	2.33	0.45
1:A:1153:U:C6	1:A:1154:C:C5	3.04	0.45
1:A:1503:2MG:HM21	1:A:1506:MA6:N7	2.31	0.45
4:F:26:TYR:O	4:F:29:VAL:HG12	2.16	0.45
4:F:30:ILE:HD11	4:F:75:LEU:HD22	1.98	0.45
12:P:115:ALA:CB	12:P:116:PRO:CD	2.91	0.45
15:I:57:ASP:OD1	15:I:59:VAL:HG12	2.16	0.45
19:S:26:ARG:NH1	19:S:46:GLU:OE2	2.49	0.45
19:S:37:PHE:CZ	19:S:44:LEU:HD22	2.50	0.45
23:d:69:PRO:HG3	49:a:2969:C:H1'	1.96	0.45
45:0:29:ASN:C	45:0:31:ARG:H	2.23	0.45
48:4:32:THR:C	48:4:33:LEU:HD12	2.39	0.45
49:a:60:G:N2	49:a:92:G:H22	2.13	0.45
49:a:1171:A:H5''	49:a:1172:G:H5'	1.98	0.45
49:a:1354:C:H2'	49:a:1355:G:C8	2.51	0.45
49:a:2430:C:OP2	58:a:3401:HOH:O	2.20	0.45
1:A:109:A:C6	1:A:328:G:C6	3.04	0.45
1:A:922:A:N3	1:A:1363:U:O2'	2.39	0.45
1:A:1400:A:H2	1:A:1474:G:H22	1.63	0.45
1:A:1441:U:H2'	1:A:1442:G:C8	2.51	0.45
5:H:53:GLU:HG2	5:H:54:PRO:HD2	1.99	0.45
14:G:26:LYS:H	14:G:27:GLN:NE2	2.14	0.45
17:M:36:VAL:HB	17:M:75:ASP:O	2.17	0.45
21:B:73:LYS:O	21:B:77:GLN:HG2	2.16	0.45
28:j:64:ARG:HB2	28:j:83:ALA:HB3	1.98	0.45
28:j:93:PRO:HG3	28:j:114:ILE:HG13	1.97	0.45
34:p:4:VAL:HG22	49:a:1276:C:H1'	1.97	0.45
36:r:10:ARG:NH2	36:r:79:GLU:OE2	2.49	0.45
37:s:65:LYS:HA	37:s:80:ASP:OD2	2.17	0.45
49:a:26:G:N2	49:a:600:G:H1'	2.31	0.45
49:a:35:G:N3	49:a:539:G:O2'	2.49	0.45
49:a:1081:C:N4	58:a:3414:HOH:O	2.49	0.45
4:F:20:ASP:O	4:F:24:GLU:HG3	2.17	0.45
22:c:211:ARG:HG2	22:c:214:TRP:CZ2	2.51	0.45
26:g:42:THR:OG1	26:g:54:GLU:HG2	2.16	0.45
45:0:29:ASN:HD21	49:a:2467:C:P	2.38	0.45
49:a:491:A:H2'	49:a:492:U:O4'	2.16	0.45
1:A:66:U:O2'	1:A:381:C:O2	2.31	0.45
1:A:505:A:C2	7:L:88:LYS:HB3	2.52	0.45
2:D:4:TYR:HE2	2:D:11:LYS:HG3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:185:LEU:O	24:e:186:ASN:ND2	2.49	0.45
25:f:107:GLU:OE2	48:4:25:ARG:NH1	2.49	0.45
29:k:58:MET:HE2	49:a:257:G:H4'	1.98	0.45
34:p:92:ARG:HH22	49:a:1081:C:P	2.39	0.45
37:s:6:ILE:HD11	42:x:18:ARG:HG2	1.97	0.45
49:a:682:U:H2'	49:a:683:G:C8	2.52	0.45
6:K:51:ALA:HB2	6:K:79:ARG:NH2	2.31	0.45
24:e:40:VAL:HG13	24:e:188:TYR:HD1	1.81	0.45
24:e:137:LYS:HG3	24:e:137:LYS:O	2.17	0.45
29:k:23:ARG:HA	49:a:896:U:H2'	1.99	0.45
34:p:66:ASN:ND2	49:a:1094:G:OP2	2.42	0.45
35:q:21:GLU:OE2	35:q:92:TYR:HB2	2.17	0.45
39:u:52:LEU:HD22	39:u:55:ARG:NH1	2.29	0.45
43:y:47:MET:O	43:y:51:VAL:HG22	2.17	0.45
49:a:432:A:O5'	49:a:433:G:N2	2.49	0.45
49:a:634:U:O2'	49:a:635:G:H8	1.98	0.45
49:a:1347:C:H5''	49:a:1348:G:H5'	1.98	0.45
2:D:191:ASN:OD1	2:D:194:ALA:N	2.40	0.45
3:E:200:ASP:O	3:E:203:ALA:HB3	2.17	0.45
5:H:43:GLU:HG3	5:H:106:ILE:HD13	1.98	0.45
15:I:30:ILE:HD13	15:I:105:VAL:HG13	1.99	0.45
17:M:30:THR:HA	17:M:33:GLY:O	2.16	0.45
20:U:68:GLY:HA3	48:4:57:ARG:HH12	1.82	0.45
25:f:151:ASP:OD2	25:f:154:LYS:HB3	2.16	0.45
44:z:8:MET:HE3	44:z:8:MET:HB2	1.84	0.45
45:0:7:ASP:OD1	45:0:7:ASP:N	2.49	0.45
47:2:19:SER:OG	49:a:737:G:OP1	2.29	0.45
49:a:2052:G:H1	49:a:2054:A:H5''	1.82	0.45
49:a:2282:G:H1	49:a:2371:U:H3	1.65	0.45
49:a:2718:G:O2'	49:a:2719:U:H6	1.99	0.45
3:E:118:MET:O	3:E:148:ALA:HA	2.17	0.45
14:G:41:TRP:HZ3	14:G:86:VAL:HG23	1.81	0.45
19:S:37:PHE:CZ	19:S:44:LEU:HD13	2.50	0.45
21:B:100:MET:HG2	21:B:107:ILE:HG13	1.97	0.45
23:d:37:PRO:HB3	23:d:101:GLU:OE2	2.16	0.45
26:g:95:TYR:HA	26:g:108:ASN:O	2.16	0.45
26:g:105:LEU:HG	26:g:125:PHE:CD2	2.52	0.45
31:m:46:PRO:O	31:m:50:LYS:HG2	2.16	0.45
49:a:310:C:H2'	49:a:311:A:C8	2.51	0.45
1:A:1345:C:O5'	1:A:1345:C:H6	2.00	0.45
20:U:27:THR:HG23	20:U:47:HIS:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:262:LYS:HG3	22:c:263:ALA:N	2.24	0.45
32:n:93:LYS:NZ	32:n:98:THR:HA	2.31	0.45
39:u:143:VAL:HG11	39:u:176:VAL:HG11	1.98	0.45
45:0:11:LYS:HB2	45:0:11:LYS:HE2	1.79	0.45
49:a:828:C:O2'	49:a:1843:U:OP1	2.30	0.45
49:a:1230:U:H2'	49:a:1231:A:C8	2.52	0.45
49:a:2495:C:H2'	49:a:2496:A:H8	1.82	0.45
52:Y:19:U:OP1	52:Y:19:U:H4'	2.16	0.45
1:A:256:G:O2'	9:Q:25:ASN:O	2.35	0.45
1:A:378:G:O3'	12:P:6:ARG:NH1	2.49	0.45
7:L:19:ASN:OD1	7:L:20:LYS:N	2.49	0.45
12:P:115:ALA:HB3	12:P:116:PRO:HD3	1.96	0.45
17:M:51:VAL:HG21	19:S:44:LEU:HD23	1.99	0.45
28:j:73:ASP:OD2	33:o:80:ILE:HD13	2.17	0.45
31:m:69:THR:HG22	31:m:70:ILE:N	2.32	0.45
31:m:106:ASP:OD2	49:a:1833:G:O2'	2.30	0.45
44:z:53:PRO:HB3	49:a:3065:A:H5'	1.99	0.45
49:a:2141:C:H2'	49:a:2142:G:H8	1.81	0.45
50:b:14:U:OP2	50:b:70:C:O2'	2.35	0.45
1:A:1075:U:O2'	1:A:1157:C:O2'	2.34	0.45
7:L:90:LEU:HD23	7:L:90:LEU:HA	1.83	0.45
12:P:5:ILE:HG12	12:P:22:VAL:HG22	1.99	0.45
15:I:113:GLU:HB3	15:I:119:ARG:HG2	1.97	0.45
17:M:36:VAL:HG12	17:M:76:ILE:HA	1.99	0.45
25:f:148:LEU:HD11	48:4:33:LEU:HD23	1.99	0.45
26:g:148:ALA:HB2	49:a:2927:C:H5'	1.99	0.45
28:j:24:VAL:HG12	28:j:30:ARG:HD3	1.98	0.45
30:l:83:MET:HB2	49:a:2432:G:C5	2.52	0.45
36:r:1:MET:HE3	36:r:1:MET:HB3	1.72	0.45
40:v:41:ARG:HH21	40:v:56:ASP:HB2	1.82	0.45
46:1:25:ARG:NH1	49:a:1443:A:O3'	2.49	0.45
47:2:26:LYS:HD3	47:2:48:THR:HB	1.98	0.45
49:a:1984:G:H3'	49:a:1985:A:H5'	1.98	0.45
49:a:2654:G:O2'	49:a:2660:A:N6	2.50	0.45
49:a:2656:U:H3'	49:a:2657:C:C6	2.52	0.45
9:Q:35:ARG:NH1	9:Q:46:THR:HG1	2.15	0.44
16:J:100:GLU:HG3	16:J:101:GLY:N	2.26	0.44
19:S:3:LYS:HB2	19:S:6:LEU:HD12	1.98	0.44
20:U:9:PRO:HG3	48:4:65:TYR:CE2	2.53	0.44
24:e:136:ASP:OD1	24:e:137:LYS:N	2.44	0.44
28:j:63:VAL:HG11	28:j:102:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:l:14:HIS:CD2	30:l:74:MET:HE1	2.52	0.44
32:n:14:ARG:HD3	50:b:30:C:OP1	2.17	0.44
38:t:29:VAL:HG13	38:t:36:VAL:HG12	1.99	0.44
44:z:39:HIS:ND1	44:z:40:LEU:O	2.48	0.44
48:4:29:GLN:O	48:4:31:GLY:N	2.50	0.44
49:a:277:A:OP2	49:a:320:G:N2	2.45	0.44
49:a:373:G:H22	49:a:437:G:H22	1.65	0.44
49:a:1359:G:O2'	49:a:1361:G:N7	2.44	0.44
49:a:1698:G:H1	49:a:1915:G:N2	2.09	0.44
1:A:78:G:H2'	1:A:79:C:C6	2.51	0.44
1:A:679:U:O2'	1:A:767:G:O2'	2.35	0.44
16:J:170:TYR:HE2	16:J:172:LYS:HB2	1.82	0.44
32:n:8:ARG:NH1	50:b:17:U:OP2	2.49	0.44
35:q:42:ASP:HB3	35:q:45:SER:OG	2.17	0.44
36:r:52:MET:SD	44:z:24:ALA:HB1	2.57	0.44
38:t:78:VAL:HG21	38:t:85:ASP:HB3	1.99	0.44
49:a:214:A:H2'	49:a:215:C:O4'	2.17	0.44
49:a:753:A:H2'	49:a:755:A:H62	1.82	0.44
49:a:2091:U:O2'	53:C:12:G:H5''	2.17	0.44
49:a:2650:G:C2	49:a:2663:G:N3	2.85	0.44
1:A:96:G:H2'	1:A:97:C:H6	1.83	0.44
1:A:718:U:H2'	1:A:719:C:C6	2.52	0.44
14:G:60:SER:O	14:G:61:GLU:HG3	2.17	0.44
18:N:4:LEU:HD23	18:N:9:LEU:HD13	2.00	0.44
21:B:130:LEU:HD23	21:B:135:LEU:HD13	1.99	0.44
22:c:213:ARG:HD2	22:c:213:ARG:HA	1.73	0.44
23:d:108:SER:OG	23:d:111:ASP:OD2	2.28	0.44
23:d:183:VAL:HG22	23:d:195:VAL:HG22	1.99	0.44
45:0:35:ASP:OD1	45:0:35:ASP:N	2.47	0.44
1:A:692:G:H5''	4:F:54:LYS:NZ	2.32	0.44
1:A:806:U:H2'	1:A:807:A:C8	2.52	0.44
1:A:1418:C:H2'	1:A:1419:G:O4'	2.16	0.44
2:D:145:LYS:HB3	12:P:122:LYS:HD2	1.98	0.44
2:D:171:ASN:O	12:P:119:ALA:HA	2.18	0.44
5:H:121:ALA:HB1	5:H:126:VAL:O	2.16	0.44
24:e:157:LEU:HD12	24:e:182:ALA:HA	1.99	0.44
24:e:159:VAL:HG21	24:e:205:ALA:CB	2.47	0.44
26:g:45:LYS:HE3	26:g:48:GLU:HA	1.98	0.44
27:i:4:TYR:CG	34:p:100:VAL:HG11	2.52	0.44
28:j:105:GLU:OE2	28:j:105:GLU:N	2.45	0.44
33:o:6:ASP:O	33:o:10:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:15:ASP:OD1	33:o:15:ASP:N	2.46	0.44
39:u:152:ILE:HB	39:u:174:ALA:HB3	2.00	0.44
47:2:12:LYS:NZ	49:a:256:C:O2	2.40	0.44
49:a:1698:G:N2	49:a:1915:G:H22	2.14	0.44
49:a:2095:A:H62	49:a:2100:PSU:HN3	1.65	0.44
49:a:2871:U:H5''	49:a:2872:G:H21	1.82	0.44
1:A:157:C:H2'	1:A:158:A:C8	2.52	0.44
1:A:1288:U:O4	18:N:14:ARG:HD3	2.18	0.44
7:L:110:ARG:NH2	7:L:112:GLN:O	2.51	0.44
21:B:174:ILE:HG21	21:B:196:GLU:HB3	1.98	0.44
23:d:155:CYS:C	23:d:157:THR:N	2.75	0.44
28:j:2:ILE:HD12	28:j:6:THR:HG21	1.99	0.44
29:k:4:GLU:OE1	29:k:6:HIS:NE2	2.42	0.44
30:l:108:GLY:HA3	39:u:118:ILE:HG21	1.99	0.44
31:m:28:LEU:HD13	31:m:113:ILE:HG23	1.99	0.44
43:y:46:GLY:HA3	49:a:937:G:H5'	2.00	0.44
48:4:18:CYS:HB2	48:4:41:CYS:SG	2.53	0.44
49:a:314:U:H3'	49:a:315:G:C8	2.52	0.44
49:a:373:G:N2	49:a:437:G:H1	2.13	0.44
49:a:631:G:H4'	49:a:632:U:H3'	1.99	0.44
49:a:861:G:N2	49:a:2423:A:OP1	2.51	0.44
49:a:1124:U:H2'	49:a:1125:G:H8	1.82	0.44
49:a:2247:C:H2'	49:a:2248:C:C6	2.51	0.44
49:a:2449:A:H5''	49:a:2450:A:H5'	1.98	0.44
1:A:25:G:H2'	1:A:26:G:C8	2.53	0.44
9:Q:1:MET:HB2	9:Q:2:SER:H	1.52	0.44
12:P:122:LYS:HZ2	12:P:125:GLU:HG2	1.82	0.44
14:G:24:ALA:HB1	14:G:27:GLN:NE2	2.33	0.44
26:g:32:THR:O	26:g:33:LEU:HD23	2.17	0.44
26:g:68:LEU:HD21	49:a:2940:A:C4	2.53	0.44
30:l:17:ARG:HD2	50:b:90:A:O2'	2.18	0.44
36:r:33:LYS:NZ	49:a:2195:G:N7	2.56	0.44
49:a:304:G:H2'	49:a:305:U:C4	2.52	0.44
49:a:461:G:O2'	49:a:489:G:O6	2.30	0.44
49:a:1128:U:O2	49:a:1130:G:N1	2.51	0.44
49:a:2872:G:O2'	49:a:2873:C:P	2.75	0.44
50:b:28:C:H2'	50:b:29:A:O4'	2.17	0.44
1:A:816:G:H5''	10:R:49:VAL:HG21	1.99	0.44
1:A:1006:U:H2'	1:A:1007:G:H8	1.82	0.44
2:D:42:LYS:HA	2:D:42:LYS:HD3	1.77	0.44
6:K:26:GLN:HA	6:K:88:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:117:ARG:O	12:P:120:ILE:HG13	2.17	0.44
12:P:123:LYS:HG3	12:P:124:SER:N	2.31	0.44
14:G:70:ALA:HA	14:G:105:VAL:HG22	1.99	0.44
25:f:89:ARG:NH1	53:C:56:C:N3	2.66	0.44
25:f:131:PHE:CE2	25:f:137:TYR:HB2	2.52	0.44
45:O:32:ASN:HD22	45:O:32:ASN:N	2.16	0.44
49:a:1493:G:H1'	49:a:1769:G:N1	2.33	0.44
49:a:2051:U:H3	49:a:2056:G:H1	1.64	0.44
49:a:2245[A]:A:C6	55:a:3101:V7A:OBE	2.71	0.44
1:A:831:G:H5'	1:A:832:G:OP2	2.18	0.44
1:A:1445:G:OP1	11:T:30:THR:OG1	2.30	0.44
15:I:27:VAL:O	15:I:31:LEU:HB2	2.18	0.44
18:N:23:TYR:HE1	18:N:70:LEU:HD22	1.83	0.44
21:B:75:GLN:HA	21:B:208:ILE:HG13	2.00	0.44
21:B:215:THR:HA	21:B:218:ILE:HG12	1.99	0.44
22:c:221:VAL:HG21	49:a:867:A:N7	2.33	0.44
24:e:207:VAL:O	24:e:211:SER:HB3	2.17	0.44
25:f:40:LEU:HA	25:f:167:THR:HG22	2.00	0.44
35:q:79:LYS:HE3	49:a:654:A:O2'	2.17	0.44
36:r:63:PRO:O	36:r:67:VAL:HG23	2.18	0.44
49:a:547:G:O2'	49:a:558:G:O6	2.27	0.44
1:A:1497:C:OP1	13:X:11:ARG:HB2	2.18	0.44
3:E:67:GLY:O	3:E:97:VAL:N	2.50	0.44
8:O:74:GLU:H	8:O:74:GLU:CD	2.26	0.44
9:Q:23:LYS:HE3	9:Q:23:LYS:HB3	1.70	0.44
9:Q:88:LYS:HG3	9:Q:90:LYS:HG3	1.99	0.44
14:G:115:VAL:HG12	14:G:199:VAL:HG21	2.00	0.44
14:G:141:MET:HE1	14:G:147:GLY:HA2	1.99	0.44
15:I:58:PRO:HA	15:I:61:THR:HG22	1.99	0.44
18:N:19:LEU:HD23	18:N:19:LEU:HA	1.84	0.44
21:B:54:TYR:O	21:B:58:LYS:HG2	2.18	0.44
28:j:88:LYS:HG2	28:j:94:ARG:HG2	1.99	0.44
34:p:65:ILE:CD1	34:p:92:ARG:HG3	2.48	0.44
36:r:95:GLU:O	49:a:23:G:O2'	2.31	0.44
43:y:39:GLU:N	43:y:39:GLU:OE1	2.50	0.44
49:a:172:U:H2'	49:a:173:A:C8	2.53	0.44
49:a:430:U:H4'	49:a:431:A:C8	2.51	0.44
49:a:827:U:H2'	49:a:828:C:C6	2.53	0.44
49:a:2758:G:O2'	49:a:2761:C:OP2	2.27	0.44
53:C:15:G:H2'	53:C:59:A:N1	2.33	0.44
1:A:392:U:H2'	1:A:393:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:U:O4	2:D:2:ALA:N	2.51	0.43
1:A:813:U:H5''	21:B:21:ARG:HD2	1.98	0.43
1:A:1367:U:C4	15:I:3:ARG:HD2	2.53	0.43
8:O:68:ILE:HG22	8:O:76:TYR:HB2	1.99	0.43
15:I:78:ARG:HA	15:I:78:ARG:HD2	1.83	0.43
23:d:158:PRO:HB2	23:d:160:LYS:HG2	2.00	0.43
23:d:214:LYS:O	23:d:216:ALA:N	2.49	0.43
30:l:118:MET:HG3	30:l:131:PHE:HD1	1.82	0.43
49:a:581:G:H2'	49:a:582:G:O4'	2.18	0.43
49:a:2433:OMG:HM23	49:a:2433:OMG:H1'	1.60	0.43
49:a:2655:C:H5'	49:a:2657:C:N4	2.32	0.43
1:A:278:G:OP1	9:Q:21:SER:OG	2.29	0.43
1:A:528:G:H4'	1:A:530:G:O3'	2.19	0.43
1:A:845:G:H4'	5:H:19:GLN:NE2	2.33	0.43
17:M:25:ILE:HD13	17:M:90:LEU:HD11	1.99	0.43
32:n:73:MET:HE1	32:n:80:LYS:HA	2.00	0.43
38:t:18:ASN:ND2	49:a:394:G:H5'	2.33	0.43
39:u:178:PHE:HB3	39:u:179:PRO:CD	2.48	0.43
41:w:40:GLU:O	41:w:42:GLY:N	2.52	0.43
49:a:405:G:H4'	49:a:407:A:C8	2.53	0.43
49:a:454:G:C6	49:a:455:C:C2	3.06	0.43
49:a:693:A:H2'	49:a:694:C:O4'	2.18	0.43
49:a:1723:G:H2'	49:a:1724:G:C8	2.54	0.43
49:a:1910:C:H2'	49:a:1912:U:C2	2.53	0.43
1:A:455:G:N2	1:A:455:G:OP2	2.50	0.43
1:A:563:G:N1	1:A:741:A:OP2	2.39	0.43
1:A:700:A:C5	6:K:124:HIS:CD2	3.05	0.43
5:H:55:LYS:NZ	5:H:56:GLU:OE2	2.37	0.43
18:N:97:PRO:HB3	18:N:101:GLN:HE21	1.83	0.43
29:k:6:HIS:HB3	49:a:1280:U:O2	2.19	0.43
30:l:67:ASN:OD1	30:l:105:GLU:HG3	2.18	0.43
32:n:66:MET:HE2	50:b:27:A:H4'	1.99	0.43
35:q:53:LEU:HA	35:q:56:VAL:HG12	2.01	0.43
49:a:314:U:O2	49:a:314:U:H2'	2.18	0.43
49:a:430:U:H5''	49:a:431:A:H5'	1.99	0.43
49:a:1110:A:N3	58:a:3417:HOH:O	2.37	0.43
