



Full wwPDB EM Validation Report ⓘ

May 4, 2026 – 11:30 AM EDT

PDB ID : 9PJ8 / pdb_00009pj8
EMDB ID : EMD-71683
Title : C. acnes 70S ribosome bound to Sarecycline
Authors : Devarkar, S.C.; Lomakin, I.B.; Bunick, C.G.
Deposited on : 2025-07-12
Resolution : 2.50 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:

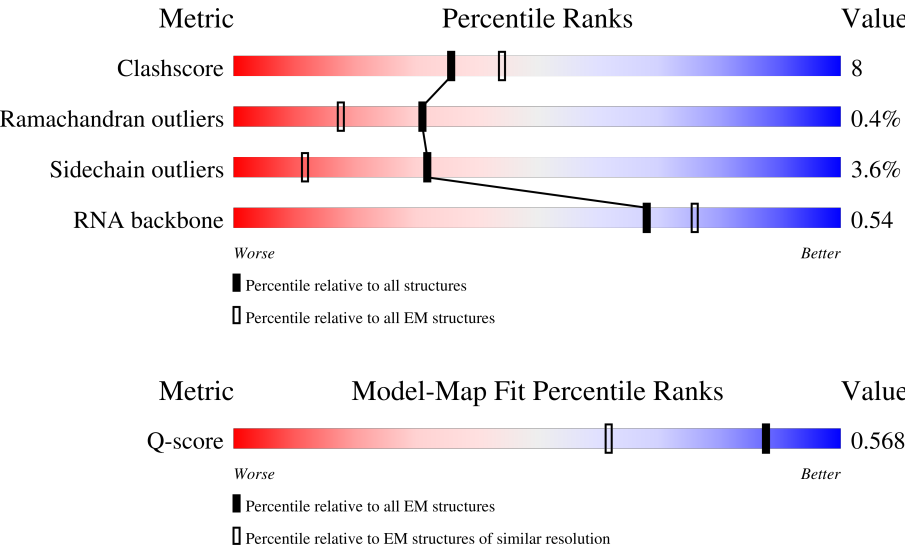
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.50 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	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	0	56	
2	1	44	
3	2	68	

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Mol	Chain	Length	Quality of chain
4	3	37	
5	4	69	
6	A	1537	
7	B	283	
8	C	77	
9	D	201	
10	E	215	
11	F	96	
12	G	269	
13	H	135	
14	I	156	
15	J	173	
16	K	135	
17	L	123	
18	M	103	
19	N	123	
20	O	87	
21	P	147	
22	Q	90	
23	R	79	
24	S	61	
25	T	88	
26	U	93	
27	V	24	
28	X	33	

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Mol	Chain	Length	Quality of chain
29	Y	22	
30	a	3086	
31	b	120	
32	c	278	
33	d	223	
34	e	301	
35	f	210	
36	g	180	
37	i	147	
38	j	122	
39	k	146	
40	l	139	
41	m	187	
42	n	127	
43	o	117	
44	p	123	
45	q	102	
46	r	153	
47	s	102	
48	t	122	
49	u	205	
50	v	89	
51	w	61	
52	x	77	
53	y	60	

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Mol	Chain	Length	Quality of chain
54	z	63	<div><div></div><div>78%</div><div>21%</div><div></div></div>

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 144415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	50	Total	C	N	O	S	0	0
			423	253	91	73	6		

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

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

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	67	Total	C	N	O	S	0	0
			513	315	110	87	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	37	Total	C	N	O	S	0	0
			302	184	66	47	5		

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

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

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

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

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

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

- Molecule 8 is a RNA chain called initiator tRNA Met (76-MER).

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

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

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

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

- Molecule 11 is a protein called 30S ribosomal protein S6.

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

- Molecule 12 is a protein called 30S ribosomal protein S3.

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

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S7.

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

- Molecule 15 is a protein called 30S ribosomal protein S9.

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

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

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

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 19 is a protein called 30S ribosomal protein S13.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S16.

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

- Molecule 22 is a protein called 30S ribosomal protein S17.

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

- Molecule 23 is a protein called 30S ribosomal protein S18.

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

- Molecule 24 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 25 is a protein called 30S ribosomal protein S20.

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

- Molecule 26 is a protein called 30S ribosomal protein S19.

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

- Molecule 27 is a protein called 50S ribosomal protein bL37.

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

- Molecule 28 is a protein called AURKAIP1/COX24 domain-containing protein.

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

- Molecule 29 is a RNA chain called mRNA 32MF.

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

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2903	Total	C	N	O	P	1	0
			62432	27805	11391	20332	2904		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	63	A	G	conflict	GB CP012350
a	524	C	G	conflict	GB CP012350
a	1038	PSU	G	conflict	GB CP012350

- Molecule 31 is a RNA chain called 5S rRNA.

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

- Molecule 32 is a protein called 50S ribosomal protein L2.

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

- Molecule 33 is a protein called 50S ribosomal protein L3.

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

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

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

- Molecule 36 is a protein called 50S ribosomal protein L6.

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

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	124	ALA	THR	conflict	UNP A0A8B2VJI7
m	185	PRO	SER	conflict	UNP A0A8B2VJI7

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL21.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	52	ALA	VAL	conflict	UNP Q6A9I3

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

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

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

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

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

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

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

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

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

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

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

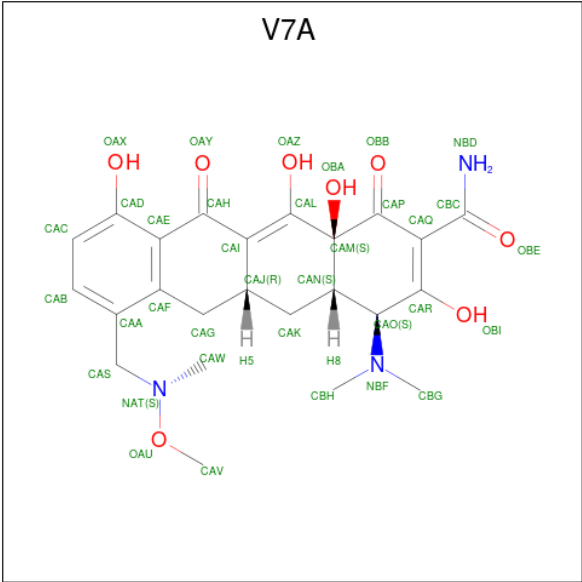
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	0	1	Total	Zn	0
			1	1	
55	3	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	
55	S	1	Total	Zn	0
			1	1	
55	w	1	Total	Zn	0
			1	1	
55	z	1	Total	Zn	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
56	A	63	Total	Mg	0
			63	63	
56	a	233	Total	Mg	0
			233	233	
56	b	2	Total	Mg	0
			2	2	
56	c	1	Total	Mg	0
			1	1	
56	d	1	Total	Mg	0
			1	1	
56	k	1	Total	Mg	0
			1	1	

- Molecule 57 is Sarecycline (CCD ID: V7A) (formula: C₂₄H₂₉N₃O₈) (labeled as "Ligand of Interest" by depositor).