49:a:1137:A:H2'	49:a:1138:G:H8	1.83	0.43
49:a:1493:G:H5'	49:a:1595:A:H4'	1.99	0.43
49:a:2284:G:H2'	49:a:2285:A:H8	1.84	0.43
1:A:1058:U:OP2	3:E:85:LYS:NZ	2.34	0.43
1:A:1509:U:OP1	6:K:134:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:24:ALA:O	25:f:27:GLU:HG3	2.18	0.43
25:f:112:LEU:HD23	25:f:117:LEU:HD22	2.00	0.43
27:i:70:THR:HG23	27:i:71:ASP:OD2	2.19	0.43
49:a:344:U:O2	49:a:347:C:N4	2.51	0.43
49:a:400:G:H2'	49:a:401:U:O4'	2.18	0.43
49:a:409:U:H2'	49:a:410:G:O4'	2.18	0.43
53:C:4:G:H1	53:C:69:C:N4	2.16	0.43
1:A:77:G:H1	1:A:97:C:H42	1.65	0.43
1:A:1045:U:C5	14:G:2:GLY:HA2	2.54	0.43
15:I:58:PRO:O	15:I:61:THR:HG22	2.19	0.43
15:I:113:GLU:O	15:I:119:ARG:HD3	2.19	0.43
17:M:42:LEU:HB2	17:M:71:LYS:HB2	2.00	0.43
30:l:83:MET:HE3	30:l:83:MET:HB3	1.93	0.43
31:m:100:ILE:HD11	31:m:112:VAL:HG12	1.99	0.43
38:t:27:LEU:N	38:t:37:VAL:O	2.47	0.43
49:a:2486:G:H22	49:a:2494:U:H3	1.67	0.43
49:a:2717:G:H2'	49:a:2718:G:O5'	2.19	0.43
1:A:406:G:N7	2:D:2:ALA:HB3	2.33	0.43
1:A:512:G:C4	52:Y:22:U:H3'	2.53	0.43
1:A:1294:U:OP1	18:N:98:VAL:HG22	2.19	0.43
2:D:54:GLN:NE2	2:D:58:TYR:HE2	2.15	0.43
18:N:35:LYS:HG3	18:N:35:LYS:HZ3	1.75	0.43
21:B:12:SER:HB2	21:B:209:ARG:HE	1.83	0.43
21:B:77:GLN:O	21:B:93:ASN:ND2	2.41	0.43
23:d:57:GLY:O	23:d:58:TYR:HB3	2.18	0.43
24:e:56:THR:O	24:e:60:VAL:HG23	2.18	0.43
25:f:59:MET:HE3	25:f:93:PRO:HB2	2.01	0.43
43:y:12:SER:HB2	43:y:32:ILE:HD11	2.00	0.43
45:0:20:LYS:N	45:0:20:LYS:HD2	2.34	0.43
49:a:302:A:C8	49:a:303:G:C8	3.07	0.43
49:a:373:G:H1	49:a:437:G:H1	1.66	0.43
49:a:1393:G:H2'	49:a:1394:G:C8	2.53	0.43
49:a:2036:A:N1	49:a:2269:G:H1'	2.34	0.43
49:a:2718:G:C2	49:a:2719:U:C2	3.07	0.43
17:M:32:THR:OG1	17:M:83:THR:HG22	2.18	0.43
21:B:60:THR:HA	21:B:63:LYS:HE2	1.99	0.43
21:B:167:THR:OG1	21:B:174:ILE:HD12	2.19	0.43
25:f:107:GLU:OE2	48:4:9:TYR:OH	2.30	0.43
25:f:161:MET:HB3	25:f:161:MET:HE2	1.82	0.43
26:g:161:GLY:O	26:g:162:LYS:C	2.62	0.43
49:a:130:G:H1	49:a:154:G:H1	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:373:G:N2	49:a:437:G:H22	2.16	0.43
49:a:1903:G:H2'	49:a:1904:U:C5	2.54	0.43
49:a:1972:A:H2'	49:a:1973:C:O4'	2.18	0.43
1:A:90:U:H4'	1:A:91:G:OP1	2.19	0.43
1:A:1274:A:N3	1:A:1338:C:O2'	2.49	0.43
2:D:169:ARG:HH11	12:P:115:ALA:HB3	1.83	0.43
9:Q:6:ALA:O	9:Q:8:ARG:N	2.46	0.43
28:j:20:LEU:HB3	28:j:42:THR:HG22	2.00	0.43
39:u:97:ARG:HA	39:u:97:ARG:HD3	1.78	0.43
49:a:359:C:H2'	49:a:360:A:H8	1.83	0.43
49:a:771:U:H2'	49:a:873:A:N1	2.34	0.43
1:A:1091:G:O2'	14:G:168:ARG:NH2	2.51	0.43
2:D:182:THR:OG1	2:D:184:ASP:OD2	2.30	0.43
3:E:171:GLU:HG2	3:E:179:ARG:NH1	2.33	0.43
5:H:48:ASP:OD2	5:H:49:TYR:N	2.45	0.43
7:L:68:PRO:O	7:L:99:ARG:NH1	2.52	0.43
16:J:46:ALA:O	16:J:103:TYR:OH	2.30	0.43
16:J:69:GLN:HG3	16:J:104:ASP:OD1	2.19	0.43
17:M:28:THR:HA	17:M:31:ARG:CZ	2.48	0.43
22:c:179:SER:OG	49:a:1982:G:N7	2.43	0.43
23:d:105:ASP:HB3	23:d:188:ALA:HB2	2.00	0.43
26:g:73:ILE:HD13	26:g:76:MET:HE3	2.01	0.43
26:g:174:LYS:HA	26:g:174:LYS:HD2	1.33	0.43
28:j:64:ARG:NE	28:j:81:GLU:OE2	2.31	0.43
32:n:29:ILE:HG21	32:n:103:ASP:HB2	1.99	0.43
36:r:98:THR:HG23	36:r:100:ARG:HH12	1.84	0.43
49:a:314:U:C3'	49:a:315:G:H8	2.32	0.43
49:a:2606:C:O2	49:a:2611:G:O2'	2.35	0.43
49:a:2694:C:H2'	49:a:2695:G:O4'	2.19	0.43
49:a:2706:G:N1	49:a:2721:C:H5	2.17	0.43
53:C:9:G:N3	53:C:45:G:H2'	2.34	0.43
1:A:1082:C:H5''	21:B:140:ARG:NH2	2.34	0.43
2:D:99:ARG:NH2	2:D:106:ARG:HH22	2.17	0.43
3:E:180:ARG:NH2	5:H:43:GLU:OE1	2.52	0.43
4:F:23:MET:SD	4:F:61:VAL:HG11	2.59	0.43
12:P:109:LEU:HD23	12:P:109:LEU:HA	1.85	0.43
29:k:56:ILE:HG13	29:k:57:HIS:H	1.83	0.43
39:u:38:HIS:NE2	39:u:94:THR:HG21	2.34	0.43
45:0:29:ASN:O	45:0:31:ARG:N	2.48	0.43
48:4:59:ALA:HA	48:4:62:GLU:OE2	2.19	0.43
49:a:249:G:O2'	49:a:261:G:O6	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:b:13:A:N1	50:b:69:G:O2'	2.40	0.43
1:A:500:C:O2'	1:A:512:G:N2	2.52	0.42
1:A:504:C:OP2	7:L:66:TYR:OH	2.30	0.42
1:A:528:G:O2'	1:A:530:G:O2'	2.32	0.42
11:T:33:ARG:HG2	11:T:33:ARG:NH1	2.33	0.42
18:N:29:ARG:HD2	18:N:64:TYR:CZ	2.54	0.42
21:B:42:ASP:OD1	21:B:45:GLN:NE2	2.45	0.42
21:B:58:LYS:NZ	21:B:221:ALA:O	2.30	0.42
22:c:29:PRO:HG2	22:c:34:LEU:HD11	2.01	0.42
26:g:156:PRO:HD3	26:g:164:VAL:O	2.19	0.42
27:i:146:ALA:O	27:i:147:GLN:HG2	2.19	0.42
28:j:4:GLN:HG2	28:j:5:GLU:HG2	2.01	0.42
35:q:34:GLU:OE1	35:q:34:GLU:N	2.52	0.42
48:4:12:THR:HG21	48:4:33:LEU:HD13	2.00	0.42
49:a:2051:U:H2'	49:a:2052:G:O4'	2.19	0.42
49:a:2571:G:H5''	49:a:2572:U:O4'	2.18	0.42
49:a:2719:U:C4	49:a:2720:C:N4	2.87	0.42
1:A:1006:U:H2'	1:A:1007:G:C8	2.54	0.42
2:D:20:VAL:HG21	2:D:105:THR:OG1	2.18	0.42
9:Q:8:ARG:HG3	9:Q:10:THR:OG1	2.19	0.42
12:P:45:ASP:HB2	12:P:46:PRO:CD	2.34	0.42
14:G:26:LYS:H	14:G:27:GLN:HE21	1.67	0.42
23:d:32:VAL:HG22	23:d:194:LEU:HD22	2.01	0.42
24:e:155:LYS:HZ1	24:e:190:VAL:N	2.17	0.42
26:g:157:GLU:CD	26:g:160:LYS:H	2.26	0.42
27:i:37:ARG:HD2	27:i:109:MET:HG3	2.01	0.42
28:j:64:ARG:HD3	28:j:101:PRO:HG2	2.01	0.42
29:k:74:TYR:CD1	29:k:110:LYS:HB2	2.55	0.42
49:a:2050:G:H3'	49:a:2051:U:H6	1.84	0.42
49:a:2089:G:OP2	49:a:2113:G:H5'	2.19	0.42
1:A:729:U:H2'	1:A:730:U:O4'	2.19	0.42
1:A:996:C:H2'	1:A:997:A:C8	2.54	0.42
3:E:36:GLU:HA	3:E:61:VAL:O	2.19	0.42
6:K:90:VAL:HG13	6:K:116:ILE:HA	2.00	0.42
7:L:79:MET:N	7:L:103:ASP:OD2	2.48	0.42
22:c:14:ARG:NH2	49:a:1879:G:N7	2.60	0.42
34:p:58:ARG:HA	34:p:61:TRP:CE3	2.54	0.42
39:u:122:GLU:HG3	39:u:172:VAL:HG23	2.01	0.42
49:a:311:A:O2'	49:a:312:U:OP1	2.29	0.42
49:a:1894:U:H2'	49:a:1895:G:O4'	2.19	0.42
49:a:2042:A:H8	49:a:2042:A:O5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:67:CYS:SG	4:F:71:THR:OG1	2.78	0.42
12:P:122:LYS:CE	12:P:125:GLU:HG2	2.50	0.42
15:I:75:VAL:CG2	15:I:144:MET:HE3	2.48	0.42
16:J:89:ILE:HG12	16:J:122:ARG:HD2	2.01	0.42
22:c:226:MET:HG2	49:a:867:A:C2	2.54	0.42
26:g:120:PRO:HD2	26:g:123:ILE:HB	2.01	0.42
30:l:36:ALA:HB2	30:l:103:LEU:HD11	2.00	0.42
34:p:77:ASN:OD1	34:p:78:ARG:N	2.51	0.42
42:x:70:ASP:HA	42:x:71:PRO:HD2	1.91	0.42
43:y:15:ALA:HA	49:a:1052:G:O3'	2.20	0.42
49:a:903:G:N1	49:a:1265:U:OP2	2.34	0.42
49:a:1222:G:O2'	49:a:1227:A:N1	2.48	0.42
49:a:2713:A:C2	49:a:2714:G:H1'	2.54	0.42
49:a:2861:A:H2'	49:a:2862:C:O4'	2.20	0.42
49:a:2870:G:O2'	49:a:2872:G:C2	2.72	0.42
1:A:673:G:OP2	6:K:34:ASN:ND2	2.52	0.42
1:A:861:C:OP1	5:H:85:LYS:HE2	2.19	0.42
2:D:169:ARG:O	2:D:170:PRO:C	2.62	0.42
5:H:118:ASP:OD2	5:H:118:ASP:N	2.52	0.42
16:J:128:ALA:O	16:J:132:VAL:HG23	2.20	0.42
25:f:160:GLY:HA3	49:a:2487:U:C2	2.54	0.42
28:j:108:GLU:HB2	28:j:110:LYS:HZ2	1.83	0.42
48:4:10:ARG:NH2	48:4:30:SER:HA	2.35	0.42
48:4:59:ALA:HA	48:4:62:GLU:CD	2.44	0.42
49:a:1142:G:N2	49:a:1163:C:O2	2.52	0.42
49:a:1906:C:H2'	49:a:1907:A:C8	2.54	0.42
49:a:2653:C:H2'	49:a:2654:G:O4'	2.19	0.42
49:a:2658:A:H2'	49:a:2658:A:N3	2.35	0.42
49:a:2722:C:H5''	49:a:2722:C:H6	1.84	0.42
52:Y:22:U:H6	52:Y:22:U:H2'	1.72	0.42
1:A:403:C:O2'	1:A:603:A:N3	2.43	0.42
1:A:639:G:H21	8:O:20:THR:HG23	1.85	0.42
1:A:874:G:O2'	1:A:890:A:N6	2.52	0.42
20:U:9:PRO:HG3	48:4:65:TYR:CD2	2.55	0.42
40:v:39:ARG:NH2	49:a:2545:U:O2'	2.52	0.42
45:0:14:LEU:HD21	45:0:39:MET:SD	2.59	0.42
47:2:50:LEU:HD23	47:2:54:GLU:HB3	2.01	0.42
49:a:1257:U:H2'	49:a:1258:G:O4'	2.20	0.42
49:a:1719:U:O2'	49:a:1720:U:OP1	2.29	0.42
1:A:1130:G:H21	1:A:1132:A:H62	1.67	0.42
1:A:1315:A:OP1	18:N:29:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1516:G:N7	13:X:7:LYS:HE3	2.34	0.42
8:O:30:LEU:O	8:O:34:ILE:HG13	2.20	0.42
12:P:46:PRO:O	12:P:47:SER:C	2.62	0.42
21:B:160:GLN:O	21:B:183:PRO:HG2	2.19	0.42
34:p:98:LEU:HD22	34:p:105:ALA:HB3	2.02	0.42
48:4:60:ARG:O	48:4:64:ARG:HG2	2.19	0.42
49:a:98:U:H5'	49:a:99:G:O4'	2.20	0.42
49:a:2533:G:H1'	49:a:2548:A:N6	2.34	0.42
54:3:22:ARG:HD3	54:3:35:ARG:HD3	2.00	0.42
1:A:405:C:H5''	2:D:128:PRO:HD2	2.00	0.42
1:A:810:A:N3	21:B:25:PRO:HG2	2.34	0.42
1:A:868:U:H4'	1:A:869:G:H5''	2.02	0.42
5:H:118:ASP:O	5:H:119:LYS:C	2.61	0.42
12:P:112:ALA:C	12:P:116:PRO:HD2	2.44	0.42
16:J:70:TRP:CD2	16:J:77:LEU:HD12	2.54	0.42
18:N:90:ARG:HA	18:N:93:ARG:NH1	2.35	0.42
34:p:59:SER:O	34:p:63:GLN:HG3	2.20	0.42
35:q:78:ASN:OD1	35:q:78:ASN:N	2.53	0.42
36:r:53:LEU:HB2	36:r:65:ARG:HG3	2.02	0.42
49:a:335:U:H1'	49:a:447:U:C4	2.55	0.42
49:a:603:A:H1'	49:a:664:C:H1'	2.01	0.42
49:a:2473:U:OP1	49:a:2562:U:O2'	2.33	0.42
49:a:2546:C:H2'	49:a:2547:G:O4'	2.20	0.42
1:A:700:A:C4	6:K:124:HIS:CD2	3.07	0.42
1:A:737:G:OP2	8:O:63:ARG:HD2	2.20	0.42
1:A:765:C:H2'	1:A:766:A:H8	1.84	0.42
1:A:958:U:P	19:S:29:ARG:HH21	2.41	0.42
1:A:1047:U:H2'	1:A:1048:C:C6	2.55	0.42
1:A:1134:U:H4'	16:J:60:ARG:HD2	2.01	0.42
1:A:1134:U:H2'	1:A:1135:C:O4'	2.19	0.42
1:A:1282:C:H4'	1:A:1288:U:O4	2.20	0.42
1:A:1361:A:O2'	15:I:31:LEU:HD23	2.20	0.42
12:P:117:ARG:C	12:P:119:ALA:N	2.72	0.42
22:c:212:ASN:HA	22:c:215:LYS:HB2	2.02	0.42
40:v:10:SER:OG	49:a:2459:G:OP2	2.26	0.42
40:v:37:ILE:HG21	40:v:78:VAL:HG11	2.02	0.42
44:z:35:CYS:SG	44:z:48:CYS:HB3	2.60	0.42
48:4:27:THR:O	48:4:29:GLN:N	2.53	0.42
49:a:359:C:H2'	49:a:360:A:C8	2.55	0.42
49:a:814:G:H5'	49:a:815:U:H5''	2.02	0.42
49:a:1176:G:O2'	49:a:1181:A:N6	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:1492:C:H2'	49:a:1493:G:N7	2.34	0.42
53:C:62:C:H2'	53:C:63:G:C8	2.55	0.42
1:A:11:G:N1	3:E:118:MET:HE2	2.35	0.42
1:A:92:G:O2'	1:A:93:G:H5'	2.19	0.42
1:A:1121:U:O2'	1:A:1122:U:H5'	2.19	0.42
3:E:104:ILE:O	3:E:121:PRO:HB3	2.20	0.42
6:K:23:VAL:O	6:K:86:LYS:N	2.51	0.42
6:K:56:VAL:O	6:K:56:VAL:HG23	2.20	0.42
13:X:16:LYS:HA	13:X:16:LYS:HD2	1.86	0.42
16:J:63:ILE:HG22	16:J:105:VAL:HG23	2.01	0.42
19:S:13:LYS:HE3	19:S:13:LYS:HB3	1.44	0.42
22:c:25:THR:O	22:c:25:THR:OG1	2.27	0.42
22:c:44:ASN:OD1	22:c:45:ASN:N	2.51	0.42
32:n:97:ILE:C	32:n:98:THR:HG1	2.28	0.42
36:r:89:SER:HB2	36:r:125:GLU:HG3	2.02	0.42
48:4:47:GLY:HA3	48:4:50:LYS:NZ	2.34	0.42
49:a:279:A:O2'	49:a:456:C:O2'	2.27	0.42
49:a:982:C:H2'	49:a:983:G:O4'	2.19	0.42
49:a:2870:G:O2'	49:a:2872:G:N1	2.52	0.42
1:A:1055:U:H5'	3:E:53:ARG:NH1	2.36	0.41
1:A:1271:G:H1'	1:A:1272:G:OP2	2.20	0.41
6:K:60:GLY:O	6:K:63:LYS:HG2	2.19	0.41
10:R:23:TYR:HE2	10:R:65:LEU:HD23	1.85	0.41
16:J:122:ARG:NH2	16:J:146:MET:HG2	2.35	0.41
19:S:32:SER:OG	19:S:41:ARG:HB2	2.20	0.41
21:B:6:THR:HG22	21:B:10:LEU:HG	2.02	0.41
21:B:83:GLN:OE1	21:B:219:ALA:HB2	2.19	0.41
22:c:183:ARG:NH2	49:a:1983:C:OP2	2.53	0.41
22:c:212:ASN:OD1	49:a:1974:A:H5''	2.19	0.41
22:c:214:TRP:CD1	49:a:1749:G:O4'	2.73	0.41
22:c:265:SER:OG	22:c:266:ARG:NH1	2.44	0.41
27:i:36:LEU:HD11	27:i:122:LEU:HB2	2.01	0.41
32:n:11:LEU:O	32:n:16:LYS:HE3	2.19	0.41
49:a:258:A:C5	49:a:259:G:H1'	2.55	0.41
49:a:868:A:H8	49:a:1961:U:O2'	2.02	0.41
49:a:1200:U:H2'	49:a:1201:C:C6	2.55	0.41
49:a:2660:A:H3'	49:a:2661:G:H8	1.85	0.41
49:a:2872:G:HO2'	49:a:2873:C:P	2.43	0.41
49:a:2937:C:O2'	49:a:2938:U:H2'	2.20	0.41
1:A:403:C:H5''	2:D:69:ARG:HD2	2.02	0.41
4:F:8:ILE:HG22	4:F:10:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:133:TYR:O	5:H:135:TRP:HE3	2.03	0.41
22:c:182:MET:HB2	22:c:269:VAL:HG12	2.01	0.41
23:d:26:ARG:HE	28:j:72:PRO:HB3	1.84	0.41
24:e:144:LYS:O	24:e:145:ALA:C	2.63	0.41
31:m:85:PRO:O	31:m:88:GLU:HG2	2.20	0.41
33:o:52:GLY:HA2	33:o:57:GLU:HG2	2.02	0.41
39:u:168:ASP:OD1	39:u:169:ALA:N	2.53	0.41
49:a:309:G:N3	49:a:310:C:H5	2.18	0.41
49:a:2050:G:H3'	49:a:2051:U:C6	2.54	0.41
49:a:2982:U:OP2	49:a:2983:C:N4	2.53	0.41
1:A:161:A:H2'	1:A:162:A:O4'	2.20	0.41
1:A:201:U:H4'	9:Q:4:ASN:ND2	2.35	0.41
1:A:1154:C:C4	1:A:1155:A:C5	3.08	0.41
2:D:91:SER:HB3	2:D:180:LEU:HD11	2.02	0.41
2:D:169:ARG:NH2	12:P:109:LEU:O	2.52	0.41
3:E:36:GLU:HB3	3:E:62:VAL:HG22	2.02	0.41
3:E:100:VAL:HG21	3:E:192:MET:HG3	2.01	0.41
12:P:45:ASP:O	12:P:47:SER:N	2.52	0.41
18:N:43:LEU:HD23	18:N:43:LEU:H	1.84	0.41
21:B:134:GLU:HA	21:B:137:MET:HE2	2.02	0.41
23:d:17:MET:HE1	49:a:2862:C:O2'	2.20	0.41
28:j:110:LYS:HG3	28:j:111:PHE:H	1.85	0.41
39:u:33:MET:HA	39:u:92:LEU:O	2.20	0.41
49:a:263:A:H2'	49:a:264:A:C8	2.54	0.41
49:a:315:G:C6	49:a:316:C:C4	3.08	0.41
49:a:439:C:H2'	49:a:440:A:H8	1.85	0.41
49:a:2042:A:H2'	49:a:2043:A:O4'	2.21	0.41
49:a:2525:U:O3'	49:a:2555:A:H4'	2.20	0.41
1:A:123:C:OP1	1:A:313:C:O2'	2.31	0.41
1:A:428:U:H2'	1:A:429:U:C6	2.56	0.41
5:H:116:LEU:HD22	5:H:120:GLN:HB3	2.01	0.41
11:T:31:TYR:CE2	11:T:57:GLN:HG3	2.56	0.41
16:J:113:GLY:O	16:J:117:GLN:HG3	2.20	0.41
26:g:55:ARG:HB2	26:g:62:ASN:HB3	2.01	0.41
36:r:58:GLN:NE2	49:a:2192:G:OP1	2.54	0.41
40:v:72:ARG:NH2	50:b:10:G:H5''	2.35	0.41
41:w:6:ASP:OD1	41:w:48:ASN:N	2.53	0.41
41:w:19:PRO:HG2	49:a:2262:A:H4'	2.03	0.41
44:z:3:VAL:HG23	49:a:2198:A:C2	2.55	0.41
1:A:246:U:O4	1:A:890:A:H1'	2.20	0.41
1:A:695:G:H2'	1:A:696:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:PRO:HA	2:D:151:VAL:HG22	2.02	0.41
14:G:55:GLU:HB3	14:G:66:PHE:HB2	2.02	0.41
22:c:44:ASN:HB2	22:c:50:THR:HG23	2.01	0.41
25:f:31:TYR:OH	25:f:174:GLU:OE1	2.25	0.41
26:g:109:LEU:HD13	26:g:154:ARG:HB2	2.01	0.41
26:g:155:LYS:NZ	26:g:155:LYS:HB3	2.36	0.41
35:q:49:ASP:O	35:q:53:LEU:HD23	2.20	0.41
39:u:119:ALA:HA	39:u:176:VAL:HG12	2.03	0.41
49:a:631:G:H5'	49:a:632:U:C5	2.56	0.41
49:a:1189:G:C6	49:a:1190:G:C5	3.08	0.41
49:a:1194:A:N3	49:a:1195:G:H1'	2.34	0.41
4:F:14:VAL:CG2	4:F:84:LYS:HE3	2.51	0.41
4:F:69:PRO:HA	4:F:72:ILE:HG22	2.03	0.41
21:B:229:ARG:HE	21:B:229:ARG:HB3	1.72	0.41
24:e:159:VAL:HA	24:e:182:ALA:H	1.85	0.41
24:e:165:GLU:HB3	24:e:169:LEU:HD12	2.01	0.41
26:g:9:ILE:O	26:g:51:ILE:N	2.53	0.41
28:j:31:ARG:HH22	49:a:2858:C:P	2.43	0.41
37:s:7:ARG:HH21	37:s:12:ILE:HG13	1.86	0.41
48:4:12:THR:CG2	48:4:33:LEU:HD13	2.50	0.41
49:a:311:A:H2'	49:a:312:U:C6	2.55	0.41
49:a:956:A:H2'	49:a:957:U:C6	2.56	0.41
49:a:1711:G:O6	49:a:1725:G:H2'	2.21	0.41
49:a:2504:A:H2'	49:a:2505:G:O4'	2.21	0.41
49:a:2718:G:C5	49:a:2719:U:C4	3.08	0.41
1:A:406:G:O2'	1:A:480:A:N1	2.43	0.41
1:A:1065:A:OP1	3:E:75:LYS:HD3	2.21	0.41
3:E:206:ALA:O	3:E:207:ARG:C	2.63	0.41
9:Q:9:THR:OG1	9:Q:10:THR:N	2.52	0.41
14:G:141:MET:HG3	14:G:169:GLU:OE2	2.21	0.41
17:M:19:ASP:HB3	17:M:23:ARG:NH1	2.34	0.41
18:N:77:ASP:OD2	18:N:80:ARG:NH2	2.53	0.41
23:d:14:LYS:HB2	23:d:207:LEU:HD11	2.02	0.41
49:a:277:A:OP2	49:a:320:G:N1	2.49	0.41
49:a:418:G:HO2'	49:a:419:U:P	2.41	0.41
49:a:440:A:H2'	49:a:441:C:C6	2.56	0.41
49:a:1345:A:H2'	49:a:1346:G:O4'	2.21	0.41
49:a:1364:U:C4	49:a:1403:U:H1'	2.56	0.41
49:a:1417:G:C2	49:a:1474:C:H4'	2.55	0.41
49:a:2205:U:O2'	49:a:2799:C:H5'	2.20	0.41
49:a:2268:U:H2'	49:a:2269:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:2560:A:C5	49:a:2561:G:H1'	2.55	0.41
50:b:88:G:H2'	50:b:89:G:O4'	2.21	0.41
54:3:29:ASN:HB3	54:3:32:HIS:ND1	2.35	0.41
1:A:995:U:H3	1:A:1004:G:H1	1.67	0.41
14:G:26:LYS:O	14:G:27:GLN:HB3	2.21	0.41
15:I:118:GLU:HA	15:I:121:MET:HB3	2.01	0.41
20:U:23:ASN:HD22	20:U:23:ASN:HA	1.66	0.41
21:B:81:VAL:HG23	21:B:91:TYR:CE2	2.55	0.41
21:B:122:PHE:HA	21:B:125:VAL:HG12	2.03	0.41
22:c:210:GLY:HA2	49:a:849:A:H5'	2.02	0.41
23:d:17:MET:HG2	23:d:31:THR:HA	2.03	0.41
24:e:139:SER:HA	24:e:142:GLN:CD	2.46	0.41
25:f:47:MET:HE3	25:f:66:ILE:HB	2.02	0.41
25:f:83:ILE:HB	25:f:88:LEU:HD21	2.02	0.41
26:g:64:SER:HB3	49:a:2939:A:C2	2.55	0.41
29:k:93:THR:HA	29:k:97:LEU:HD12	2.02	0.41
39:u:129:GLN:N	39:u:164:SER:O	2.51	0.41
39:u:142:ASP:OD1	39:u:144:THR:OG1	2.24	0.41
49:a:694:C:H2'	49:a:695:C:H6	1.85	0.41
49:a:1067:G:H2'	51:V:22:PRO:HG3	2.03	0.41
49:a:2872:G:O2'	49:a:2873:C:C6	2.71	0.41
1:A:102:G:O2'	1:A:152:A:N3	2.50	0.41
1:A:478:A:H2	1:A:480:A:H62	1.66	0.41
1:A:485:C:O2'	1:A:492:A:N1	2.41	0.41
1:A:537:C:H2'	1:A:538:C:C6	2.56	0.41
1:A:729:U:C4	1:A:730:U:C5	3.09	0.41
1:A:845:G:H4'	5:H:19:GLN:HE22	1.85	0.41
1:A:960:G:OP1	19:S:32:SER:N	2.54	0.41
1:A:1045:U:H5	14:G:2:GLY:HA2	1.85	0.41
1:A:1503:2MG:HM21	1:A:1506:MA6:C8	2.50	0.41
8:O:81:ALA:HA	8:O:85:LEU:HD12	2.03	0.41
18:N:105:THR:HG23	18:N:106:ASN:N	2.35	0.41
21:B:54:TYR:CE2	21:B:221:ALA:HB2	2.56	0.41
22:c:213:ARG:NH1	49:a:849:A:N3	2.64	0.41
23:d:139:THR:OG1	49:a:2176:U:H4'	2.21	0.41
23:d:161:VAL:HG21	49:a:2800:G:H21	1.86	0.41
25:f:14:LYS:HE3	25:f:18:ARG:HE	1.86	0.41
25:f:42:LYS:O	25:f:43:ILE:HD13	2.20	0.41
25:f:128:SER:HB3	25:f:176:LYS:NZ	2.36	0.41
27:i:4:TYR:CD2	34:p:100:VAL:HG11	2.55	0.41
28:j:69:HIS:ND1	28:j:105:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:m:45:ARG:HG3	31:m:95:THR:OG1	2.20	0.41
33:o:103:ARG:HH22	49:a:1938:A:P	2.44	0.41
35:q:6:ARG:HG2	35:q:7:SER:N	2.35	0.41
40:v:15:ASP:OD1	40:v:16:SER:N	2.52	0.41
40:v:44:HIS:HD2	40:v:45:PHE:CE2	2.39	0.41
47:2:29:LYS:HD2	47:2:41:THR:HG23	2.02	0.41
48:4:49:GLN:CD	48:4:50:LYS:H	2.29	0.41
49:a:142:G:N2	49:a:147:G:H1	2.17	0.41
49:a:222:G:H4'	49:a:223:A:H4'	2.03	0.41
49:a:332:U:H2'	49:a:333:U:O4'	2.21	0.41
49:a:405:G:H4'	49:a:407:A:N7	2.36	0.41
49:a:441:C:H2'	49:a:442:U:C6	2.56	0.41
49:a:721:C:H2'	49:a:722:G:O4'	2.21	0.41
49:a:771:U:H6	49:a:873:A:N1	2.18	0.41
49:a:949:G:H21	49:a:951:A:N6	2.16	0.41
49:a:1232:U:H2'	49:a:1233:C:C6	2.55	0.41
49:a:1629:C:H5'	49:a:1727:G:H1'	2.02	0.41
49:a:2469:A:O2'	49:a:2470:A:H3'	2.21	0.41
49:a:2655:C:H5''	49:a:2656:U:H5	1.86	0.41
49:a:2656:U:C4	49:a:2657:C:C2	3.09	0.41
49:a:2931:A:N1	49:a:2932:A:N6	2.69	0.41
49:a:3050:C:H2'	49:a:3051:U:O4'	2.21	0.41
2:D:174:ARG:HD3	2:D:176:LEU:HD21	2.03	0.41
9:Q:15:ARG:HD2	9:Q:32:VAL:HG11	2.02	0.41
12:P:72:ALA:O	12:P:76:ARG:HD3	2.21	0.41
16:J:75:ARG:NH2	16:J:80:TYR:HA	2.36	0.41
16:J:92:GLU:HG2	16:J:93:PRO:HD3	2.03	0.41
17:M:64:HIS:HB3	19:S:59:SER:OG	2.20	0.41
19:S:25:GLN:NE2	19:S:38:GLY:HA3	2.35	0.41
25:f:36:LEU:HA	25:f:36:LEU:HD23	1.87	0.41
26:g:7:LEU:HA	26:g:8:PRO:HD3	1.95	0.41
42:x:3:LYS:HA	42:x:3:LYS:HD3	1.84	0.41
42:x:12:LEU:O	42:x:63:ARG:NH2	2.51	0.41
49:a:431:A:H2'	49:a:432:A:O4'	2.21	0.41
49:a:715:C:H5''	49:a:736:C:O2'	2.22	0.41
49:a:1151:G:H21	49:a:1178:A:H2'	1.86	0.41
49:a:1717:G:O2'	49:a:1718:G:O4'	2.36	0.41
49:a:2281:U:H1'	49:a:2373:G:N2	2.35	0.41
49:a:2661:G:H2'	49:a:2662:C:O4'	2.21	0.41
49:a:2938:U:OP2	54:3:19:ARG:NH2	2.52	0.41
50:b:89:G:OP1	51:V:12:ARG:NH2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:U:P	7:L:12:ARG:HH21	2.44	0.40
1:A:1119:C:H2'	1:A:1120:G:O4'	2.20	0.40
9:Q:21:SER:HB3	9:Q:29:THR:HB	2.03	0.40
12:P:108:ALA:HA	12:P:111:GLU:CB	2.43	0.40
15:I:26:LEU:HB2	15:I:101:MET:HE1	2.03	0.40
18:N:40:SER:HB3	18:N:43:LEU:HD22	2.03	0.40
29:k:66:PHE:H	49:a:717:A:HO2'	1.67	0.40
49:a:272:A:O2'	49:a:273:G:H4'	2.20	0.40
49:a:463:A:C2	49:a:464:G:H1'	2.56	0.40
49:a:483:U:H2'	49:a:484:C:C6	2.55	0.40
49:a:2291:U:H5'	49:a:2363:G:N2	2.37	0.40
49:a:2427:U:H5''	49:a:2428:G:H5'	2.03	0.40
1:A:91:G:O2'	1:A:92:G:H8	2.04	0.40
1:A:969:C:H2'	1:A:970:U:H6	1.87	0.40
2:D:52:GLU:OE1	2:D:191:ASN:N	2.54	0.40
6:K:22:VAL:O	6:K:24:ALA:N	2.54	0.40
8:O:37:LEU:HD23	8:O:54:LEU:HB2	2.03	0.40
9:Q:44:VAL:O	9:Q:44:VAL:HG13	2.21	0.40
12:P:97:GLU:C	12:P:98:ARG:HD3	2.46	0.40
13:X:22:LYS:NZ	13:X:25:ARG:HH22	2.19	0.40
21:B:214:LEU:HA	21:B:217:ILE:HG12	2.03	0.40
24:e:92:VAL:HG12	24:e:93:HIS:CG	2.56	0.40
29:k:92:ILE:HG23	29:k:92:ILE:O	2.21	0.40
32:n:72:GLU:OE1	32:n:72:GLU:N	2.53	0.40
34:p:11:LYS:O	34:p:15:ARG:HG3	2.21	0.40
49:a:343:C:H2'	49:a:344:U:C6	2.56	0.40
49:a:443:G:H8	49:a:443:G:O5'	2.04	0.40
49:a:978:U:H3'	49:a:979:U:O4'	2.22	0.40
49:a:1130:G:H21	49:a:1194:A:N6	2.18	0.40
49:a:2498:G:H2'	49:a:2499:U:O4'	2.21	0.40
49:a:2789:G:H2'	49:a:2790:G:O4'	2.20	0.40
49:a:2804:C:O2'	49:a:3005:G:N7	2.53	0.40
1:A:91:G:O2'	1:A:92:G:H5'	2.21	0.40
1:A:545:A:O2'	1:A:548:G:O3'	2.38	0.40
1:A:619:U:H2'	1:A:620:C:C6	2.56	0.40
10:R:22:ASP:O	10:R:25:ASP:N	2.43	0.40
17:M:33:GLY:O	17:M:34:ALA:C	2.64	0.40
20:U:62:VAL:HA	20:U:66:MET:HG3	2.02	0.40
23:d:145:LYS:NZ	49:a:2760:G:OP2	2.53	0.40
24:e:93:HIS:CD2	49:a:670:G:H5'	2.56	0.40
24:e:137:LYS:HB3	24:e:166:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:k:132:ALA:O	29:k:136:ILE:HG13	2.20	0.40
32:n:76:ASP:OD2	50:b:50:G:H5''	2.20	0.40
38:t:100:ARG:HH11	38:t:104:GLY:HA2	1.87	0.40
49:a:443:G:H2'	49:a:444:G:C8	2.56	0.40
49:a:622:U:H2'	49:a:623:C:C6	2.55	0.40
49:a:1712:C:H42	49:a:1724:G:H1	1.67	0.40
49:a:2662:C:N4	49:a:2663:G:C6	2.89	0.40
49:a:2713:A:C6	49:a:2714:G:C4	3.08	0.40
49:a:2980:G:H2'	49:a:2981:U:C2	2.57	0.40
50:b:88:G:H8	50:b:88:G:OP1	2.03	0.40
1:A:1187:A:H1'	1:A:1188:U:OP2	2.21	0.40
2:D:31:TYR:HA	2:D:32:PRO:HD3	1.96	0.40
3:E:33:GLU:HG2	3:E:34:TYR:N	2.37	0.40
3:E:157:ILE:CG2	3:E:161:HIS:CE1	3.01	0.40
7:L:76:GLU:HB3	7:L:77:HIS:ND1	2.36	0.40
13:X:20:LEU:O	13:X:24:THR:OG1	2.35	0.40
22:c:235:GLY:HA3	49:a:2780:A:H5''	2.03	0.40
24:e:45:ALA:O	24:e:48:ARG:HB2	2.21	0.40
25:f:173:GLU:HG2	25:f:174:GLU:N	2.35	0.40
26:g:146:THR:O	26:g:150:ILE:HG12	2.22	0.40
32:n:26:ARG:NH2	32:n:54:ASP:OD1	2.55	0.40
39:u:56:THR:HG23	39:u:59:PRO:HG3	2.03	0.40
49:a:11:G:O6	49:a:613:U:H2'	2.21	0.40
49:a:146:U:HO2'	49:a:147:G:P	2.45	0.40
49:a:1251:C:H2'	49:a:1252:C:C6	2.57	0.40
1:A:1022:U:H2'	1:A:1023:C:C6	2.56	0.40
4:F:27:LEU:HD22	4:F:37:VAL:HG11	2.04	0.40
6:K:71:MET:O	6:K:74:GLU:HG2	2.21	0.40
14:G:59:ARG:HH22	17:M:91:ASP:CG	2.29	0.40
16:J:170:TYR:CE2	16:J:172:LYS:HB2	2.56	0.40
24:e:4:THR:HG22	24:e:4:THR:O	2.22	0.40
25:f:17:TYR:HA	25:f:21:ILE:CG1	2.52	0.40
26:g:2:SER:OG	26:g:55:ARG:NH1	2.55	0.40
34:p:34:LYS:HE3	49:a:2201:G:O2'	2.21	0.40
45:0:39:MET:HE1	49:a:2468:A:N6	2.35	0.40
47:2:31:HIS:NE2	49:a:2574:A:OP2	2.49	0.40
49:a:285:U:O2	49:a:313:G:N2	2.55	0.40
49:a:291:U:H5''	49:a:308:U:C5	2.56	0.40
49:a:1305:G:O3'	49:a:1306:U:H3'	2.21	0.40
49:a:2792[B]:C:H6	49:a:2792[B]:C:H2'	1.74	0.40
50:b:34:G:O2'	50:b:35:U:P	2.80	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	D	198/201 (98%)	187 (94%)	10 (5%)	1 (0%)	24	52
3	E	177/215 (82%)	166 (94%)	10 (6%)	1 (1%)	21	47
4	F	94/96 (98%)	91 (97%)	2 (2%)	1 (1%)	11	32
5	H	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
6	K	115/135 (85%)	99 (86%)	15 (13%)	1 (1%)	14	37
7	L	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
8	O	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
9	Q	88/90 (98%)	79 (90%)	5 (6%)	4 (4%)	2	5
10	R	65/79 (82%)	58 (89%)	7 (11%)	0	100	100
11	T	85/88 (97%)	85 (100%)	0	0	100	100
12	P	126/147 (86%)	111 (88%)	9 (7%)	6 (5%)	2	5
13	X	30/33 (91%)	29 (97%)	0	1 (3%)	3	9
14	G	204/269 (76%)	196 (96%)	7 (3%)	1 (0%)	24	52
15	I	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
16	J	132/173 (76%)	114 (86%)	17 (13%)	1 (1%)	16	40
17	M	96/103 (93%)	91 (95%)	3 (3%)	2 (2%)	5	17
18	N	120/123 (98%)	110 (92%)	10 (8%)	0	100	100
19	S	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	22
20	U	82/93 (88%)	77 (94%)	4 (5%)	1 (1%)	10	30
21	B	231/283 (82%)	214 (93%)	16 (7%)	1 (0%)	30	57
22	c	272/278 (98%)	254 (93%)	16 (6%)	2 (1%)	18	44
23	d	212/223 (95%)	198 (93%)	13 (6%)	1 (0%)	24	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	e	208/301 (69%)	184 (88%)	19 (9%)	5 (2%)	4	15
25	f	182/210 (87%)	167 (92%)	15 (8%)	0	100	100
26	g	175/180 (97%)	162 (93%)	12 (7%)	1 (1%)	21	47
27	i	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
28	j	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
29	k	142/146 (97%)	120 (84%)	22 (16%)	0	100	100
30	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
31	m	118/187 (63%)	112 (95%)	5 (4%)	1 (1%)	16	40
32	n	124/127 (98%)	120 (97%)	3 (2%)	1 (1%)	16	40
33	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
34	p	117/123 (95%)	109 (93%)	7 (6%)	1 (1%)	14	37
35	q	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
36	r	130/153 (85%)	123 (95%)	6 (5%)	1 (1%)	16	40
37	s	93/102 (91%)	87 (94%)	5 (5%)	1 (1%)	11	32
38	t	103/122 (84%)	99 (96%)	3 (3%)	1 (1%)	12	35
39	u	177/205 (86%)	168 (95%)	7 (4%)	2 (1%)	11	32
40	v	76/89 (85%)	73 (96%)	3 (4%)	0	100	100
41	w	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	22
42	x	67/77 (87%)	62 (92%)	4 (6%)	1 (2%)	8	25
43	y	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
44	z	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	7	22
45	0	48/56 (86%)	42 (88%)	6 (12%)	0	100	100
46	1	42/44 (96%)	42 (100%)	0	0	100	100
47	2	65/68 (96%)	65 (100%)	0	0	100	100
48	4	64/69 (93%)	51 (80%)	10 (16%)	3 (5%)	2	5
51	V	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
54	3	35/37 (95%)	35 (100%)	0	0	100	100
All	All	5646/6322 (89%)	5277 (94%)	324 (6%)	45 (1%)	18	40