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

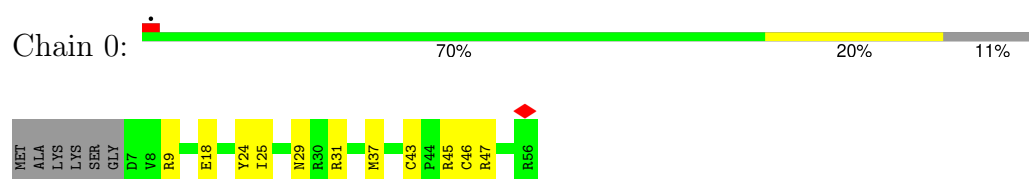
- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	A	11	Total	O	0
			11	11	
58	a	108	Total	O	0
			108	108	
58	b	1	Total	O	0
			1	1	
58	c	1	Total	O	0
			1	1	

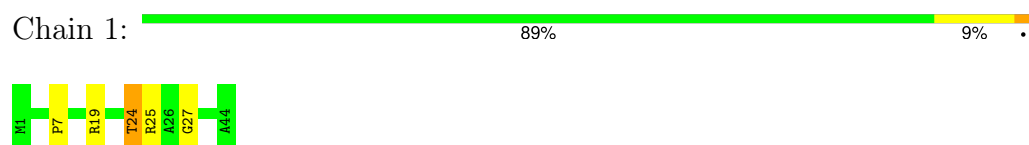
3 Residue-property plots [i](#)

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

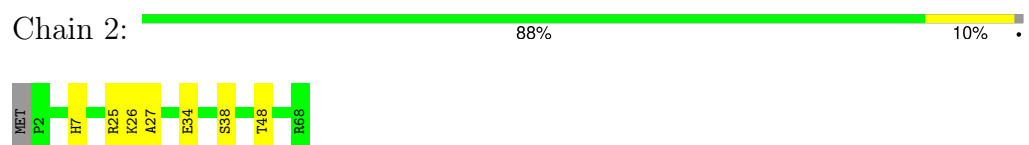
- Molecule 1: 50S ribosomal protein L33



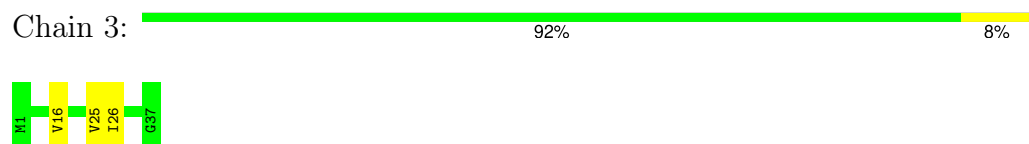
- Molecule 2: 50S ribosomal protein L34



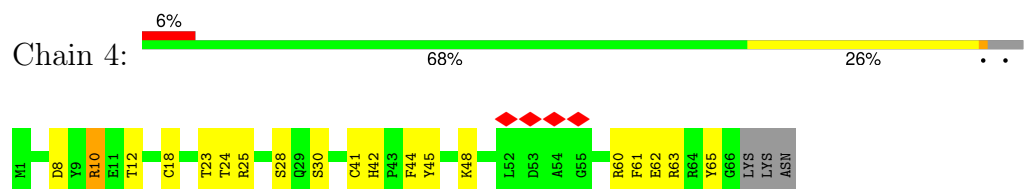
- Molecule 3: Large ribosomal subunit protein bL35



- Molecule 4: 50S ribosomal protein L36

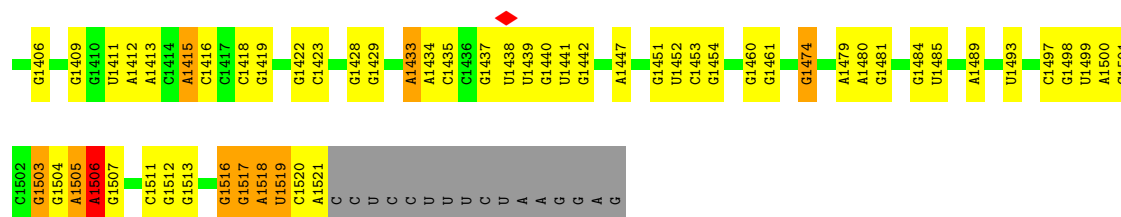


- Molecule 5: 50S ribosomal protein L31

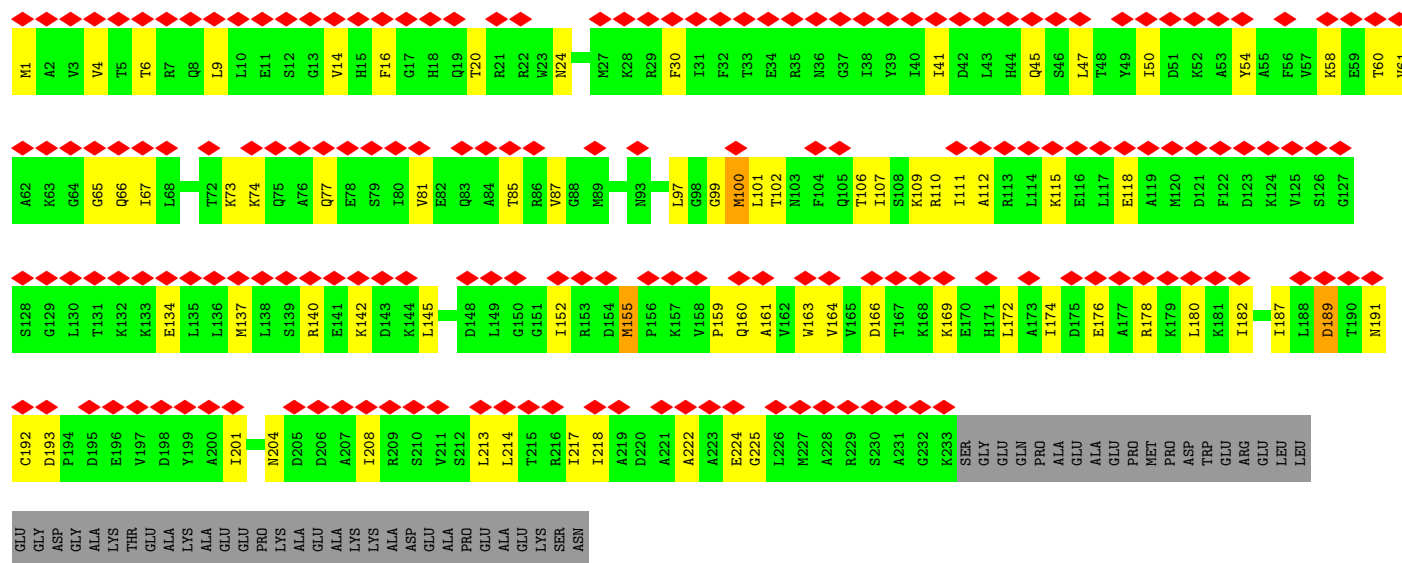


- Molecule 6: 16S rRNA





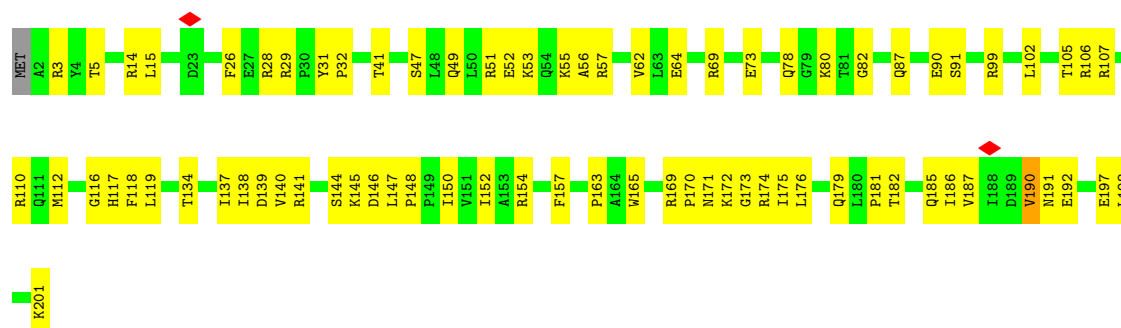
• Molecule 7: 30S ribosomal protein S2



• Molecule 8: initiator tRNA Met (76-MER)

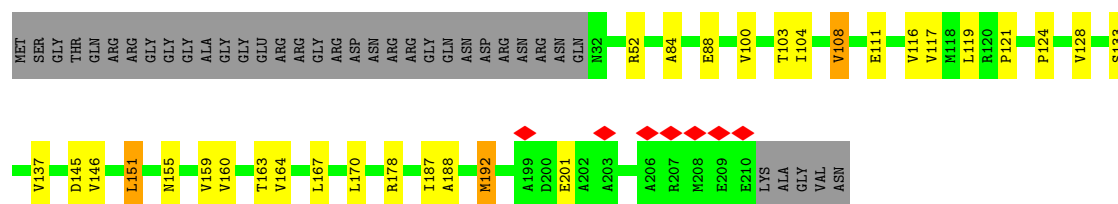


• Molecule 9: 30S ribosomal protein S4



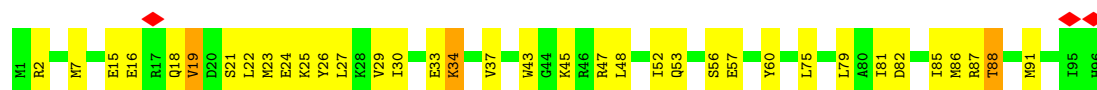
• Molecule 10: Small ribosomal subunit protein uS5