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	17	ARG

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Mol	Chain	Res	Type
12	P	46	PRO
12	P	47	SER
13	X	4	VAL
14	G	27	GLN
16	J	46	ALA
22	c	26	ARG
24	e	151	ALA
24	e	159	VAL
24	e	186	ASN
34	p	93	LYS
48	4	30	SER
9	Q	10	THR
12	P	97	GLU
12	P	112	ALA
12	P	113	ASP
17	M	34	ALA
24	e	133	VAL
32	n	5	LEU
36	r	3	LYS
39	u	97	ARG
41	w	41	ASN
9	Q	5	THR
9	Q	9	THR
19	S	23	ARG
20	U	84	VAL
48	4	28	SER
37	s	93	ARG
48	4	49	GLN
3	E	207	ARG
17	M	6	ILE
22	c	262	LYS
24	e	138	PRO
31	m	37	THR
9	Q	8	ARG
21	B	100	MET
23	d	95	GLU
38	t	64	ILE
39	u	98	GLY
42	x	5	SER
12	P	115	ALA
44	z	55	GLY
2	D	170	PRO

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Mol	Chain	Res	Type
6	K	23	VAL
26	g	161	GLY

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	D	175/176 (99%)	170 (97%)	5 (3%)	37	70
3	E	130/155 (84%)	127 (98%)	3 (2%)	44	75
4	F	89/89 (100%)	89 (100%)	0	100	100
5	H	108/109 (99%)	107 (99%)	1 (1%)	70	87
6	K	88/101 (87%)	87 (99%)	1 (1%)	65	85
7	L	103/104 (99%)	101 (98%)	2 (2%)	50	78
8	O	74/74 (100%)	74 (100%)	0	100	100
9	Q	81/81 (100%)	77 (95%)	4 (5%)	22	52
10	R	55/65 (85%)	55 (100%)	0	100	100
11	T	68/69 (99%)	68 (100%)	0	100	100
12	P	103/115 (90%)	94 (91%)	9 (9%)	9	27
13	X	28/29 (97%)	27 (96%)	1 (4%)	31	63
14	G	160/200 (80%)	156 (98%)	4 (2%)	42	73
15	I	132/133 (99%)	132 (100%)	0	100	100
16	J	97/131 (74%)	96 (99%)	1 (1%)	68	86
17	M	89/93 (96%)	83 (93%)	6 (7%)	15	39
18	N	99/100 (99%)	98 (99%)	1 (1%)	68	86
19	S	48/49 (98%)	47 (98%)	1 (2%)	47	76
20	U	72/80 (90%)	72 (100%)	0	100	100
21	B	197/234 (84%)	197 (100%)	0	100	100
22	c	216/220 (98%)	216 (100%)	0	100	100
23	d	166/172 (96%)	164 (99%)	2 (1%)	63	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	e	165/237 (70%)	164 (99%)	1 (1%)	78	91
25	f	154/175 (88%)	154 (100%)	0	100	100
26	g	150/152 (99%)	143 (95%)	7 (5%)	23	54
27	i	118/120 (98%)	118 (100%)	0	100	100
28	j	101/101 (100%)	99 (98%)	2 (2%)	48	77
29	k	111/113 (98%)	110 (99%)	1 (1%)	70	87
30	l	108/110 (98%)	108 (100%)	0	100	100
31	m	100/142 (70%)	99 (99%)	1 (1%)	68	86
32	n	95/96 (99%)	95 (100%)	0	100	100
33	o	97/99 (98%)	97 (100%)	0	100	100
34	p	98/99 (99%)	98 (100%)	0	100	100
35	q	84/84 (100%)	84 (100%)	0	100	100
36	r	105/118 (89%)	101 (96%)	4 (4%)	29	61
37	s	84/89 (94%)	84 (100%)	0	100	100
38	t	91/103 (88%)	91 (100%)	0	100	100
39	u	149/168 (89%)	145 (97%)	4 (3%)	39	71
40	v	60/67 (90%)	60 (100%)	0	100	100
41	w	52/53 (98%)	52 (100%)	0	100	100
42	x	61/68 (90%)	61 (100%)	0	100	100
43	y	53/55 (96%)	53 (100%)	0	100	100
44	z	51/52 (98%)	51 (100%)	0	100	100
45	0	47/51 (92%)	46 (98%)	1 (2%)	47	76
46	1	36/36 (100%)	36 (100%)	0	100	100
47	2	54/55 (98%)	54 (100%)	0	100	100
48	4	56/59 (95%)	54 (96%)	2 (4%)	31	63
51	V	16/17 (94%)	16 (100%)	0	100	100
54	3	35/35 (100%)	34 (97%)	1 (3%)	37	70
All	All	4709/5133 (92%)	4644 (99%)	65 (1%)	57	82

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	42	LYS

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Mol	Chain	Res	Type
2	D	45	GLU
2	D	47	SER
2	D	171	ASN
2	D	172	LYS
3	E	201	GLU
3	E	207	ARG
3	E	209	GLU
5	H	120	GLN
6	K	100	GLU
7	L	43	LYS
7	L	44	LYS
9	Q	1	MET
9	Q	7	GLU
9	Q	8	ARG
9	Q	11	ARG
12	P	46	PRO
12	P	111	GLU
12	P	114	GLU
12	P	117	ARG
12	P	118	GLU
12	P	120	ILE
12	P	122	LYS
12	P	123	LYS
12	P	125	GLU
13	X	22	LYS
14	G	25	GLU
14	G	26	LYS
14	G	27	GLN
14	G	161	MET
16	J	44	MET
17	M	31	ARG
17	M	32	THR
17	M	35	LYS
17	M	66	GLU
17	M	77	LEU
17	M	78	GLU
18	N	35	LYS
19	S	13	LYS
23	d	45	THR
23	d	94	SER
24	e	144	LYS
26	g	54	GLU

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Mol	Chain	Res	Type
26	g	155	LYS
26	g	157	GLU
26	g	160	LYS
26	g	174	LYS
26	g	175	VAL
26	g	177	LYS
28	j	23	ARG
28	j	122	ILE
29	k	27	SER
31	m	73	ARG
36	r	1	MET
36	r	2	SER
36	r	3	LYS
36	r	95	GLU
39	u	95	VAL
39	u	99	GLU
39	u	100	LYS
39	u	180	GLU
45	0	20	LYS
48	4	48	LYS
48	4	49	GLN
54	3	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	66	GLN
2	D	193	GLN
3	E	161	HIS
5	H	24	GLN
6	K	34	ASN
6	K	124	HIS
8	O	48	HIS
11	T	7	GLN
14	G	18	HIS
14	G	27	GLN
15	I	40	GLN
15	I	68	ASN
15	I	86	GLN
18	N	52	GLN
20	U	23	ASN
20	U	28	HIS

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Mol	Chain	Res	Type
21	B	24	ASN
21	B	77	GLN
21	B	204	ASN
22	c	135	ASN
23	d	25	ASN
23	d	55	GLN
24	e	93	HIS
24	e	142	GLN
26	g	22	GLN
27	i	47	HIS
27	i	118	GLN
29	k	75	GLN
32	n	110	HIS
33	o	41	GLN
33	o	56	GLN
34	p	81	ASN
34	p	119	GLN
45	0	29	ASN
48	4	20	ASN
54	3	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1537 (97%)	204 (13%)	16 (1%)
49	a	2886/3086 (93%)	484 (16%)	0
50	b	117/120 (97%)	11 (9%)	0
52	Y	9/22 (40%)	7 (77%)	0
53	C	75/77 (97%)	10 (13%)	1 (1%)
All	All	4590/4842 (94%)	716 (15%)	17 (0%)

All (716) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	9	U
1	A	10	G
1	A	13	G
1	A	36	A
1	A	43	G
1	A	51	C

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Mol	Chain	Res	Type
1	A	52	U
1	A	55	A
1	A	75	A
1	A	78	G
1	A	82	U
1	A	91	G
1	A	92	G
1	A	93	G
1	A	95	U
1	A	100	G
1	A	121	C
1	A	130	A
1	A	143	C
1	A	145	U
1	A	164	C
1	A	174	U
1	A	178	G
1	A	183	G
1	A	184	G
1	A	185	A
1	A	195	G
1	A	197	A
1	A	214	G
1	A	218	C
1	A	220	G
1	A	222	G
1	A	226	G
1	A	242	C
1	A	247	C
1	A	249	G
1	A	252	U
1	A	253	G
1	A	268	G
1	A	269	C
1	A	291	G
1	A	323	A
1	A	330	U
1	A	331	A
1	A	349	G
1	A	354	C
1	A	356	G
1	A	369	U

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Mol	Chain	Res	Type
1	A	374	C
1	A	375	A
1	A	386	G
1	A	408	G
1	A	413	A
1	A	414	U
1	A	415	G
1	A	416	A
1	A	423	U
1	A	424	C
1	A	426	G
1	A	431	U
1	A	432	A
1	A	441	U
1	A	461	G
1	A	463	G
1	A	467	G
1	A	468	U
1	A	478	A
1	A	493	C
1	A	500	C
1	A	503	G
1	A	509	G7M
1	A	513	U
1	A	529	A
1	A	541	A
1	A	544	U
1	A	546	U
1	A	554	A
1	A	555	A
1	A	558	G
1	A	559	G
1	A	600	C
1	A	614	U
1	A	635	U
1	A	647	G
1	A	703	A
1	A	704	G
1	A	716	G
1	A	729	U
1	A	730	U
1	A	737	G

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Mol	Chain	Res	Type
1	A	759	A
1	A	775	U
1	A	776	A
1	A	791	G
1	A	797	A
1	A	799	C
1	A	803	G
1	A	811	G
1	A	825	U
1	A	826	C
1	A	827	C
1	A	828	A
1	A	831	G
1	A	832	G
1	A	871	G
1	A	874	G
1	A	886	G
1	A	898	A
1	A	911	G
1	A	915	C
1	A	918	C
1	A	919	A
1	A	944	U
1	A	945	U
1	A	950	2MG
1	A	953	A
1	A	955	G
1	A	958	U
1	A	959	A
1	A	960	G
1	A	961	A
1	A	976	U
1	A	977	G
1	A	984	A
1	A	987	G
1	A	989	G
1	A	994	C
1	A	1009	G
1	A	1010	C
1	A	1012	U
1	A	1013	C
1	A	1025	G

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Mol	Chain	Res	Type
1	A	1027	U
1	A	1029	A
1	A	1030	C
1	A	1038	G
1	A	1050	U
1	A	1051	C
1	A	1053	G
1	A	1066	G
1	A	1070	U
1	A	1079	G
1	A	1080	U
1	A	1086	A
1	A	1121	U
1	A	1122	U
1	A	1124	U
1	A	1125	G
1	A	1126	G
1	A	1145	C
1	A	1146	G
1	A	1153	U
1	A	1155	A
1	A	1170	G
1	A	1182	A
1	A	1183	A
1	A	1188	U
1	A	1198	U
1	A	1199	A
1	A	1200	U
1	A	1210	U
1	A	1213	A
1	A	1224	A
1	A	1242	U
1	A	1244	G
1	A	1246	G
1	A	1256	G
1	A	1261	A
1	A	1266	A
1	A	1272	G
1	A	1273	A
1	A	1285	A
1	A	1286	G
1	A	1291	G

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Mol	Chain	Res	Type
1	A	1306	C
1	A	1332	A
1	A	1333	G
1	A	1339	G
1	A	1351	C
1	A	1368	U
1	A	1382	C
1	A	1384	C
1	A	1387	5MC
1	A	1388	G
1	A	1406	G
1	A	1409	G
1	A	1414	C
1	A	1416	C
1	A	1429	G
1	A	1433	A
1	A	1438	U
1	A	1440	G
1	A	1479	A
1	A	1480	A
1	A	1484	G
1	A	1486	A
1	A	1490	A
1	A	1493	U
1	A	1504	G
1	A	1506	MA6
1	A	1516	G
1	A	1517	G
1	A	1521	A
49	a	11	G
49	a	12	U
49	a	31	C
49	a	33	U
49	a	34	G
49	a	42	G
49	a	50	G
49	a	62	G
49	a	70	A
49	a	73	A
49	a	74	G
49	a	82	G
49	a	91	A

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Mol	Chain	Res	Type
49	a	94	G
49	a	98	U
49	a	99	G
49	a	100	U
49	a	101	G
49	a	117	A
49	a	118	A
49	a	119	U
49	a	124	A
49	a	132	A
49	a	133	A
49	a	135	G
49	a	137	C
49	a	147	G
49	a	166	A
49	a	180	U
49	a	188	A
49	a	203	A
49	a	206	A
49	a	222	G
49	a	223	A
49	a	229	A
49	a	230	A
49	a	236	U
49	a	255	G
49	a	272	A
49	a	273	G
49	a	279	A
49	a	283	U
49	a	284	G
49	a	285	U
49	a	286	G
49	a	287	U
49	a	288	G
49	a	289	U
49	a	290	G
49	a	304	G
49	a	305	U
49	a	307	U
49	a	309	G
49	a	310	C
49	a	311	A

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Mol	Chain	Res	Type
49	a	312	U
49	a	313	G
49	a	314	U
49	a	316	C
49	a	318	G
49	a	321	U
49	a	322	U
49	a	324	U
49	a	325	G
49	a	332	U
49	a	335	U
49	a	336	G
49	a	337	G
49	a	338	U
49	a	339	U
49	a	340	C
49	a	341	U
49	a	342	G
49	a	345	G
49	a	346	C
49	a	347	C
49	a	348	G
49	a	353	A
49	a	354	U
49	a	355	U
49	a	356	G
49	a	358	C
49	a	359	C
49	a	360	A
49	a	366	A
49	a	367	A
49	a	369	U
49	a	370	G
49	a	373	G
49	a	379	A
49	a	380	G
49	a	385	A
49	a	386	G
49	a	387	C
49	a	393	G
49	a	396	A
49	a	402	A

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Mol	Chain	Res	Type
49	a	408	G
49	a	415	A
49	a	419	U
49	a	423	G
49	a	431	A
49	a	432	A
49	a	433	G
49	a	434	C
49	a	435	G
49	a	447	U
49	a	453	U
49	a	454	G
49	a	460	A
49	a	475	G
49	a	476	U
49	a	477	G
49	a	480	A
49	a	494	U
49	a	500	G
49	a	501	A
49	a	532	A
49	a	533	C
49	a	544	U
49	a	545	G
49	a	546	A
49	a	570	G
49	a	592	G
49	a	593	A
49	a	596	U
49	a	618	G
49	a	619	C
49	a	620	C
49	a	621	G
49	a	632	U
49	a	633	G
49	a	635	G
49	a	639	A
49	a	646	G
49	a	656	G
49	a	658	A
49	a	674	G
49	a	675	U

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Mol	Chain	Res	Type
49	a	676	G
49	a	687	A
49	a	699	G
49	a	700	G
49	a	701	U
49	a	707	A
49	a	713	A
49	a	720	G
49	a	723	A
49	a	731	A
49	a	733	G
49	a	739	G
49	a	740	A
49	a	741	G
49	a	770	A
49	a	771	U
49	a	802	G
49	a	815	U
49	a	832	U
49	a	842	G
49	a	849	A
49	a	860	G
49	a	861	G
49	a	867	A
49	a	869	G
49	a	870	G
49	a	874	A
49	a	875	U
49	a	877	A
49	a	890	G
49	a	897	C
49	a	912	U
49	a	931	G
49	a	944	G
49	a	968	G
49	a	969	C
49	a	970	U
49	a	972	A
49	a	973	U
49	a	974	C
49	a	975	G
49	a	978	U

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Mol	Chain	Res	Type
49	a	979	U
49	a	980	A
49	a	981	C
49	a	991	C
49	a	994	A
49	a	1016	A
49	a	1028	A
49	a	1029	G
49	a	1042	A
49	a	1044	G
49	a	1057	G
49	a	1066	A
49	a	1073	A
49	a	1079	A
49	a	1096	G
49	a	1105	G
49	a	1109	G
49	a	1116	U
49	a	1119	G
49	a	1128	U
49	a	1129	A
49	a	1130	G
49	a	1141	G
49	a	1142	G
49	a	1144	U
49	a	1145	G
49	a	1149	U
49	a	1150	G
49	a	1151	G
49	a	1152	A
49	a	1153	A
49	a	1154	G
49	a	1156	A
49	a	1157	G
49	a	1161	U
49	a	1165	U
49	a	1172	G
49	a	1173	U
49	a	1177	U
49	a	1178	A
49	a	1179	A
49	a	1181	A

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Mol	Chain	Res	Type
49	a	1189	G
49	a	1190	G
49	a	1193	A
49	a	1195	G
49	a	1196	U
49	a	1215	U
49	a	1216	A
49	a	1218	C
49	a	1225	U
49	a	1226	A
49	a	1227	A
49	a	1254	G
49	a	1255	U
49	a	1256	G
49	a	1257	U
49	a	1283	G
49	a	1297	G
49	a	1306	U
49	a	1307	G
49	a	1327	G
49	a	1330	A
49	a	1333	G
49	a	1348	G
49	a	1350	G
49	a	1351	U
49	a	1365	C
49	a	1376	A
49	a	1377	U
49	a	1390	C
49	a	1428	U
49	a	1441	A
49	a	1455	U
49	a	1460	A
49	a	1471	A
49	a	1472	U
49	a	1595	A
49	a	1601	G
49	a	1607	A
49	a	1608	C
49	a	1625	U
49	a	1626	C
49	a	1630	G

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Mol	Chain	Res	Type
49	a	1633	G
49	a	1637	G
49	a	1639	U
49	a	1641	U
49	a	1642	C
49	a	1648	C
49	a	1663	G
49	a	1673	U
49	a	1674	A
49	a	1677	U
49	a	1689	G
49	a	1690	A
49	a	1691	A
49	a	1692	G
49	a	1697	A
49	a	1698	G
49	a	1706	G
49	a	1710	A
49	a	1712	C
49	a	1714	C
49	a	1717	G
49	a	1718	G
49	a	1719	U
49	a	1720	U
49	a	1721	G
49	a	1725	G
49	a	1726	U
49	a	1727	G
49	a	1743	A
49	a	1749	G
49	a	1752	A
49	a	1761	G
49	a	1768	A
49	a	1769	G
49	a	1774	C
49	a	1777	G
49	a	1792	A
49	a	1818	U
49	a	1830	A
49	a	1832	C
49	a	1837	G
49	a	1838	A

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Mol	Chain	Res	Type
49	a	1858	G
49	a	1897	G
49	a	1898	C
49	a	1904	U
49	a	1911	G
49	a	1912	U
49	a	1913	G
49	a	1914	C
49	a	1915	G
49	a	1916	G
49	a	1921	G
49	a	1939	G
49	a	1947	G
49	a	1956	A
49	a	1965	C
49	a	1969	A
49	a	1974	A
49	a	1983	C
49	a	1984	G
49	a	1985	A
49	a	1999	U
49	a	2012	A
49	a	2031	A
49	a	2041	G
49	a	2052	G
49	a	2053	U
49	a	2054	A
49	a	2055	U
49	a	2056	G
49	a	2057	C
49	a	2068	A
49	a	2089	G
49	a	2096	A
49	a	2098	3TD
49	a	2112	G
49	a	2113	G
49	a	2119	A
49	a	2120	A
49	a	2121	A
49	a	2138	U
49	a	2146	U
49	a	2150	C

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Mol	Chain	Res	Type
49	a	2153	A
49	a	2154	U
49	a	2155	G
49	a	2174	U
49	a	2176	U
49	a	2186	G
49	a	2204	U
49	a	2206	A
49	a	2210	G
49	a	2214	A
49	a	2215	G
49	a	2216	A
49	a	2222	G
49	a	2226	C
49	a	2238	C
49	a	2239	G
49	a	2243	A
49	a	2275	G
49	a	2279	A
49	a	2283	G
49	a	2287	G
49	a	2289	U
49	a	2364	A
49	a	2365	U
49	a	2366	U
49	a	2367	G
49	a	2368	U
49	a	2369	U
49	a	2384	G
49	a	2385	U
49	a	2386	G
49	a	2393	G
49	a	2394	A
49	a	2407	A
49	a	2420	G
49	a	2421	G
49	a	2461	G
49	a	2464	G
49	a	2465	C
49	a	2469	A
49	a	2487	U
49	a	2490	G

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Mol	Chain	Res	Type
49	a	2491	U
49	a	2501	G
49	a	2502	U
49	a	2503	G
49	a	2504	A
49	a	2507	G
49	a	2517	A
49	a	2518	A
49	a	2527	G
49	a	2529	C
49	a	2532	U
49	a	2536	A
49	a	2543	G
49	a	2565	G
49	a	2567	A
49	a	2588	U
49	a	2607	A
49	a	2611	G
49	a	2612	A
49	a	2613	U
49	a	2617	A
49	a	2623	C
49	a	2630	A
49	a	2652	G
49	a	2653	C
49	a	2654	G
49	a	2655	C
49	a	2656	U
49	a	2657	C
49	a	2658	A
49	a	2659	U
49	a	2660	A
49	a	2661	G
49	a	2663	G
49	a	2664	A
49	a	2673	U
49	a	2674	U
49	a	2679	A
49	a	2684	G
49	a	2687	G
49	a	2688	U
49	a	2700	A

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Mol	Chain	Res	Type
49	a	2702	C
49	a	2711	G
49	a	2712	G
49	a	2713	A
49	a	2714	G
49	a	2716	C
49	a	2717	G
49	a	2720	C
49	a	2721	C
49	a	2722	C
49	a	2748	A
49	a	2749	G
49	a	2755	C
49	a	2767	U
49	a	2784	A
49	a	2795	U
49	a	2797	U
49	a	2811	A
49	a	2871	U
49	a	2872	G
49	a	2873	C
49	a	2900	G
49	a	2908	C
49	a	2911	C
49	a	2915	U
49	a	2917	G
49	a	2926	G
49	a	2930	A
49	a	2939	A
49	a	2944	G
49	a	2947	A
49	a	2948	G
49	a	2960	A
49	a	2962	A
49	a	2971	C
49	a	2972	A
49	a	2973	C
49	a	2979	U
49	a	2981	U
49	a	2982	U
49	a	2983	C
49	a	3000	G

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Mol	Chain	Res	Type
49	a	3015	A
49	a	3041	G
49	a	3052	G
49	a	3063	A
49	a	3064	U
49	a	3066	G
49	a	3073	G
49	a	3074	A
49	a	3075	C
50	b	24	G
50	b	25	A
50	b	35	U
50	b	45	A
50	b	56	U
50	b	57	A
50	b	84	C
50	b	90	A
50	b	100	A
50	b	109	C
50	b	110	G
52	Y	14	A
52	Y	15	A
52	Y	16	A
52	Y	19	U
52	Y	20	U
52	Y	21	U
52	Y	22	U
53	C	9	G
53	C	16	C
53	C	17	C
53	C	17(A)	U
53	C	18	G
53	C	21	A
53	C	46	G
53	C	47	U
53	C	69	C
53	C	76	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U

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Mol	Chain	Res	Type
1	A	90	U
1	A	94	G
1	A	146	U
1	A	418	G
1	A	466	G
1	A	467	G
1	A	638	G
1	A	869	G
1	A	960	G
1	A	1050	U
1	A	1052	A
1	A	1187	A
1	A	1271	G
1	A	1350	A
1	A	1387	5MC
53	C	17(A)	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	G7M	A	509	1	23,26,27	2.84	9 (39%)	34,39,42	1.81	9 (26%)
1	5MC	A	1387	1	19,22,23	0.53	0	26,32,35	0.66	0
49	PSU	a	2762	49	18,21,22	1.11	2 (11%)	21,30,33	1.96	5 (23%)
49	5MC	a	2145	49	19,22,23	0.58	0	26,32,35	0.70	0
1	2MG	A	950	1	23,26,27	0.45	0	33,38,41	0.48	0
49	2MG	a	2627	49	23,26,27	0.52	0	33,38,41	0.47	0
49	2MA	a	2685	49,56	22,25,26	3.60	8 (36%)	32,37,40	2.05	9 (28%)
49	2MG	a	2018	49	23,26,27	0.47	0	33,38,41	0.55	0
49	PSU	a	1038	49	18,21,22	1.03	1 (5%)	21,30,33	2.01	3 (14%)
1	MA6	A	1505	1	23,26,27	1.38	4 (17%)	33,38,41	4.39	13 (39%)
1	PSU	A	498	1,56	18,21,22	1.10	2 (11%)	21,30,33	1.98	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	OMC	a	2680	49,56	19,22,23	0.62	0	25,31,34	0.74	0
1	5MC	A	1391	1	19,22,23	0.61	0	26,32,35	0.58	0
53	PSU	C	55	53	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
1	5MC	A	951	1	19,22,23	0.56	0	26,32,35	0.64	0
49	H2U	a	2631	49	18,21,22	0.48	0	19,30,33	1.08	1 (5%)
49	OMG	a	2433	53,49	23,26,27	0.31	0	32,38,41	0.39	0
1	MA6	A	1506	1	23,26,27	1.38	4 (17%)	33,38,41	4.53	14 (42%)
1	2MG	A	1503	1	23,26,27	0.48	0	33,38,41	0.77	0
1	UR3	A	1485	1,56	19,22,23	2.76	8 (42%)	26,32,35	1.59	4 (15%)
49	5MU	a	2122	49	19,22,23	0.47	0	27,32,35	0.47	0
49	PSU	a	2094	49	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
49	PSU	a	2786	49	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
1	4OC	A	1389	1	20,23,24	3.12	8 (40%)	25,32,35	0.92	1 (4%)
1	5MC	A	1394	1	19,22,23	0.51	0	26,32,35	0.61	0
53	5MC	C	32	53	19,22,23	0.49	0	26,32,35	0.61	0
49	PSU	a	2787	49	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
49	3TD	a	2098	49	19,22,23	4.27	6 (31%)	23,32,35	1.81	4 (17%)
53	5MU	C	54	53	19,22,23	0.38	0	27,32,35	0.62	0
49	PSU	a	2686	49	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
49	PSU	a	2100	49	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)
53	4SU	C	8	53	18,21,22	3.80	7 (38%)	25,30,33	2.30	5 (20%)
49	PSU	a	2639	49	18,21,22	1.08	2 (11%)	21,30,33	2.02	5 (23%)
49	OMU	a	2734	49	19,22,23	2.91	7 (36%)	25,31,34	1.85	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	A	509	1	-	2/7/25/26	0/3/3/3
1	5MC	A	1387	1	-	3/7/25/26	0/2/2/2
49	PSU	a	2762	49	-	0/7/25/26	0/2/2/2
49	5MC	a	2145	49	-	1/7/25/26	0/2/2/2
1	2MG	A	950	1	-	0/9/27/28	0/3/3/3
49	2MG	a	2627	49	-	1/9/27/28	0/3/3/3
49	2MA	a	2685	49,56	-	3/7/25/26	0/3/3/3
49	2MG	a	2018	49	-	0/9/27/28	0/3/3/3
49	PSU	a	1038	49	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1505	1	-	0/11/29/30	0/3/3/3
1	PSU	A	498	1,56	-	0/7/25/26	0/2/2/2
49	OMC	a	2680	49,56	-	0/9/27/28	0/2/2/2
1	5MC	A	1391	1	-	0/7/25/26	0/2/2/2
53	PSU	C	55	53	-	0/7/25/26	0/2/2/2
1	5MC	A	951	1	-	0/7/25/26	0/2/2/2
49	H2U	a	2631	49	-	0/7/38/39	0/2/2/2
49	OMG	a	2433	53,49	-	1/9/27/28	0/3/3/3
1	MA6	A	1506	1	-	2/11/29/30	0/3/3/3
1	2MG	A	1503	1	-	0/9/27/28	0/3/3/3
1	UR3	A	1485	1,56	-	0/7/25/26	0/2/2/2
49	5MU	a	2122	49	-	0/7/25/26	0/2/2/2
49	PSU	a	2094	49	-	0/7/25/26	0/2/2/2
49	PSU	a	2786	49	-	0/7/25/26	0/2/2/2
1	4OC	A	1389	1	-	1/9/29/30	0/2/2/2
1	5MC	A	1394	1	-	0/7/25/26	0/2/2/2
53	5MC	C	32	53	-	0/7/25/26	0/2/2/2
49	PSU	a	2787	49	-	0/7/25/26	0/2/2/2
49	3TD	a	2098	49	-	2/7/25/26	0/2/2/2
53	5MU	C	54	53	-	0/7/25/26	0/2/2/2
49	PSU	a	2686	49	-	0/7/25/26	0/2/2/2
49	PSU	a	2100	49	-	0/7/25/26	0/2/2/2
53	4SU	C	8	53	-	0/7/25/26	0/2/2/2
49	PSU	a	2639	49	-	0/7/25/26	0/2/2/2
49	OMU	a	2734	49	-	0/9/27/28	0/2/2/2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	a	2098	3TD	C6-C5	13.12	1.49	1.35
49	a	2685	2MA	C4-N3	10.71	1.48	1.34
49	a	2098	3TD	C2-N1	9.47	1.48	1.37
53	C	8	4SU	C2-N3	7.39	1.50	1.38
53	C	8	4SU	C2-N1	7.23	1.49	1.38
1	A	1485	UR3	C2-N1	7.19	1.48	1.38
1	A	1389	4OC	C4-N3	7.11	1.44	1.32
53	C	8	4SU	C4-N3	7.04	1.44	1.37
49	a	2734	OMU	C2-N1	6.90	1.49	1.38
49	a	2685	2MA	C2-N3	6.89	1.45	1.34
49	a	2685	2MA	C2-N1	6.86	1.45	1.34
1	A	509	G7M	C4-N3	6.68	1.49	1.34
49	a	2734	OMU	C2-N3	6.60	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	509	G7M	C2-N2	6.54	1.49	1.34
1	A	1389	4OC	C6-C5	6.24	1.49	1.35
53	C	8	4SU	C5-C4	6.15	1.49	1.42
1	A	1485	UR3	C6-C5	6.15	1.49	1.35
49	a	2098	3TD	C6-N1	6.14	1.46	1.36
1	A	1389	4OC	C2-N3	6.10	1.48	1.36
49	a	2734	OMU	C6-C5	5.79	1.48	1.35
1	A	509	G7M	C2-N3	5.66	1.46	1.33
53	C	8	4SU	C6-C5	5.61	1.48	1.35
1	A	1485	UR3	C2-N3	4.92	1.48	1.39
53	C	8	4SU	C4-S4	-4.83	1.60	1.68
49	a	2098	3TD	C2-N3	4.77	1.48	1.38
49	a	2685	2MA	C5-C6	4.66	1.54	1.41
49	a	2685	2MA	C6-N1	4.53	1.41	1.35
1	A	509	G7M	C5-N7	-4.48	1.34	1.39
1	A	1389	4OC	C4-N4	4.44	1.45	1.36
1	A	1389	4OC	C2-N1	4.04	1.48	1.40
53	C	55	PSU	C6-C5	3.79	1.39	1.35
1	A	509	G7M	C5-C6	3.77	1.53	1.43
49	a	2100	PSU	C6-C5	3.76	1.39	1.35
1	A	1389	4OC	C5-C4	3.69	1.49	1.41
49	a	2094	PSU	C6-C5	3.68	1.39	1.35
49	a	2734	OMU	C4-N3	3.47	1.44	1.38
49	a	2685	2MA	C6-N6	-3.43	1.25	1.34
49	a	2686	PSU	C6-C5	3.43	1.39	1.35
1	A	498	PSU	C6-C5	3.36	1.39	1.35
49	a	2762	PSU	C6-C5	3.33	1.39	1.35
1	A	1506	MA6	C6-N6	3.30	1.45	1.36
49	a	2786	PSU	C6-C5	3.30	1.38	1.35
49	a	2787	PSU	C6-C5	3.24	1.38	1.35
1	A	1505	MA6	C6-N6	3.20	1.45	1.36
49	a	1038	PSU	C6-C5	3.17	1.38	1.35
49	a	2639	PSU	C6-C5	3.11	1.38	1.35
1	A	1389	4OC	C6-N1	3.07	1.45	1.38
1	A	1506	MA6	C5-C4	-3.04	1.33	1.39
1	A	1505	MA6	C5-C4	-3.00	1.33	1.39
49	a	2098	3TD	C4-N3	2.98	1.46	1.40
1	A	1485	UR3	C6-N1	2.91	1.45	1.38
1	A	509	G7M	C2-N1	2.91	1.44	1.37
49	a	2734	OMU	O2-C2	-2.84	1.18	1.23
1	A	1505	MA6	C5-N7	-2.82	1.33	1.39
49	a	2685	2MA	C5-N7	-2.79	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	509	G7M	C6-N1	2.79	1.44	1.38
1	A	1389	4OC	O2-C2	-2.77	1.18	1.23
1	A	1506	MA6	C5-N7	-2.77	1.34	1.39
49	a	2734	OMU	O4-C4	-2.77	1.19	1.24
53	C	8	4SU	C6-N1	2.74	1.44	1.38
49	a	2685	2MA	C8-N7	2.71	1.36	1.31
1	A	509	G7M	O6-C6	-2.59	1.18	1.23
1	A	1506	MA6	C8-N9	-2.53	1.33	1.37
1	A	1485	UR3	C4-N3	2.46	1.45	1.40
1	A	1505	MA6	C8-N9	-2.38	1.33	1.37
1	A	1485	UR3	O4-C4	-2.28	1.18	1.23
1	A	1485	UR3	C5-C4	2.22	1.49	1.43
49	a	2098	3TD	O4-C4	-2.20	1.18	1.23
1	A	1485	UR3	O2-C2	-2.15	1.18	1.22
49	a	2762	PSU	C4-C5	-2.09	1.38	1.44
1	A	509	G7M	C8-N7	2.06	1.36	1.33
49	a	2734	OMU	C5-C4	2.06	1.48	1.43
1	A	498	PSU	C4-C5	-2.04	1.38	1.44
49	a	2639	PSU	C4-C5	-2.01	1.38	1.44