Chain E: 



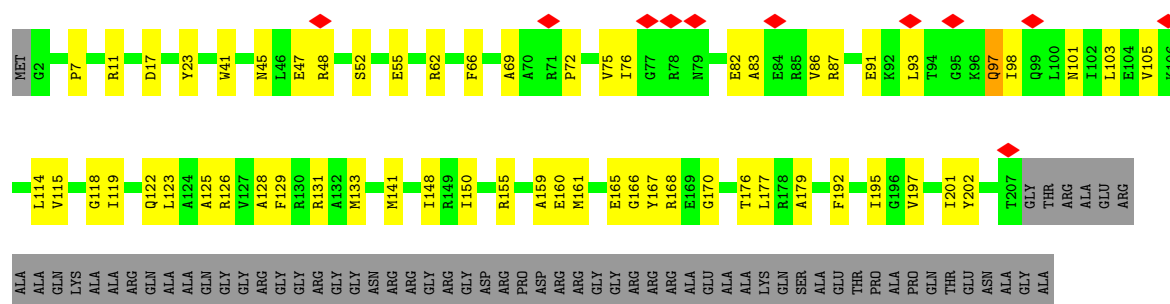
- Molecule 11: 30S ribosomal protein S6

Chain F: 




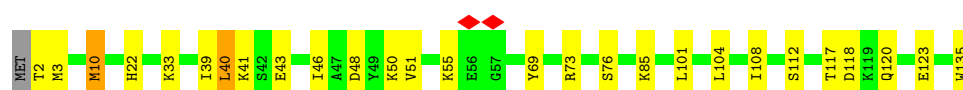
- Molecule 12: 30S ribosomal protein S3

Chain G: 



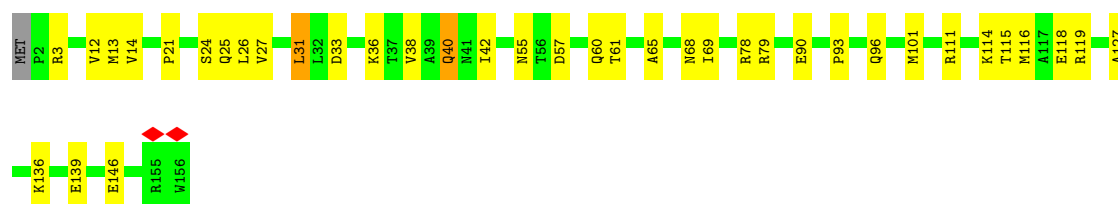
- Molecule 13: 30S ribosomal protein S8

Chain H: 

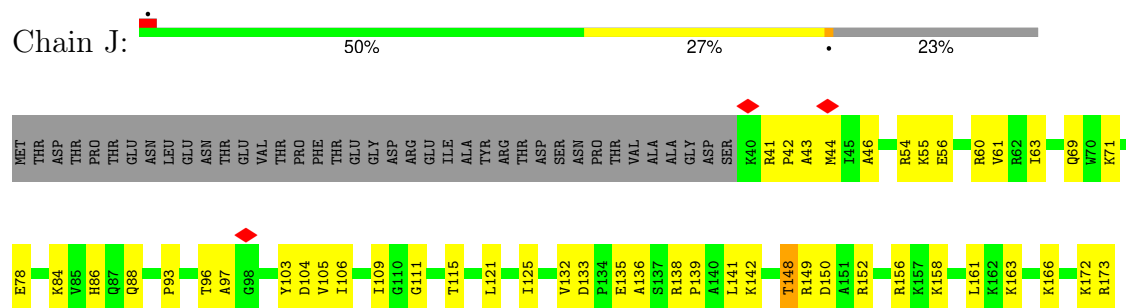


- Molecule 14: 30S ribosomal protein S7

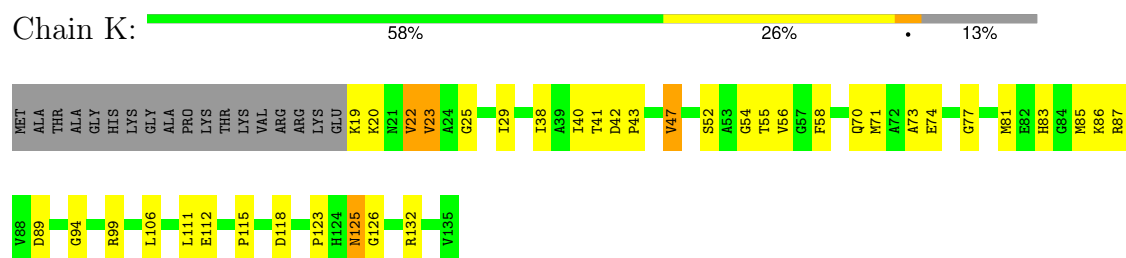
Chain I: 



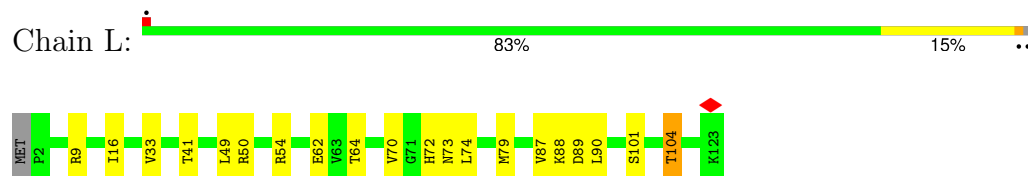
- Molecule 15: 30S ribosomal protein S9



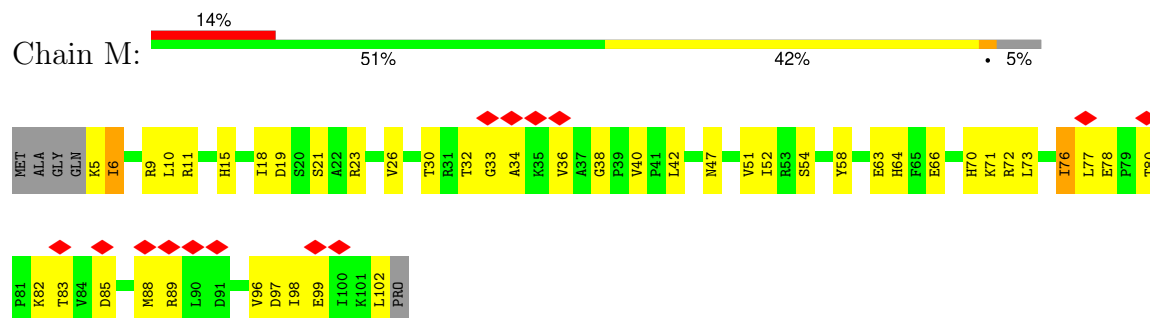
- Molecule 16: 30S ribosomal protein S11



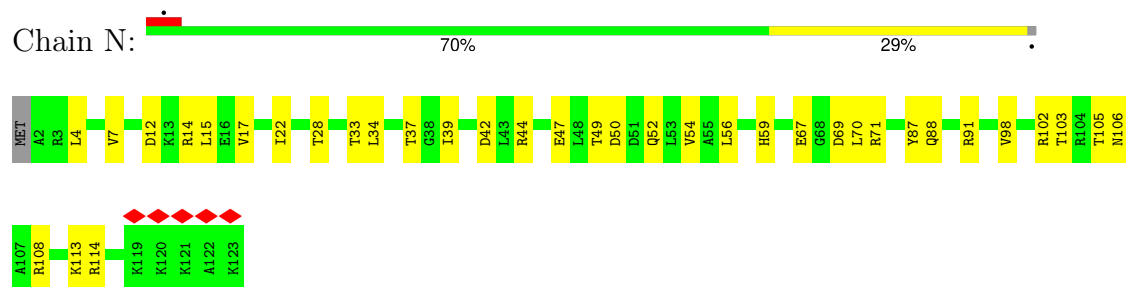
- Molecule 17: 30S ribosomal protein S12



- Molecule 18: Small ribosomal subunit protein uS10



- Molecule 19: 30S ribosomal protein S13



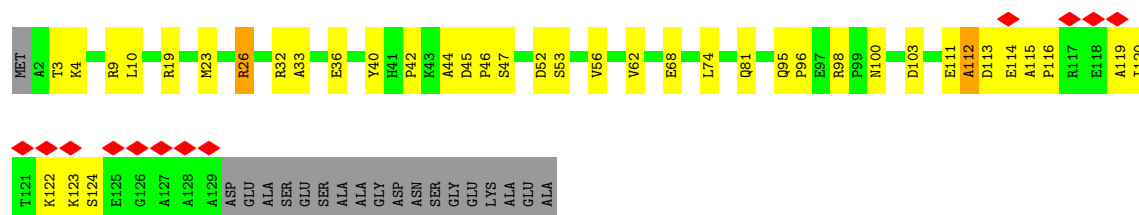
- Molecule 20: 30S ribosomal protein S15

Chain O:  75% 25%




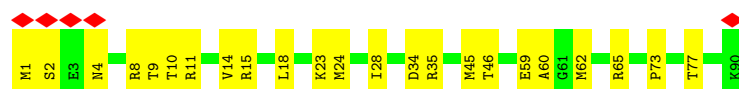
- Molecule 21: 30S ribosomal protein S16

Chain P:  8% 61% 25% 13%



- Molecule 22: 30S ribosomal protein S17

Chain Q:  6% 74% 26%



- Molecule 23: 30S ribosomal protein S18

Chain R:  9% 63% 19% 15%



- Molecule 24: 30S ribosomal protein S14 type Z

Chain S:  74% 23% 3%



- Molecule 25: 30S ribosomal protein S20

Chain T:  74% 25% 1%



- Molecule 26: 30S ribosomal protein S19

Chain U:  68% 22% 10%



- Molecule 27: 50S ribosomal protein bL37

Chain V: 75% 21% .



- Molecule 28: AURKAIP1/COX24 domain-containing protein

Chain X: 70% 27% .



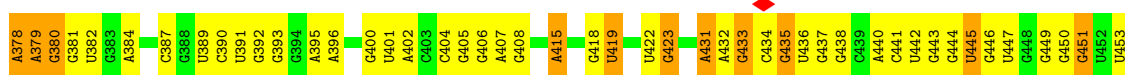
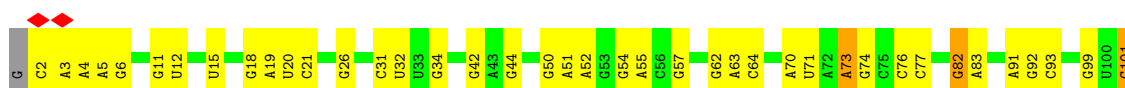
- Molecule 29: mRNA 32MF