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1506	MA6	N1-C6-N6	-16.56	96.68	116.86
1	A	1505	MA6	N1-C6-N6	-15.80	97.60	116.86
1	A	1506	MA6	C5-C6-N6	11.67	143.80	125.33
1	A	1505	MA6	C5-C6-N6	11.10	142.90	125.33
53	C	8	4SU	C4-N3-C2	-7.91	119.73	127.31
1	A	1505	MA6	C4-N9-C1'	-7.67	108.69	126.63
1	A	1506	MA6	C4-N9-C1'	-7.37	109.40	126.63
1	A	1505	MA6	C1'-N9-C8	7.04	142.72	127.09
1	A	1506	MA6	C1'-N9-C8	6.74	142.06	127.09
49	a	2685	2MA	C5-C4-N3	-6.40	120.44	127.18
49	a	2734	OMU	C4-N3-C2	-5.81	119.40	126.61
49	a	2098	3TD	N1-C2-N3	5.73	120.30	116.13
1	A	1506	MA6	N1-C2-N3	-5.60	120.10	128.58
1	A	1485	UR3	C4-N3-C2	-5.51	120.14	124.58
49	a	1038	PSU	C4-N3-C2	-5.51	118.78	126.37
1	A	1505	MA6	N1-C2-N3	-5.47	120.30	128.58
1	A	1506	MA6	C5-C4-N3	-5.44	119.23	126.72
53	C	8	4SU	C5-C4-N3	5.39	119.76	114.75
49	a	2639	PSU	N1-C2-N3	5.09	120.53	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1505	MA6	C5-C4-N3	-5.07	119.74	126.72
1	A	498	PSU	C4-N3-C2	-5.06	119.41	126.37
49	a	2786	PSU	C4-N3-C2	-5.05	119.41	126.37
49	a	2787	PSU	C4-N3-C2	-5.02	119.46	126.37
49	a	1038	PSU	N1-C2-N3	4.98	120.42	115.17
49	a	2762	PSU	C4-N3-C2	-4.96	119.53	126.37
49	a	2639	PSU	C4-N3-C2	-4.89	119.64	126.37
49	a	2786	PSU	N1-C2-N3	4.88	120.31	115.17
49	a	2686	PSU	C4-N3-C2	-4.87	119.66	126.37
49	a	2686	PSU	N1-C2-N3	4.85	120.28	115.17
1	A	498	PSU	N1-C2-N3	4.84	120.27	115.17
49	a	2094	PSU	C4-N3-C2	-4.83	119.72	126.37
49	a	2762	PSU	N1-C2-N3	4.82	120.25	115.17
53	C	55	PSU	C4-N3-C2	-4.82	119.73	126.37
49	a	2094	PSU	N1-C2-N3	4.79	120.22	115.17
49	a	2100	PSU	C4-N3-C2	-4.78	119.78	126.37
49	a	2787	PSU	N1-C2-N3	4.77	120.20	115.17
53	C	55	PSU	N1-C2-N3	4.74	120.17	115.17
49	a	2100	PSU	N1-C2-N3	4.70	120.12	115.17
1	A	1506	MA6	C4-C5-C6	4.61	120.68	115.91
1	A	1505	MA6	C4-C5-C6	4.57	120.63	115.91
1	A	509	G7M	C2-N3-C4	4.55	120.14	112.30
49	a	2685	2MA	N9-C8-N7	-4.38	107.72	113.94
1	A	1506	MA6	N9-C8-N7	-4.35	107.77	113.94
1	A	1505	MA6	N9-C8-N7	-4.23	107.94	113.94
49	a	2098	3TD	C4-N3-C2	-4.15	120.22	124.61
1	A	509	G7M	C5-C4-N3	-4.07	120.45	128.15
1	A	509	G7M	C5-C6-N1	4.07	120.26	111.84
49	a	2734	OMU	N3-C2-N1	3.87	119.93	114.89
53	C	8	4SU	C5-C4-S4	-3.86	119.90	124.31
53	C	8	4SU	N3-C2-N1	3.81	119.85	114.89
49	a	2734	OMU	C5-C4-N3	3.77	120.08	114.80
1	A	1506	MA6	N3-C4-N9	3.69	133.44	127.17
49	a	2685	2MA	N3-C4-N9	3.64	131.61	126.99
1	A	1485	UR3	C5-C4-N3	3.59	119.76	115.04
1	A	1505	MA6	N3-C4-N9	3.54	133.19	127.17
1	A	509	G7M	O6-C6-C5	-3.48	120.24	128.01
1	A	1506	MA6	C2-N3-C4	3.46	120.29	111.83
1	A	1506	MA6	C2-N1-C6	3.42	120.18	111.83
49	a	2631	H2U	C5-C4-N3	-3.41	113.06	116.69
1	A	1505	MA6	C2-N1-C6	3.38	120.08	111.83
49	a	2685	2MA	N3-C2-N1	-3.32	119.92	125.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1505	MA6	C2-N3-C4	3.25	119.76	111.83
1	A	509	G7M	C2-N1-C6	-3.14	119.42	125.11
1	A	509	G7M	N9-C4-N3	3.11	132.17	125.95
1	A	1506	MA6	C5-N7-C8	2.99	108.15	103.45
49	a	2734	OMU	O4-C4-C5	-2.98	120.02	125.16
49	a	2639	PSU	O2-C2-N1	-2.91	119.78	122.79
49	a	2685	2MA	C5-N7-C8	2.90	108.00	103.45
49	a	2686	PSU	O2-C2-N1	-2.84	119.86	122.79
49	a	2094	PSU	O2-C2-N1	-2.79	119.91	122.79
53	C	55	PSU	O2-C2-N1	-2.77	119.93	122.79
1	A	1505	MA6	C5-N7-C8	2.77	107.80	103.45
1	A	498	PSU	O2-C2-N1	-2.75	119.95	122.79
1	A	1505	MA6	C4-N9-C8	2.72	108.59	105.74
1	A	1506	MA6	C4-N9-C8	2.68	108.55	105.74
49	a	2639	PSU	C6-N1-C2	-2.67	120.21	122.69
49	a	2762	PSU	O2-C2-N1	-2.67	120.04	122.79
49	a	2786	PSU	O2-C2-N1	-2.61	120.10	122.79
49	a	2100	PSU	O2-C2-N1	-2.60	120.10	122.79
49	a	2639	PSU	C6-C5-C4	2.57	119.91	118.17
49	a	2685	2MA	C4-N9-C8	2.49	108.35	105.74
49	a	2787	PSU	O2-C2-N1	-2.46	120.25	122.79
49	a	2686	PSU	C6-N1-C2	-2.43	120.43	122.69
1	A	509	G7M	CN7-N7-C5	2.43	129.82	126.80
49	a	2094	PSU	C6-N1-C2	-2.42	120.45	122.69
49	a	2098	3TD	C6-C5-C4	2.41	119.81	118.19
49	a	1038	PSU	O2-C2-N1	-2.36	120.35	122.79
49	a	2762	PSU	C6-N1-C2	-2.35	120.51	122.69
1	A	498	PSU	C6-N1-C2	-2.34	120.52	122.69
49	a	2786	PSU	C6-C5-C4	2.33	119.75	118.17
53	C	55	PSU	C6-N1-C2	-2.33	120.53	122.69
49	a	2762	PSU	C6-C5-C4	2.31	119.73	118.17
49	a	2685	2MA	C4-C5-N7	-2.28	107.97	110.58
1	A	509	G7M	N9-C8-N7	-2.26	107.00	112.48
49	a	2786	PSU	C6-N1-C2	-2.24	120.61	122.69
49	a	2685	2MA	N6-C6-N1	2.23	120.04	117.03
49	a	2100	PSU	C6-N1-C2	-2.22	120.63	122.69
1	A	1389	4OC	C6-C5-C4	2.22	119.67	117.00
49	a	2734	OMU	O2-C2-N1	-2.20	119.93	122.80
49	a	2787	PSU	C6-N1-C2	-2.16	120.69	122.69
49	a	2094	PSU	C6-C5-C4	2.15	119.62	118.17
1	A	1485	UR3	C6-N1-C2	-2.14	120.05	121.80
53	C	8	4SU	O2-C2-N1	-2.11	120.05	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	C	55	PSU	C6-C5-C4	2.10	119.59	118.17
1	A	498	PSU	C6-C5-C4	2.10	119.59	118.17
1	A	498	PSU	O4'-C1'-C2'	2.09	108.04	105.15
49	a	2098	3TD	C1'-C5-C4	2.08	120.77	117.61
1	A	1506	MA6	C4-C5-N7	-2.08	108.21	110.58
49	a	2685	2MA	CM2-C2-N1	2.08	120.23	117.13
1	A	509	G7M	CN7-N7-C8	-2.03	121.71	124.79
1	A	1485	UR3	C1'-N1-C2	2.02	120.34	117.04

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1387	5MC	O4'-C4'-C5'-O5'
1	A	1506	MA6	O4'-C4'-C5'-O5'
49	a	2098	3TD	O4'-C4'-C5'-O5'
49	a	2433	OMG	C1'-C2'-O2'-CM2
49	a	2098	3TD	C3'-C4'-C5'-O5'
1	A	1387	5MC	C3'-C4'-C5'-O5'
1	A	1506	MA6	C3'-C4'-C5'-O5'
49	a	2685	2MA	O4'-C4'-C5'-O5'
49	a	2685	2MA	C3'-C4'-C5'-O5'
1	A	509	G7M	C3'-C4'-C5'-O5'
49	a	2627	2MG	C3'-C4'-C5'-O5'
1	A	1389	4OC	O4'-C4'-C5'-O5'
1	A	1387	5MC	C4'-C5'-O5'-P
1	A	509	G7M	C4'-C5'-O5'-P
49	a	2685	2MA	O4'-C1'-N9-C8
49	a	2145	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1387	5MC	1	0
49	a	2145	5MC	2	0
49	a	2627	2MG	1	0
49	a	2685	2MA	1	0
1	A	1505	MA6	1	0
1	A	1391	5MC	1	0
49	a	2433	OMG	1	0

Continued on next page...

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1506	MA6	4	0
1	A	1503	2MG	2	0
49	a	2100	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 393 ligands modelled in this entry, 391 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	V7A	A	1601	56	37,38,38	1.25	2 (5%)	43,60,60	2.22	6 (13%)
55	V7A	a	3101	-	37,38,38	1.05	2 (5%)	43,60,60	0.89	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	V7A	A	1601	56	-	5/13/72/72	0/4/4/4
55	V7A	a	3101	-	-	8/13/72/72	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	1601	V7A	CBC-NBD	6.21	1.51	1.33
55	a	3101	V7A	CBC-NBD	4.99	1.47	1.33
55	A	1601	V7A	OAY-CAH	2.37	1.28	1.23
55	a	3101	V7A	OAY-CAH	2.24	1.27	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A	1601	V7A	CAH-CAI-CAL	9.09	125.99	118.80
55	A	1601	V7A	CAP-CAM-CAL	7.95	119.19	109.88
55	A	1601	V7A	CBC-CAQ-CAP	3.29	124.86	120.97
55	A	1601	V7A	OBA-CAM-CAL	-2.63	105.94	110.14
55	A	1601	V7A	CAQ-CBC-NBD	2.53	123.80	118.64
55	a	3101	V7A	CAM-CAP-CAQ	2.46	119.65	115.75
55	A	1601	V7A	OBE-CBC-NBD	-2.36	117.59	122.89
55	a	3101	V7A	CAP-CAM-CAL	2.09	112.33	109.88

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	1601	V7A	CAA-CAS-NAT-OAU
55	A	1601	V7A	CAW-NAT-OAU-CAV
55	a	3101	V7A	CAN-CAO-NBF-CBH
55	a	3101	V7A	CAP-CAQ-CBC-OBE
55	a	3101	V7A	CAR-CAQ-CBC-NBD
55	a	3101	V7A	CAR-CAQ-CBC-OBE
55	a	3101	V7A	CAA-CAS-NAT-CAW
55	a	3101	V7A	CAA-CAS-NAT-OAU
55	a	3101	V7A	CAW-NAT-OAU-CAV
55	a	3101	V7A	CAP-CAQ-CBC-NBD
55	A	1601	V7A	CAF-CAA-CAS-NAT
55	A	1601	V7A	CAA-CAS-NAT-CAW
55	A	1601	V7A	CAN-CAO-NBF-CBG

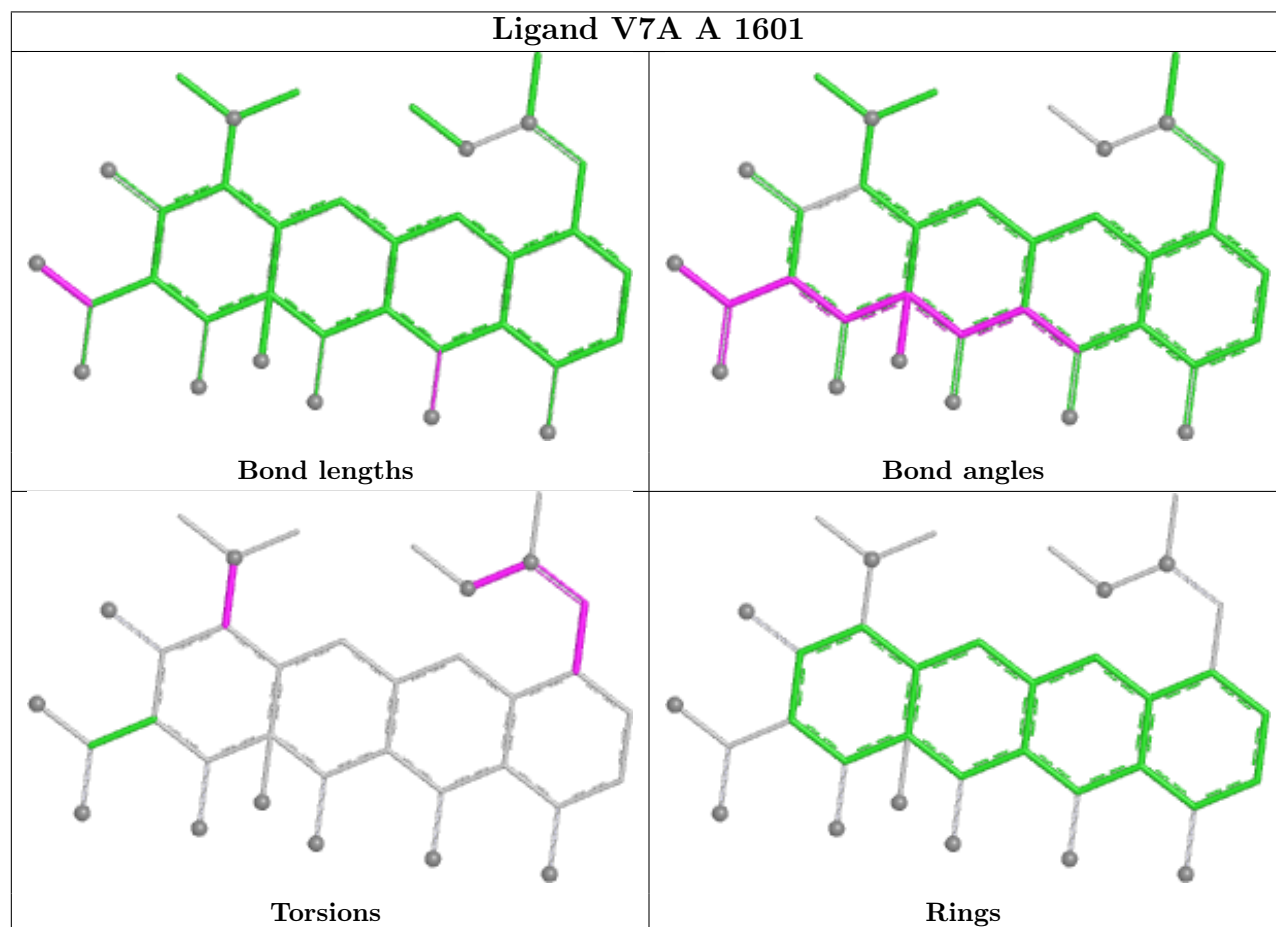
There are no ring outliers.

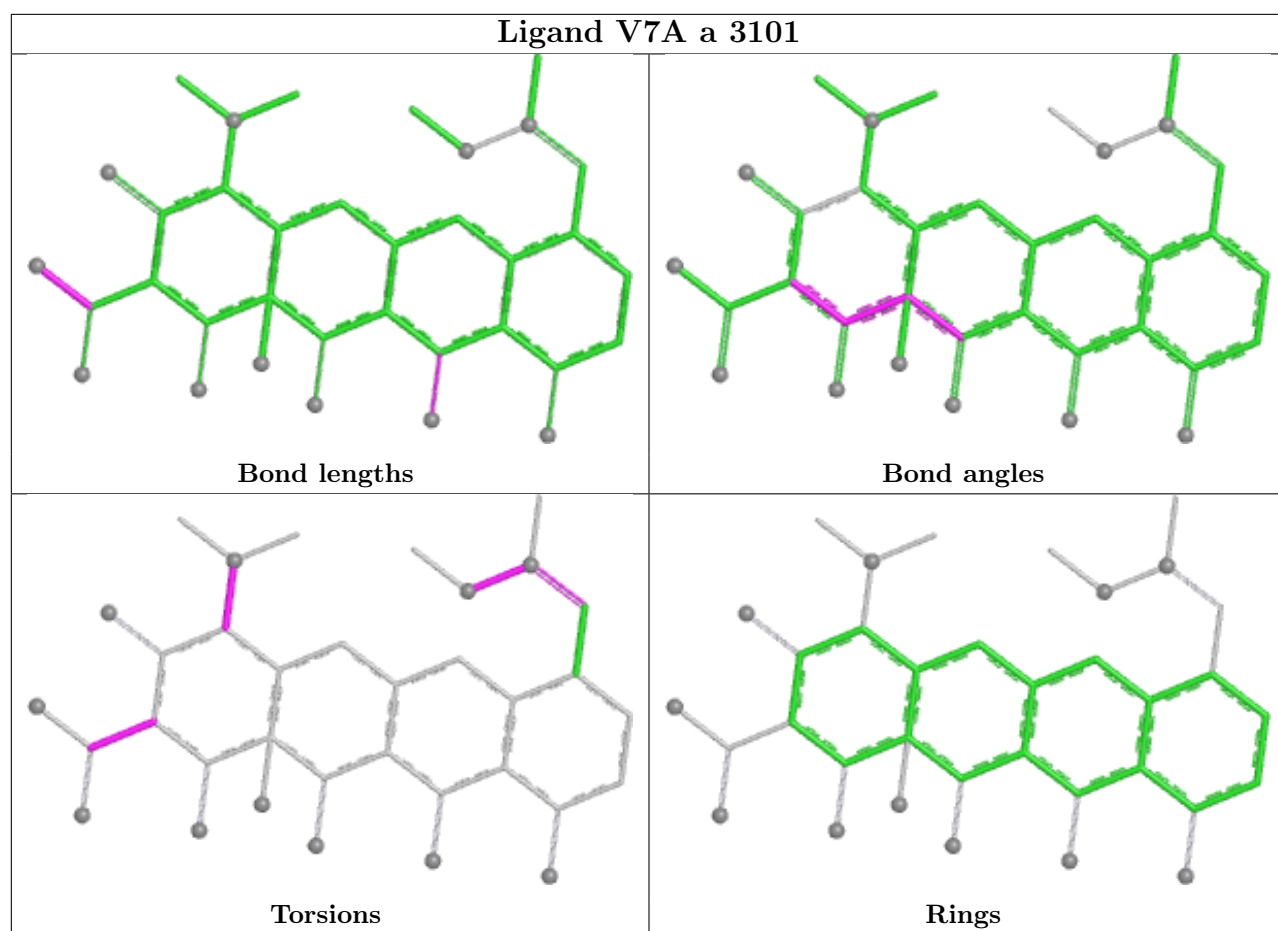
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	a	3101	V7A	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

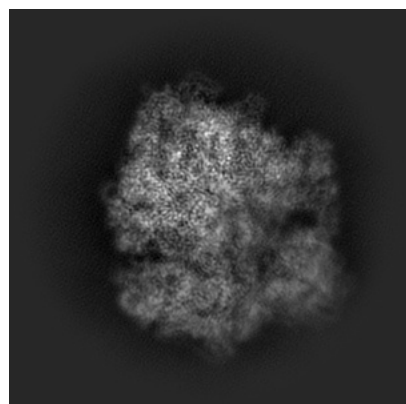
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26959. These allow visual inspection of the internal detail of the map and identification of artifacts.