Chain Y: 5% 23% 14% 9% 55%

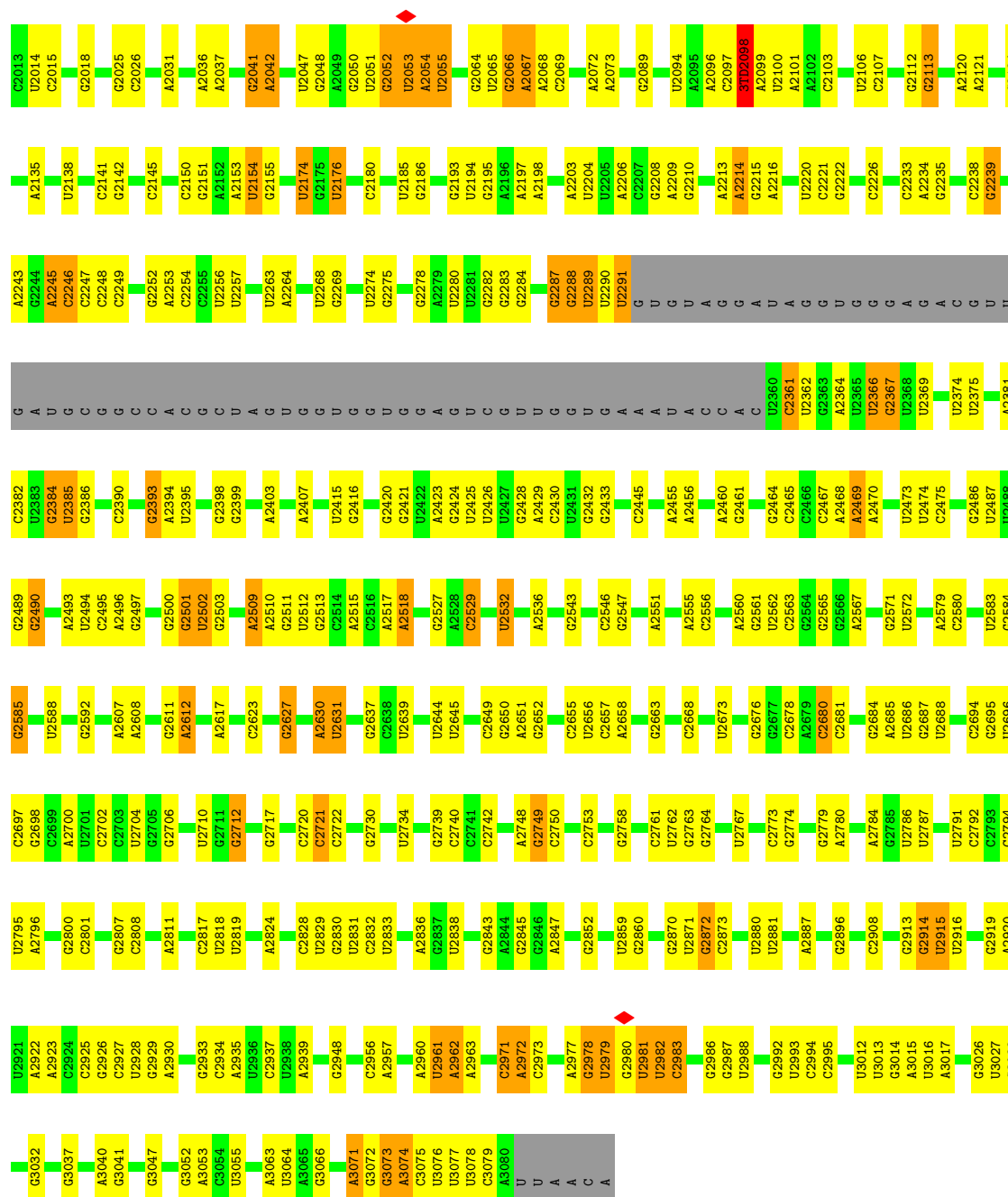


- Molecule 30: 23S rRNA

Chain a: 57% 31% 6% 6%

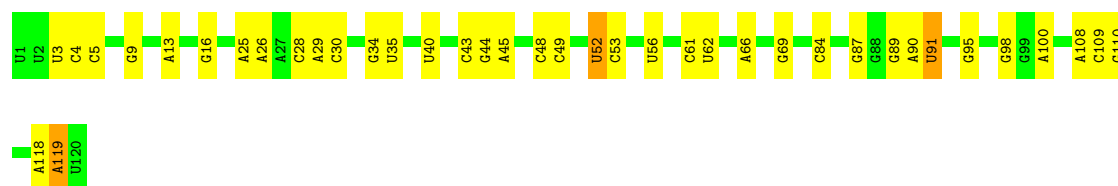


U1904	G581	A1675	G1761	G1904	U1191	A1010	A904	G794	U682	G581
G1905	U587	A1676	G1762	G1905	U1192	A1011	A905	G797	G683	U587
C1906	G588	G1685	U1763	C1906	U1128	G1014	U911	U797	G686	G588
C1908	A589	A1328	A1328	C1908	A1129	U1015	U912	U798	A687	A589
C1909	G1687	A1331	A1331	C1909	G1130	A1028	U913	U799	G687	G1687
C1910	U1688	U1332	U1332	C1910	C1135	G1029	G916	A800	A692	U1688
G1911	G1689	G1333	G1333	G1911	C1136	G1030	U917	A801	A693	G1689
U1912	U1598	G1337	G1337	U1912	A1137	A1031	G918	G802	U698	U1598
G1913	G1599	G1348	G1348	G1913	G1138	C1038	G921	U806	G699	G1599
C1914	C1600	U1349	U1349	C1914	G1140	A1042	G930	C807	G700	C1600
G1915	G1601	G1350	G1350	G1915	G1141	A1043	G931	G814	U608	G1601
G1916	A1607	U1351	U1351	G1916	U1143	G1044	U935	U815	C609	A1607
U1917	C1608	G1481	G1481	U1917	U1144	U1047	U936	C816	G704	C1608
G1918	G1609	G1482	G1482	G1918	G1145	G1052	G937	G817	U709	G1609
U1919	C1610	U1486	U1486	U1919	G1146	U1053	U938	G818	C710	U1486
G1920	A1611	G1487	G1487	G1920	C1147	G1057	U939	A824	G621	A1611
G1921	G1612	C1488	C1488	G1921	U1148	G1057	G940	C825	G622	G1612
G1922	U1613	C1489	C1489	G1922	U1149	G1057	G941	U826	A713	U1613
U1923	G1614	C1491	C1491	U1923	G1150	G1063	A942	U827	G714	U1614
G1924	U1615	G1492	G1492	G1924	G1151	A1064	G944	C828	C715	G1615
U1925	G1616	U1493	U1493	U1925	A1152	C1065	G947	U832	A718	U1616
G1926	U1617	G1494	G1494	G1926	G1153	A1066	G948	U838	A719	U1617
U1927	G1618	U1495	U1495	U1927	G1154	C1069	G949	G839	G720	U1618
A1619	U1619	C1492	C1492	A1619	C1155	G1070	G950	U848	G721	U1619
C1623	G1623	G1493	G1493	C1623	A1156	A1071	A951	A849	G722	G1623
A1624	C1624	U	U	A1624	G1157	C1078	U960	U853	G723	C1624
U1625	U1625	C	C	U1625	C1158	A1079	G966	G853	G724	U1625
C1626	G1626	U	U	C1626	U1159	C1079	G967	U852	G725	G1626
G1627	U1627	G	G	G1627	C1160	A1084	G968	G861	G726	U1627
C1628	G1628	U	U	C1628	U1161	G1085	C969	A867	G727	G1628
G1630	U1630	C	C	G1630	C1162	A1085	U970	G860	G728	U1630
U1631	G1631	G	G	U1631	U1163	G1086	G971	G867	G729	U1631
C1632	U1632	G	G	C1632	C1164	A1090	U972	A868	A731	U1632
G1633	G1633	U	U	G1633	U1165	A1091	U973	G869	G734	G1633
U1638	U1638	U	U	U1638	G1166	C1092	G974	G870	G739	U1638
C1639	C1639	G	G	C1639	A1167	U1095	G975	U875	A740	C1639
U1640	U1640	A	A	U1640	U1168	G1096	G976	C876	G741	U1640
G1641	G1641	U	U	G1641	A1169	U1096	U979	A877	U742	G1641
C1642	U1642	C	C	C1642	G1170	G1105	G981	G877	C743	U1642
U1647	G1647	U	U	U1647	U1171	U1106	U980	A881	C751	U1647
C1648	C1648	A	A	C1648	G1172	G1109	C981	C882	U752	C1648
U1649	U1649	C	C	U1649	U1173	A1110	A993	G890	A753	U1649
A1650	A1650	U	U	A1650	G1174	A1111	A994	G894	G764	A1650
A1651	U1651	A	A	A1651	C1175	A1112	C996	G894	G765	U1651
C1661	C1661	C	C	C1661	G1176	U1116	G1000	C897	U671	C1661
U1662	U1662	U	U	U1662	U1177	G1117	A1001	U898	U672	U1662
G1663	G1663	A	A	G1663	A1178	U1118	A1002	C899	A673	G1663
U1664	U1664	U	U	U1664	A1179	G1119	G1000	U899	G674	U1664
C1665	C1665	C	C	C1665	U1180	U1119	A1002	G903	U675	C1665
U1666	U1666	A	A	U1666	A1181	G1120	G1000	G903	G676	U1666
G1667	G1667	U	U	G1667	U1182	U1120	G1000	G903	G676	G1667
U1673	U1673	G	G	U1673	C1183	U1120	G1000	G903	G676	U1673
A1674	A1674	A	A	A1674	U1184	U1120	G1000	G903	G676	A1674
G1765	G1765	G	G	G1765	U1188	U1120	G1000	G903	G676	G1765
A1705	A1705	U	U	A1705	G1189	U1120	G1000	G903	G676	A1705
U1706	U1706	C	C	U1706	U1189	U1120	G1000	G903	G676	U1706
G1707	G1707	U	U	G1707	U1189	U1120	G1000	G903	G676	G1707
U1708	U1708	A	A	U1708	U1189	U1120	G1000	G903	G676	U1708
G1709	G1709	U	U	G1709	U1189	U1120	G1000	G903	G676	G1709
A1710	A1710	C	C	A1710	U1189	U1120	G1000	G903	G676	A1710
G1711	G1711	U	U	G1711	U1189	U1120	G1000	G903	G676	G1711
U1712	U1712	U	U	U1712	U1189	U1120	G1000	G903	G676	U1712
C1713	C1713	C	C	C1713	U1189	U1120	G1000	G903	G676	C1713
G1714	G1714	U	U	G1714	U1189	U1120	G1000	G903	G676	G1714
A1715	A1715	G	G	A1715	U1189	U1120	G1000	G903	G676	A1715
C1716	C1716	U	U	C1716	U1189	U1120	G1000	G903	G676	C1716
U1717	U1717	G	G	U1717	U1189	U1120	G1000	G903	G676	U1717
G1718	G1718	U	U	G1718	U1189	U1120	G1000	G903	G676	G1718
U1719	U1719	C	C	U1719	U1189	U1120	G1000	G903	G676	U1719
G1720	G1720	G	G	G1720	U1189	U1120	G1000	G903	G676	G1720
U1721	U1721	C	C	U1721	U1189	U1120	G1000	G903	G676	U1721
G1724	G1724	U	U	G1724	U1189	U1120	G1000	G903	G676	G1724
U1725	U1725	G	G	U1725	U1189	U1120	G1000	G903	G676	U1725
G1726	G1726	A	A	G1726	U1189	U1120	G1000	G903	G676	G1726
U1727	U1727	U	U	U1727	U1189	U1120	G1000	G903	G676	U1727
A1728	A1728	G	G	A1728	U1189	U1120	G1000	G903	G676	A1728
G1729	G1729	U	U	G1729	U1189	U1120	G1000	G903	G676	G1729
U1730	U1730	C	C	U1730	U1189	U1120	G1000	G903	G676	U1730
G1731	G1731	A	A	G1731	U1189	U1120	G1000	G903	G676	G1731
U1734	U1734	U	U	U1734	U1189	U1120	G1000	G903	G676	U1734
G1735	G1735	C	C	G1735	U1189	U1120	G1000	G903	G676	G1735
A1736	A1736	U	U	A1736	U1189	U1120	G1000	G903	G676	A1736
U1737	U1737	A	A	U1737	U1189	U1120	G1000	G903	G676	U1737
A1743	A1743	C	C	A1743	U1189	U1120	G1000	G903	G676	A1743
G1749	G1749	U	U	G1749	U1189	U1120	G1000	G903	G676	G1749
A1752	A1752	A	A	A1752	U1189	U1120	G1000	G903	G676	A1752
U1753	U1753	U	U	U1753	U1189	U1120	G1000	G903	G676	U1753
A1754	A1754	C	C	A1754	U1189	U1120	G1000	G903	G676	A1754
G1755	G1755	G	G	G1755	U1189	U1120	G1000	G903	G676	G1755
U1977	U1977	U	U	U1977	U1189	U1120	G1000	G903	G676	U1977
C1978	C1978	G	G	C1978	U1189	U1120	G1000	G903	G676	C1978
G1979	G1979	A	A	G1979	U1189	U1120	G1000	G903	G676	G1979
U1980	U1980	U	U	U1980	U1189	U1120	G1000	G903	G676	U1980
G1981	G1981	C	C	G1981	U1189	U1120	G1000	G903	G676	G1981
U1982	U1982	U	U	U1982	U1189	U1120	G1000	G903	G676	U1982
C1983	C1983	G	G	C1983	U1189	U1120	G1000	G903	G676	C1983
G1984	G1984	A	A	G1984	U1189	U1120	G1000	G903	G676	G1984
A1985	A1985	U	U	A1985	U1189	U1120	G1000	G903	G676	A1985
U1986	U1986	C	C	U1986	U1189	U1120	G1000	G903	G676	U1986
A1995	A1995	U	U	A1995	U1189	U1120	G1000	G903	G676	A1995
C1996	C1996	C	C	C1996	U1189	U1120	G1000	G903	G676	C1996
U1999	U1999	A	A	U1999	U1189	U1120	G1000	G903	G676	U1999
G2000	G2000	U	U	G2000	U1189	U1120	G1000	G903	G676	G2000
U2001	U2001	C	C	U2001	U1189	U1120	G1000	G903	G676	U2001
A2008	A2008	A	A	A2008	U1189	U1120	G1000	G903	G676	A2008
C2009	C2009	U	U	C2009	U1189	U1120	G1000	G903	G676	C2009
U2010	U2010	C	C	U2010	U1189	U1120	G1000	G903	G676	U2010
G2011	G2011	U	U	G2011	U1189	U1120	G1000	G903	G676	G2011
A2012	A2012	A	A	A2012	U1189	U1120	G1000	G903	G676	A2012