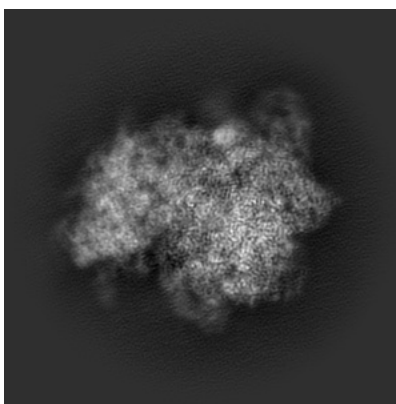
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

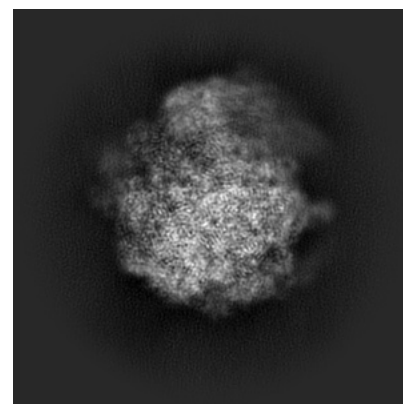
6.1.1 Primary map



X

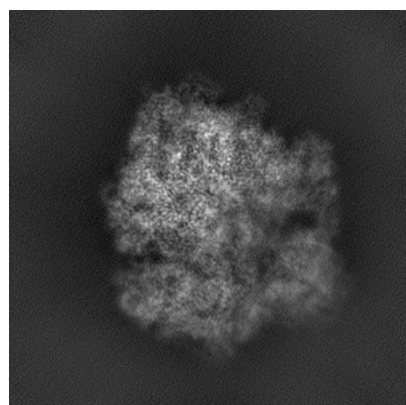


Y

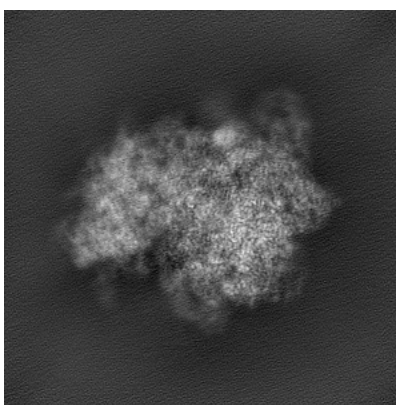


Z

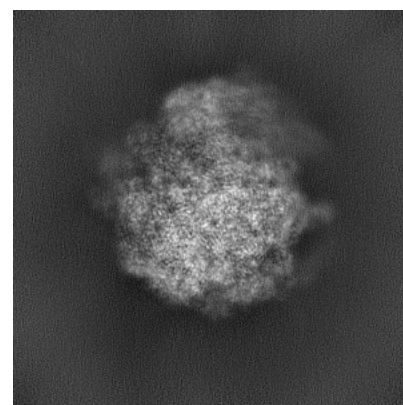
6.1.2 Raw map



X



Y

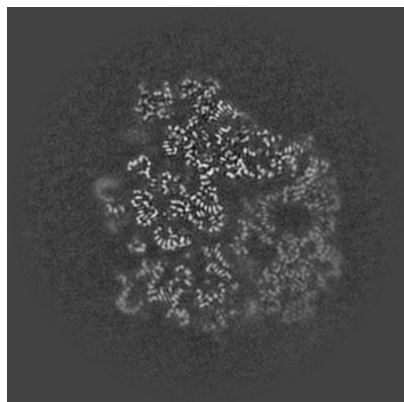


Z

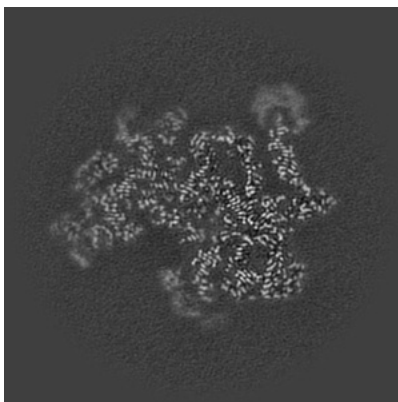
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

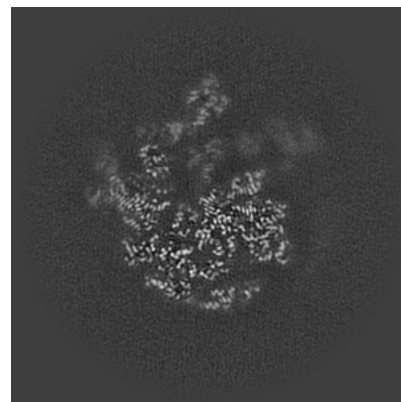
6.2.1 Primary map



X Index: 170

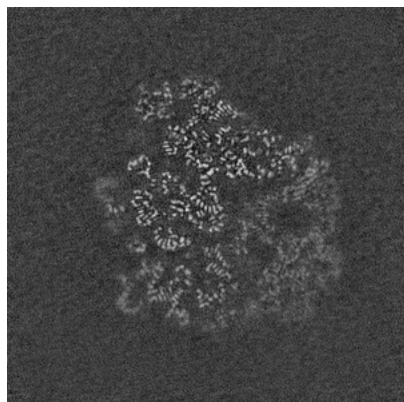


Y Index: 170

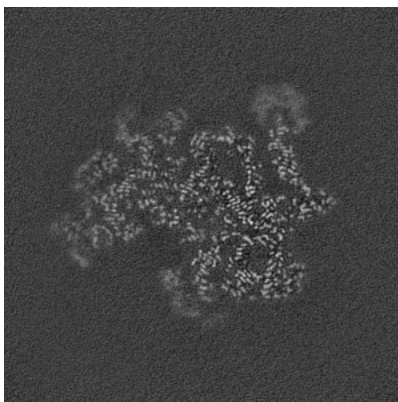


Z Index: 170

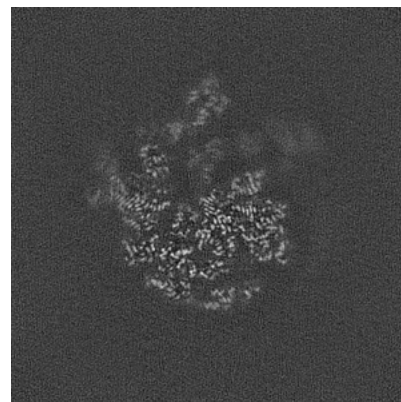
6.2.2 Raw map



X Index: 170



Y Index: 170

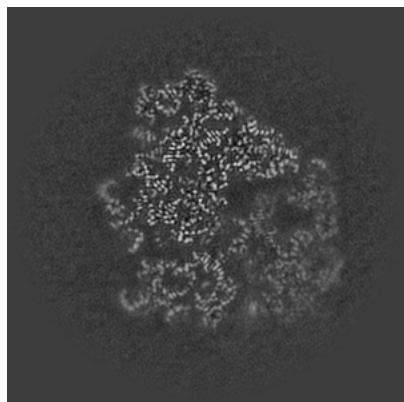


Z Index: 170

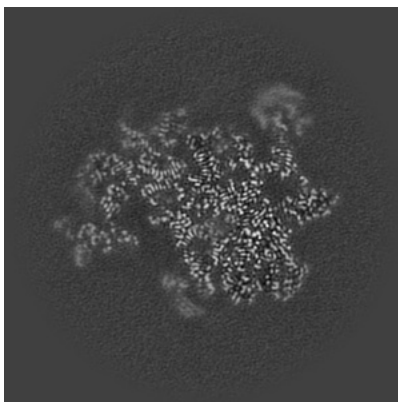
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

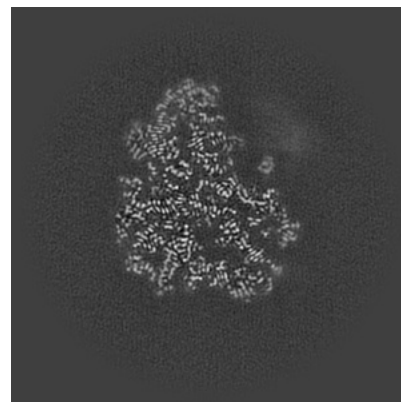
6.3.1 Primary map



X Index: 175

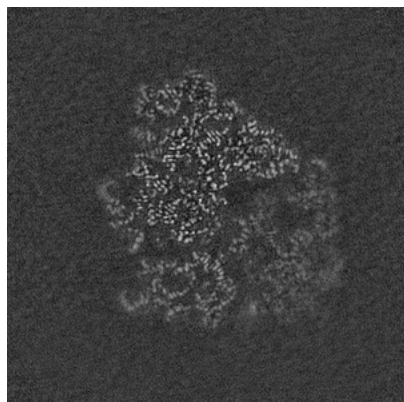


Y Index: 165

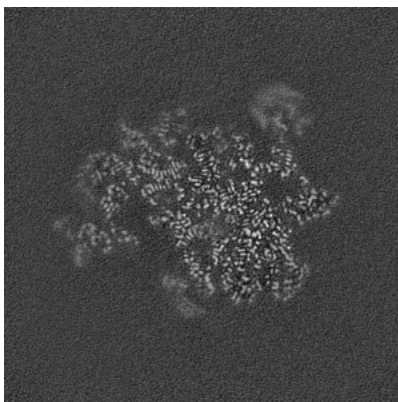


Z Index: 203

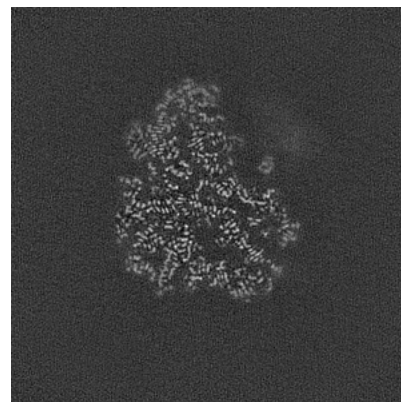
6.3.2 Raw map



X Index: 175



Y Index: 165

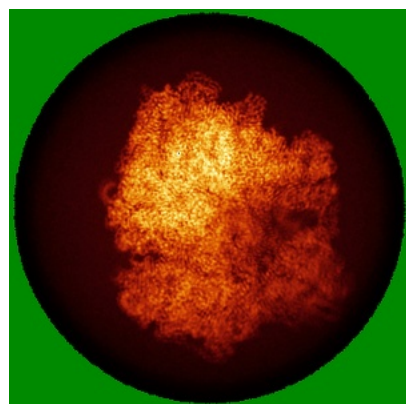


Z Index: 203

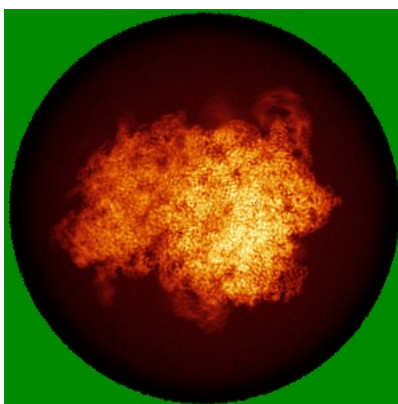
The images above show the largest variance slices of the map in three orthogonal directions.

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

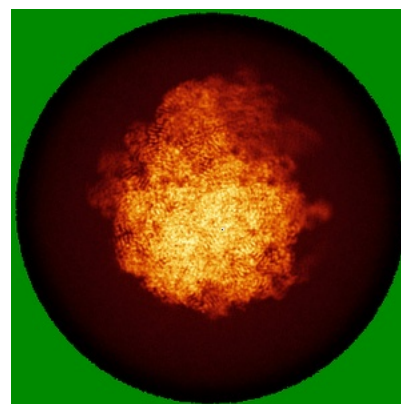
6.4.1 Primary map



X

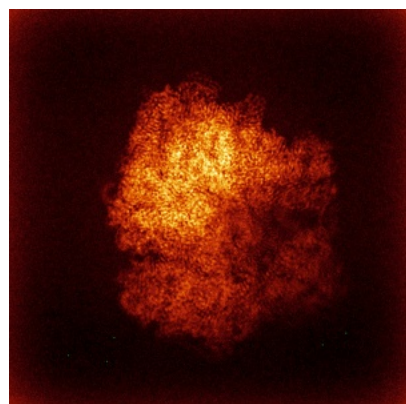


Y

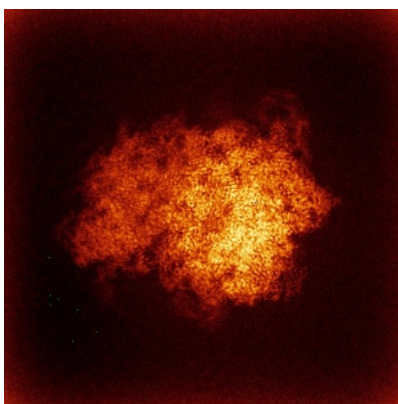


Z

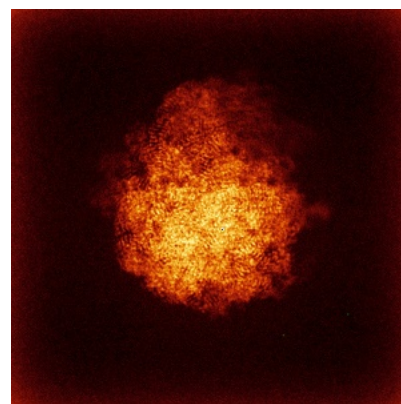
6.4.2 Raw map



X



Y

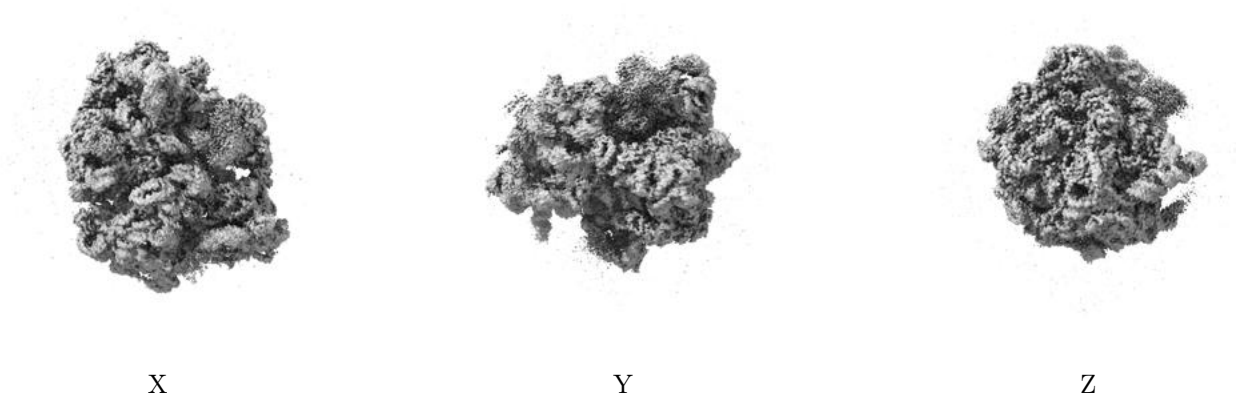


Z

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

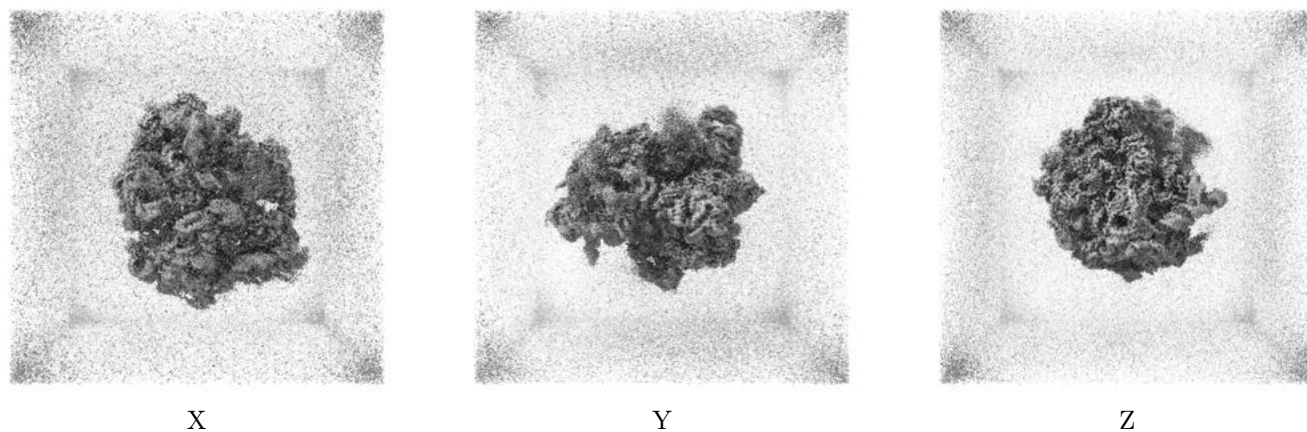
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

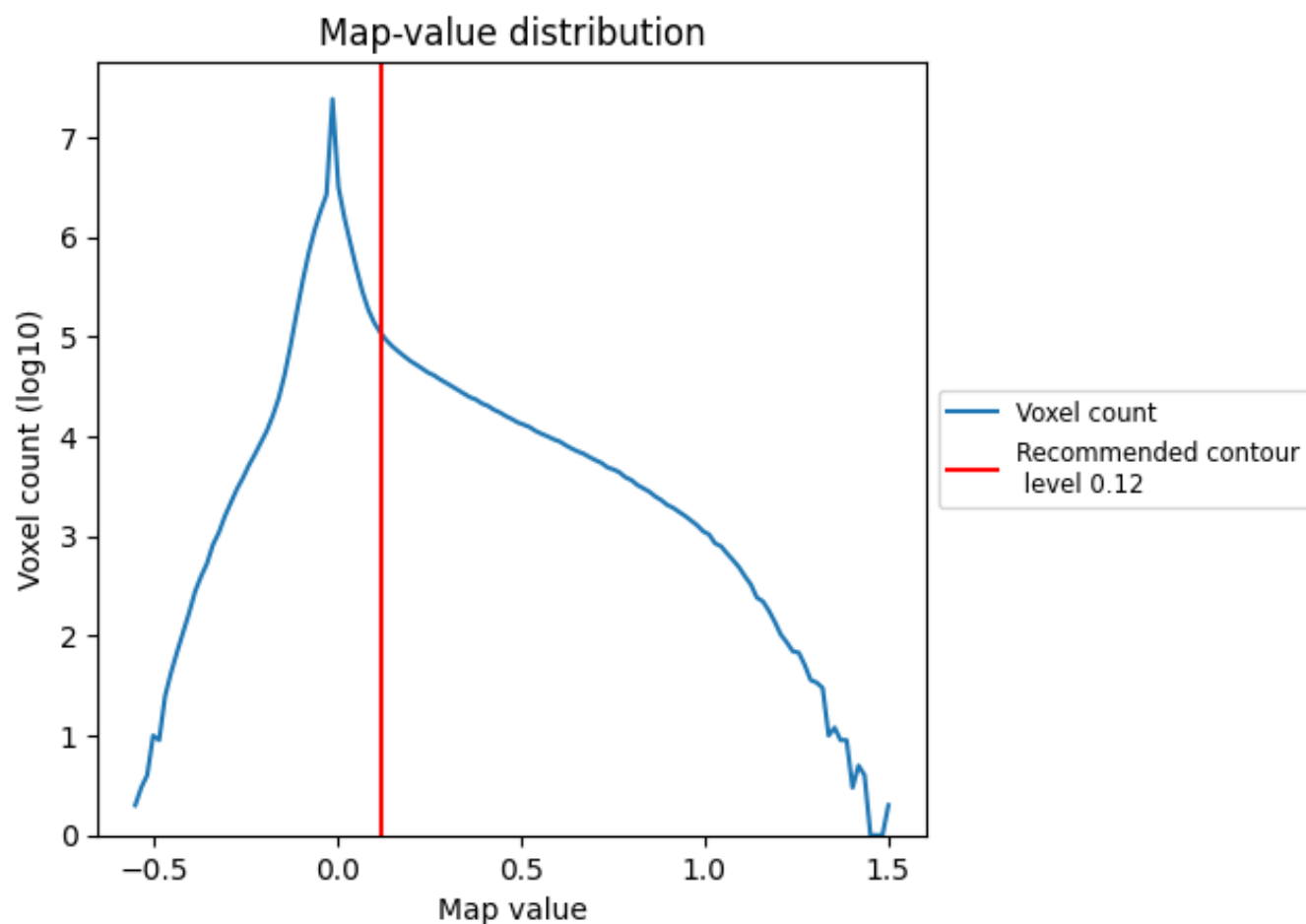
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

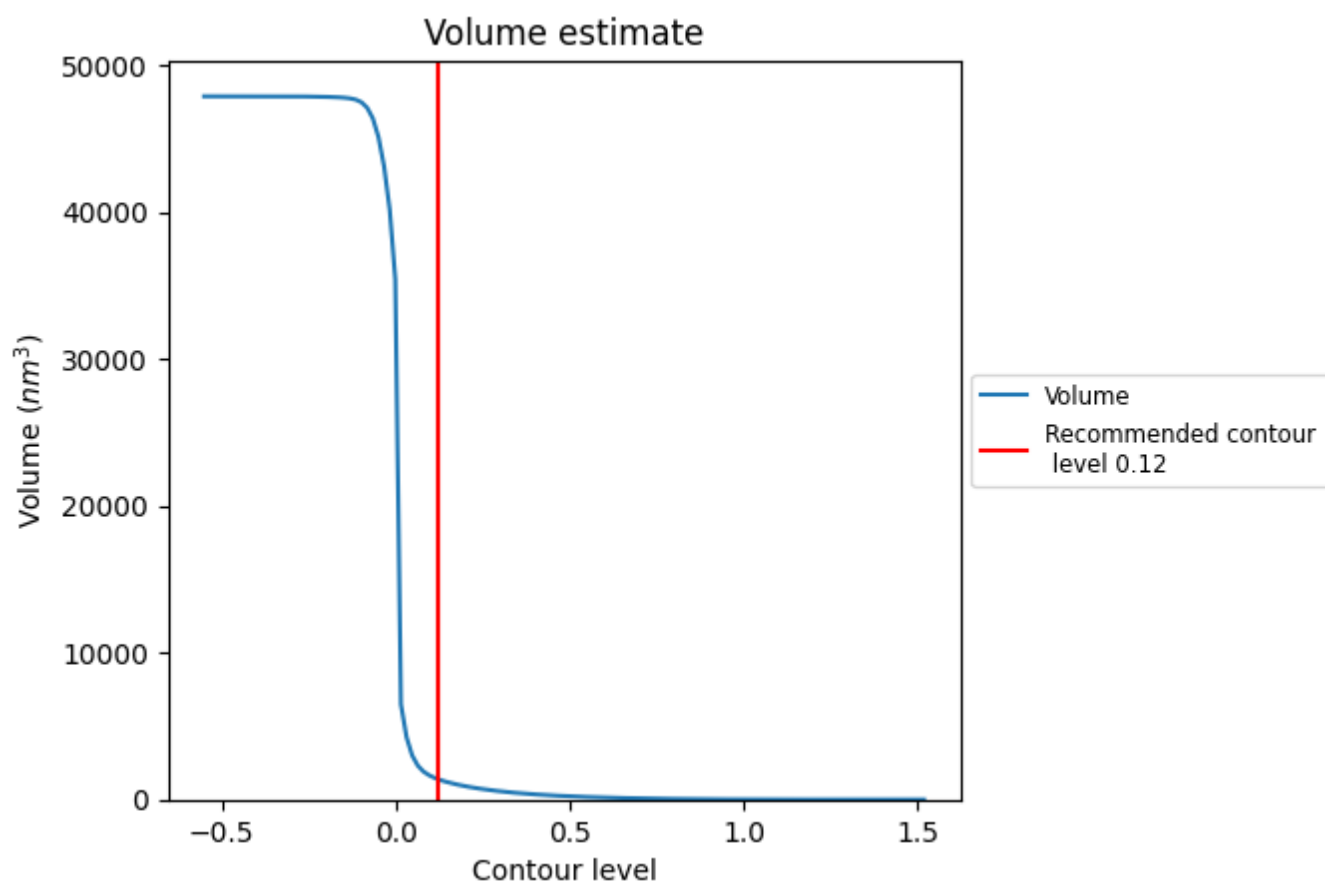
This section contains the results of statistical analysis of the map.

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.

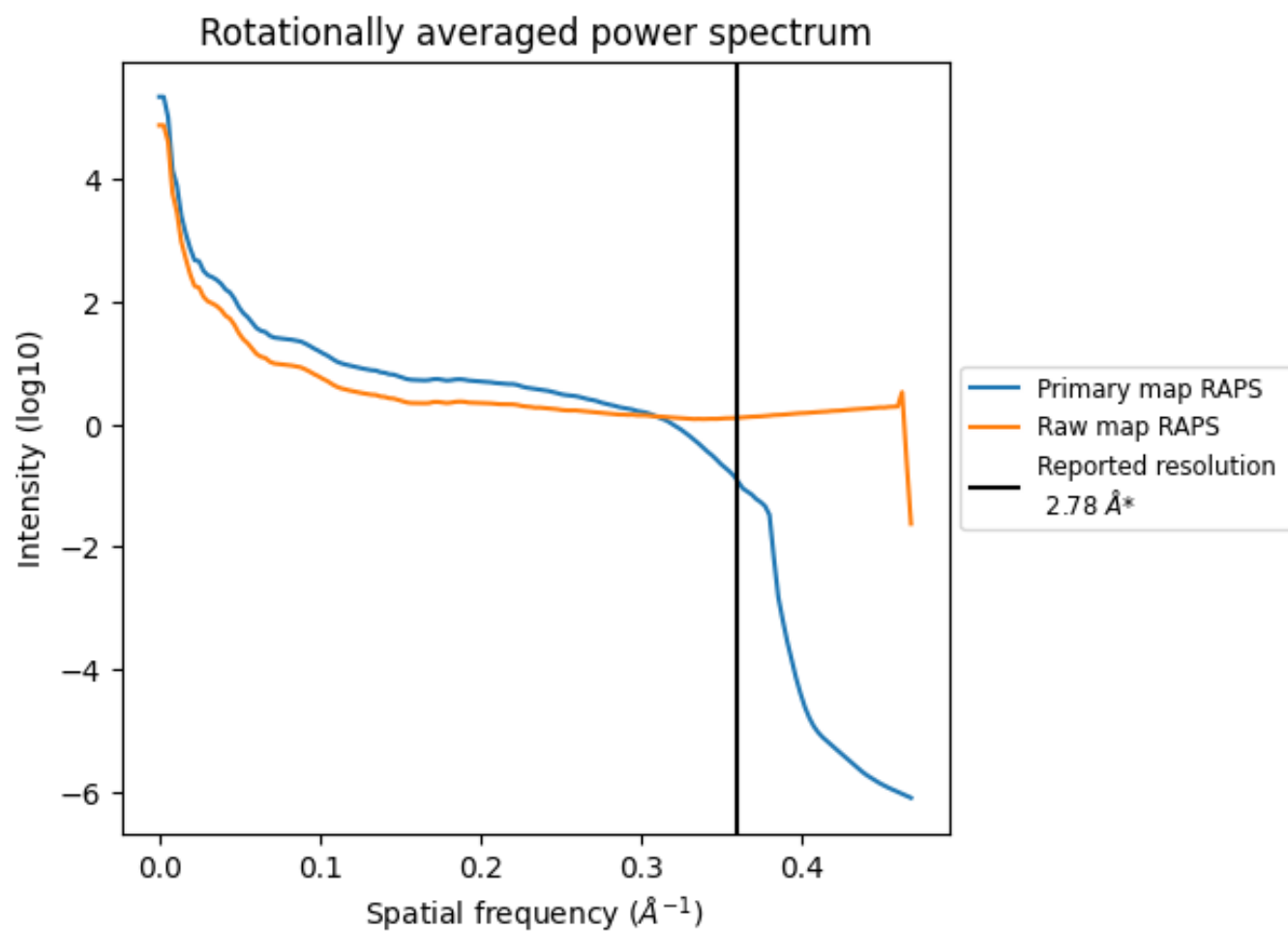
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1399 nm³; this corresponds to an approximate mass of 1263 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 ⓘ

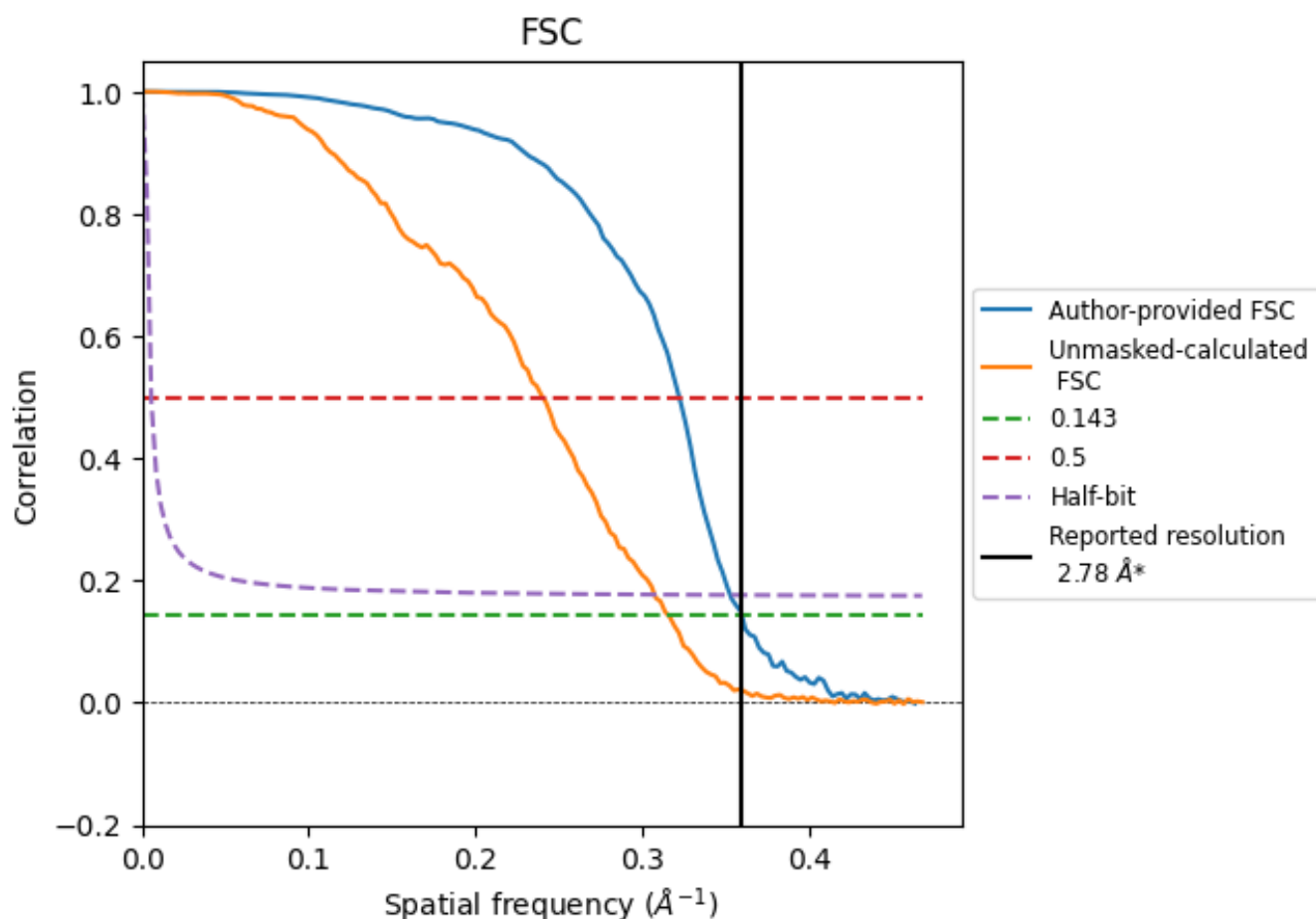


*Reported resolution corresponds to spatial frequency of $0.360 \text{ \AA}^{-1}$

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 0.360 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.10	2.83
Unmasked-calculated*	3.17	4.16	3.25

*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 3.17 differs from the reported value 2.78 by more than 10 %

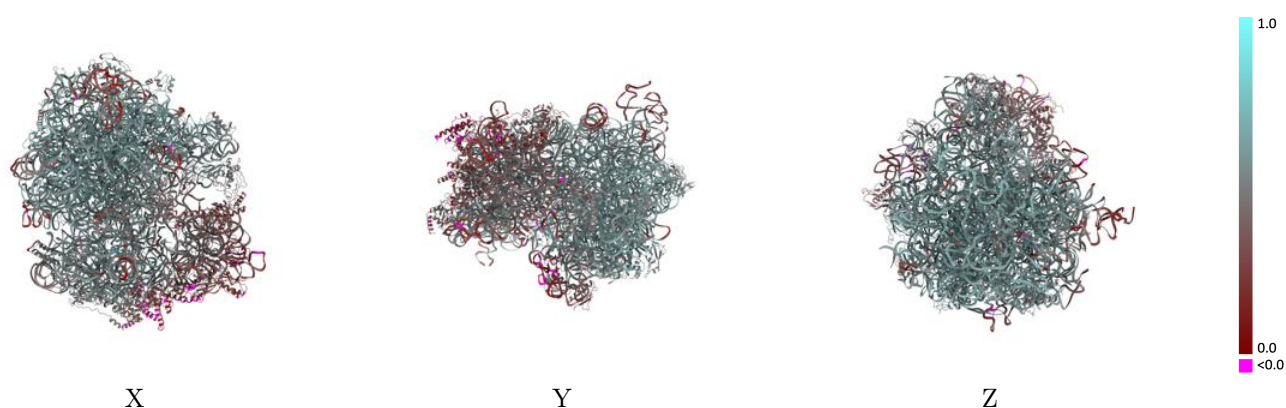
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26959 and PDB model 8CRX. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

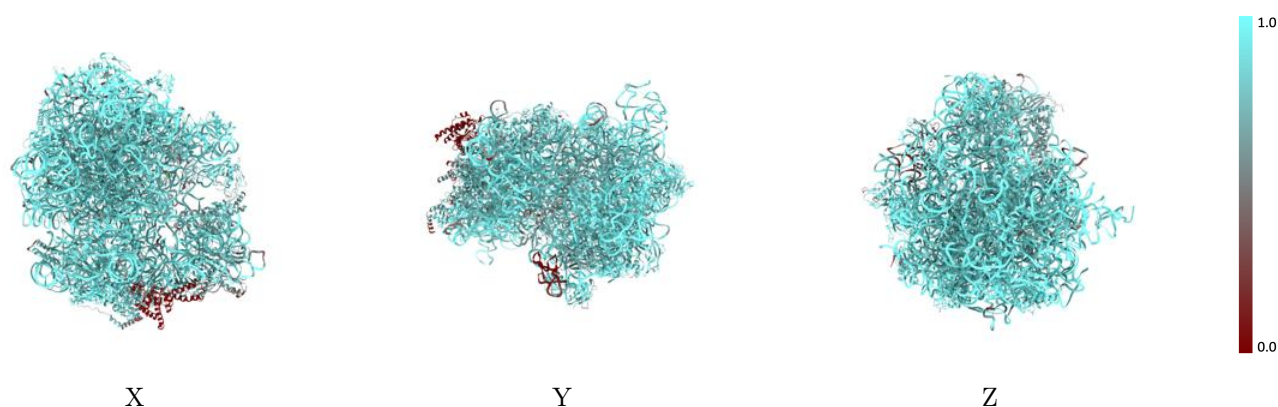
This section was not generated.

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



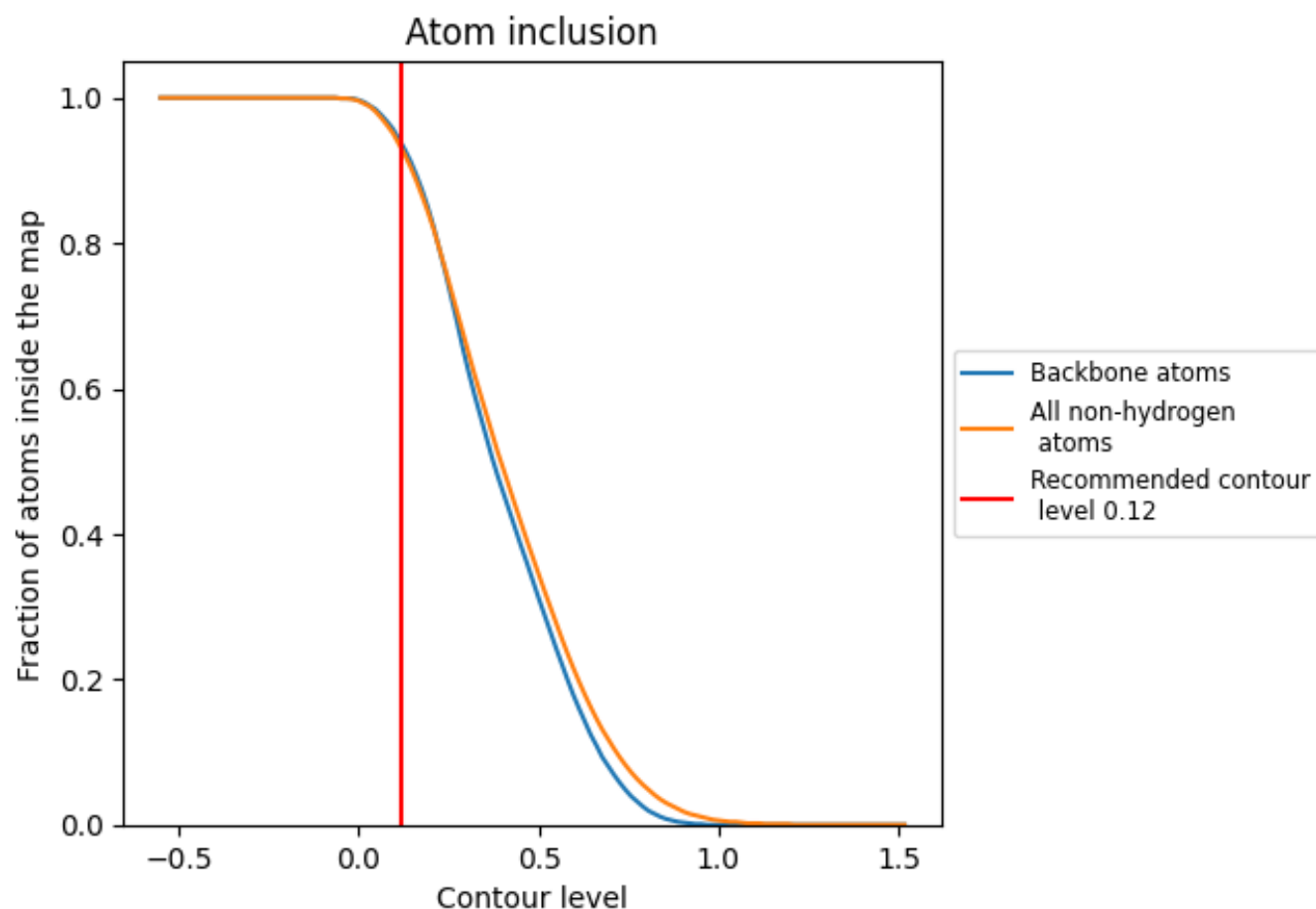
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.5190
0	 0.9260	 0.5600
1	 0.9790	 0.6190
2	 0.9760	 0.6050
3	 0.5750	 0.4940
4	 0.6410	 0.3670
A	 0.9670	 0.4880
B	 0.0710	 0.1600
C	 0.8760	 0.4990
D	 0.8780	 0.4550
E	 0.8540	 0.4620
F	 0.8530	 0.3820
G	 0.7280	 0.3440
H	 0.9270	 0.5190
I	 0.7330	 0.3060
J	 0.7540	 0.2820
K	 0.8900	 0.4290
L	 0.9110	 0.5300
M	 0.6180	 0.2970
N	 0.7460	 0.3380
O	 0.8990	 0.4870
P	 0.8130	 0.4330
Q	 0.8760	 0.4990
R	 0.8030	 0.4040
S	 0.7980	 0.3910
T	 0.9020	 0.4950
U	 0.7700	 0.3380
V	 0.9650	 0.6190
X	 0.8530	 0.5450
Y	 0.7110	 0.3600
a	 0.9670	 0.5610
b	 0.9970	 0.5580
c	 0.9700	 0.5940
d	 0.9730	 0.5900
e	 0.9430	 0.5450



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Chain	Atom inclusion	Q-score
f	 0.9140	 0.4730
g	 0.8580	 0.4050
i	 0.9790	 0.5990
j	 0.9480	 0.5740
k	 0.9510	 0.5700
l	 0.9640	 0.5890
m	 0.9640	 0.5870
n	 0.9410	 0.5310
o	 0.9410	 0.5680
p	 0.9690	 0.5990
q	 0.9420	 0.5720
r	 0.9600	 0.5900
s	 0.9560	 0.5700
t	 0.9630	 0.5560
u	 0.7710	 0.4720
v	 0.9610	 0.5980
w	 0.9850	 0.6060
x	 0.9340	 0.5420
y	 0.9670	 0.5880
z	 0.9630	 0.5980