• Molecule 31: 5S rRNA

Chain b: 68% 30%




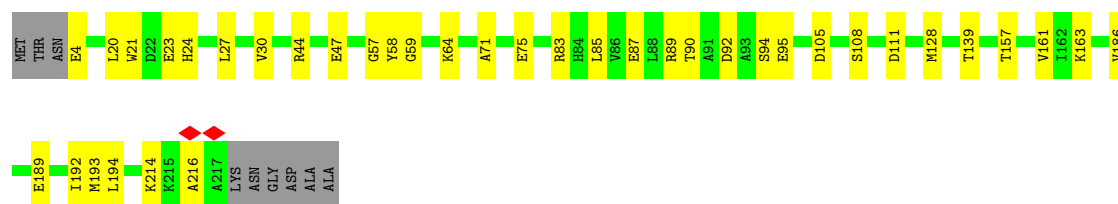
• Molecule 32: 50S ribosomal protein L2

Chain c:  85% 13% ..



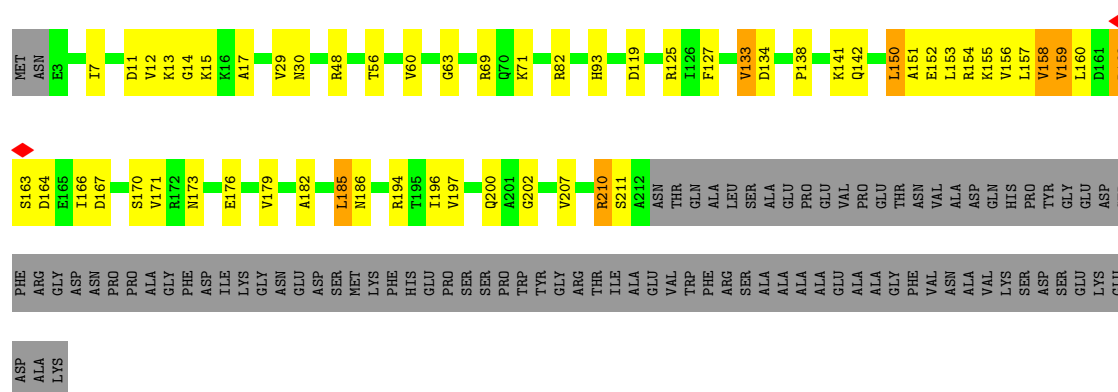
- Molecule 33: 50S ribosomal protein L3

Chain d:  79% 17% .



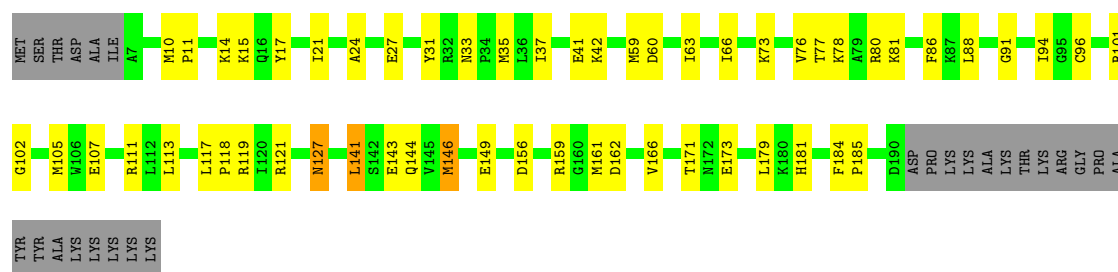
- Molecule 34: 50S ribosomal protein L4

Chain e:  51% 17% . 30%

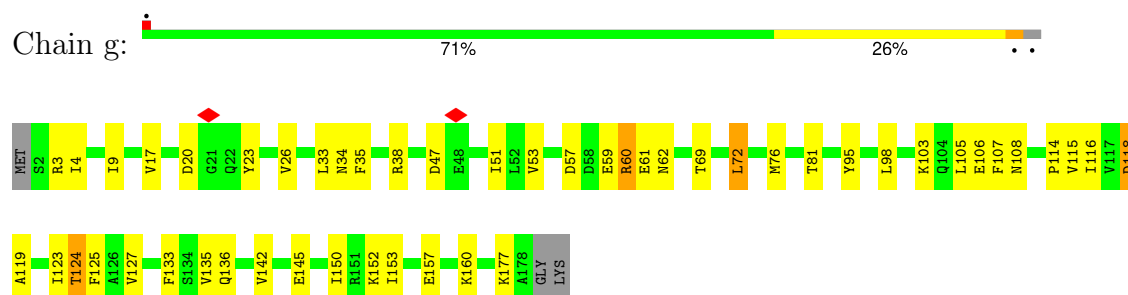


- Molecule 35: 50S ribosomal protein L5

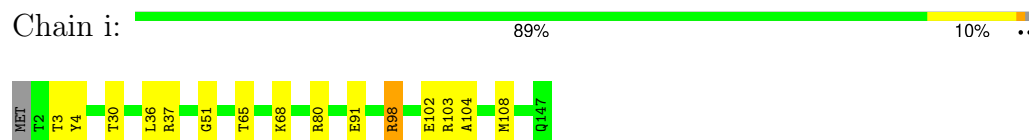
Chain f:  61% 25% . 12%



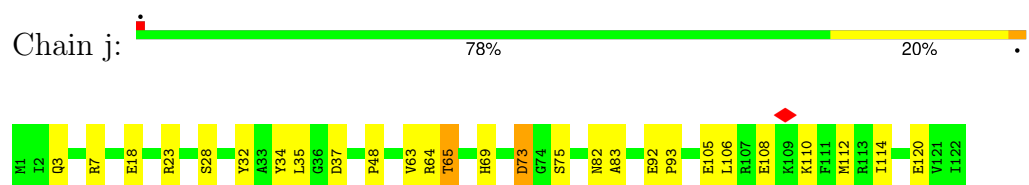
- Molecule 36: 50S ribosomal protein L6



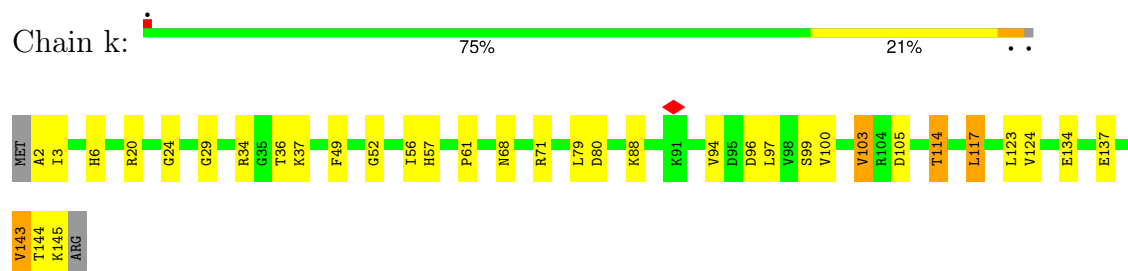
- Molecule 37: 50S ribosomal protein L13



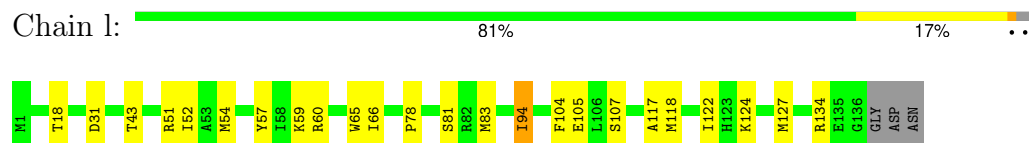
- Molecule 38: 50S ribosomal protein L14



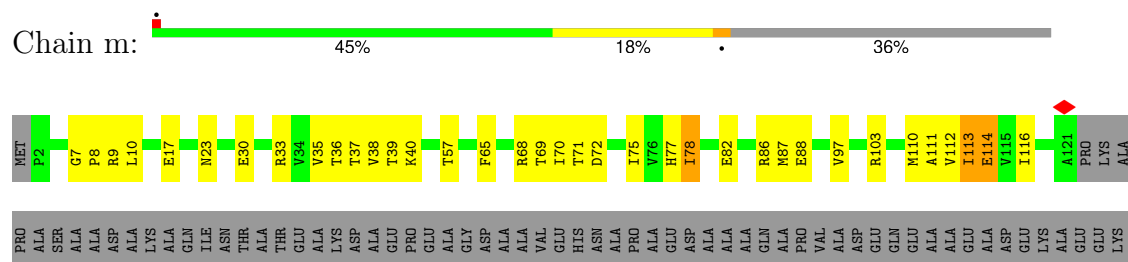
- Molecule 39: 50S ribosomal protein L15



- Molecule 40: 50S ribosomal protein L16



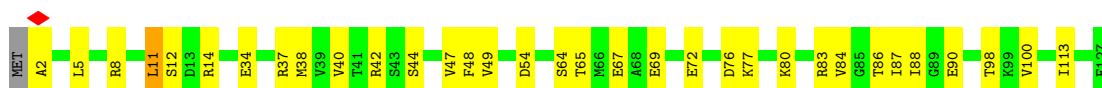
- Molecule 41: Large ribosomal subunit protein bL17




PRO
GLU
ALA

- Molecule 42: 50S ribosomal protein L18

Chain n:  73% 25%



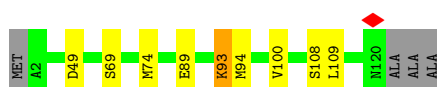
- Molecule 43: 50S ribosomal protein L19

Chain o:  81% 16%




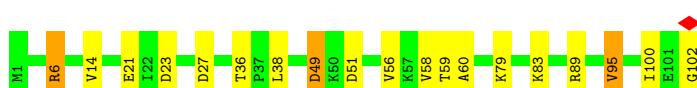
- Molecule 44: 50S ribosomal protein L20

Chain p:  89% 7%



- Molecule 45: Large ribosomal subunit protein bL21

Chain q:  81% 16%



- Molecule 46: 50S ribosomal protein L22

Chain r:  69% 17% 14%



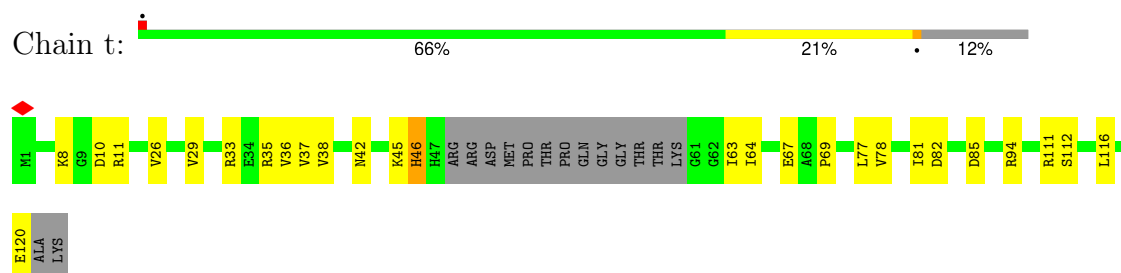
ALA
ALA
LYS
SER
GLU
THR
GLY
LYS
GLY
ALA

- Molecule 47: 50S ribosomal protein L23

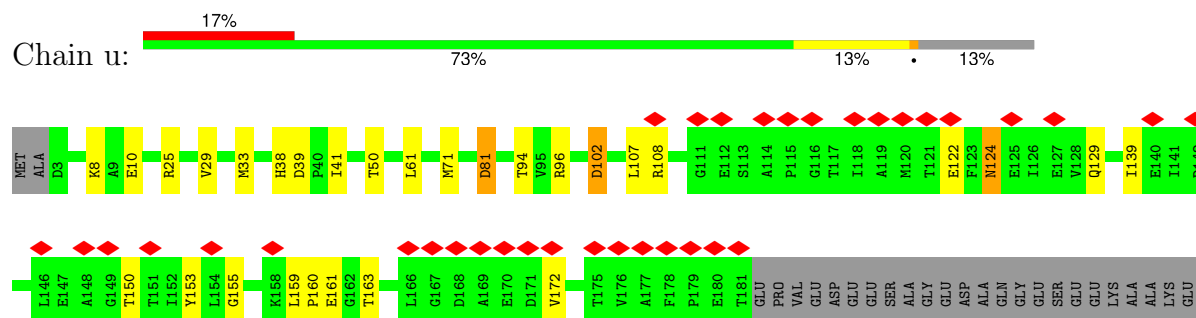
Chain s:  67% 26% 7%



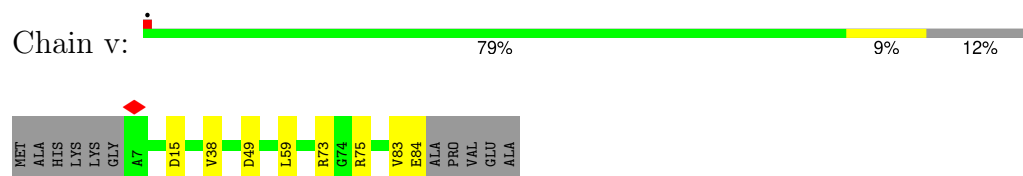
- Molecule 48: Large ribosomal subunit protein uL24



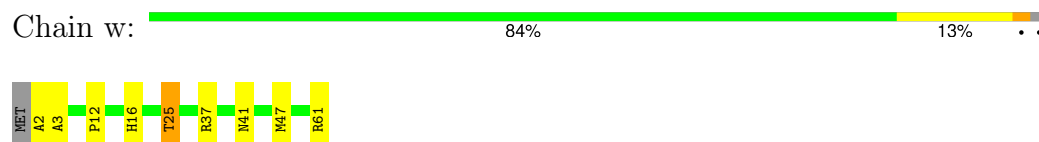
- Molecule 49: 50S ribosomal protein L25



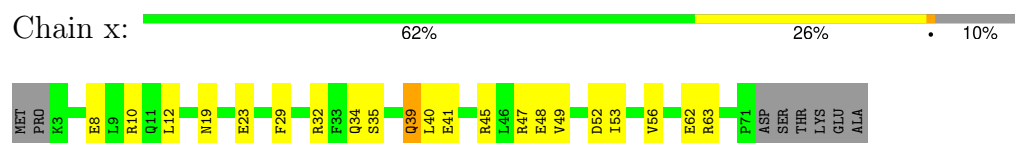
- Molecule 50: 50S ribosomal protein L27



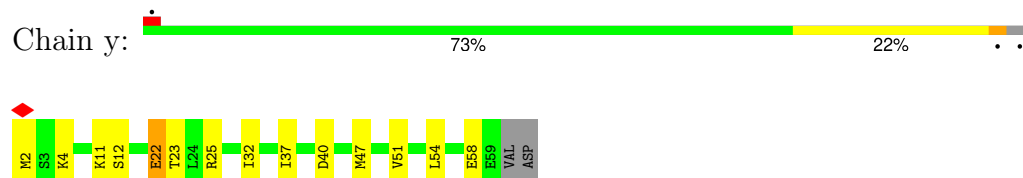
- Molecule 51: 50S ribosomal protein L28



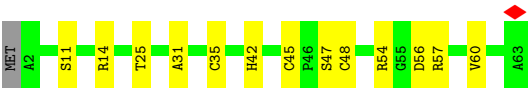
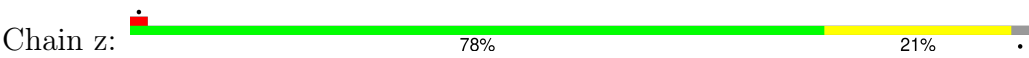
- Molecule 52: 50S ribosomal protein L29



- Molecule 53: 50S ribosomal protein L30



● Molecule 54: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.654	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.21	0/429	0.42	0/569
2	1	0.20	0/365	0.26	0/478
3	2	0.20	0/519	0.30	0/682
4	3	0.18	0/305	0.31	0/401
5	4	0.28	0/521	0.46	0/700
6	A	0.21	0/35898	0.30	0/56012
7	B	0.14	0/1864	0.40	1/2509 (0.0%)
8	C	0.27	0/1725	0.35	0/2689
9	D	0.25	0/1662	0.45	0/2239
10	E	0.16	0/1325	0.34	0/1789
11	F	0.20	0/794	0.56	1/1069 (0.1%)
12	G	0.17	0/1638	0.41	0/2201
13	H	0.20	0/1036	0.44	0/1395
14	I	0.17	0/1246	0.43	0/1679
15	J	0.19	0/1027	0.45	0/1376
16	K	0.20	0/874	0.46	0/1177
17	L	0.26	0/960	0.44	0/1283
18	M	0.20	0/800	0.55	0/1080
19	N	0.17	0/985	0.39	0/1317
20	O	0.20	0/718	0.44	0/959
21	P	0.38	0/1013	0.59	0/1370
22	Q	0.18	0/734	0.41	0/978
23	R	0.21	0/532	0.41	0/713
24	S	0.62	0/484	0.88	1/644 (0.2%)
25	T	0.19	0/676	0.30	0/897
26	U	0.19	0/675	0.47	0/908
27	V	0.21	0/184	0.30	0/236
28	X	0.19	0/277	0.36	0/355
29	Y	0.50	0/235	0.64	0/363
30	a	0.26	0/69472	0.35	3/108408 (0.0%)
31	b	0.22	0/2871	0.29	0/4475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.22	0/2132	0.38	1/2871 (0.0%)
33	d	0.22	0/1611	0.41	0/2172
34	e	0.30	0/1600	0.56	0/2165
35	f	0.20	0/1493	0.44	0/2001
36	g	0.16	0/1398	0.38	0/1884
37	i	0.29	0/1164	0.48	0/1574
38	j	0.21	0/957	0.37	0/1282
39	k	0.31	0/1090	0.57	0/1465
40	l	0.22	0/1108	0.40	0/1488
41	m	0.42	0/949	0.63	1/1277 (0.1%)
42	n	0.21	0/959	0.44	0/1281
43	o	0.20	0/909	0.31	0/1216
44	p	0.22	0/969	0.28	0/1292
45	q	0.20	0/785	0.42	0/1050
46	r	0.20	0/1028	0.33	0/1379
47	s	0.22	0/759	0.42	0/1022
48	t	0.19	0/840	0.43	0/1123
49	u	0.17	0/1396	0.39	0/1896
50	v	0.20	0/598	0.35	0/800
51	w	0.22	0/483	0.34	0/648
52	x	0.20	0/567	0.38	0/759
53	y	0.18	0/471	0.31	0/627
54	z	0.20	0/487	0.29	0/654
All	All	0.24	0/155597	0.36	8/232877 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	P	0	1
24	S	0	2
34	e	0	1
37	i	0	2
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	152	ILE	N-CA-C	-6.23	106.70	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1898	C	O3'-P-O5'	-6.21	94.69	104.00
32	c	274	SER	CB-CA-C	-5.51	110.20	116.54
30	a	739	G	C4'-C3'-O3'	5.20	117.19	109.40
30	a	2961	U	O3'-P-O5'	5.18	111.78	104.00
24	S	26	ARG	CA-C-O	-5.17	115.54	120.92
41	m	78	ILE	CA-C-O	-5.06	116.14	121.41
11	F	34	LYS	CA-CB-CG	5.04	124.19	114.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	P	26	ARG	Sidechain
24	S	23	ARG	Sidechain
24	S	45	ARG	Sidechain
34	e	162	ARG	Sidechain
37	i	103	ARG	Sidechain
37	i	98	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	423	0	429	9	0
2	1	362	0	388	4	0
3	2	513	0	565	5	0
4	3	302	0	330	2	0
5	4	512	0	499	14	0
6	A	32340	0	16267	392	0
7	B	1836	0	1902	46	0
8	C	1625	0	829	8	0
9	D	1632	0	1663	55	0
10	E	1309	0	1349	22	0
11	F	785	0	818	27	0
12	G	1613	0	1626	41	0
13	H	1021	0	1059	17	0
14	I	1225	0	1275	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	1012	0	1069	34	0
16	K	858	0	884	27	0
17	L	948	0	1031	14	0
18	M	786	0	823	37	0
19	N	976	0	1031	26	0
20	O	708	0	737	23	0
21	P	994	0	1008	29	0
22	Q	728	0	772	14	0
23	R	527	0	580	11	0
24	S	474	0	499	11	0
25	T	673	0	726	14	0
26	U	658	0	671	15	0
27	V	183	0	202	5	0
28	X	277	0	338	5	0
29	Y	211	0	106	4	0
30	a	62432	0	31308	621	0
31	b	2567	0	1297	23	0
32	c	2091	0	2150	24	0
33	d	1586	0	1634	31	0
34	e	1577	0	1619	51	0
35	f	1468	0	1487	43	0
36	g	1376	0	1421	34	0
37	i	1139	0	1163	8	0
38	j	946	0	1011	16	0
39	k	1072	0	1106	30	0
40	l	1082	0	1117	16	0
41	m	936	0	997	22	0
42	n	952	0	995	21	0
43	o	896	0	928	15	0
44	p	958	0	986	6	0
45	q	778	0	824	9	0
46	r	1017	0	1070	14	0
47	s	751	0	803	20	0
48	t	833	0	883	15	0
49	u	1376	0	1397	19	0
50	v	591	0	581	4	0
51	w	474	0	487	5	0
52	x	564	0	582	15	0
53	y	467	0	504	8	0
54	z	477	0	479	11	0
55	0	1	0	0	0	0
55	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	4	1	0	0	0	0
55	S	1	0	0	0	0
55	w	1	0	0	0	0
55	z	1	0	0	0	0
56	A	63	0	0	0	0
56	a	233	0	0	0	0
56	b	2	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
56	k	1	0	0	0	0
57	A	35	0	0	0	0
57	a	35	0	0	0	0
58	A	11	0	0	0	0
58	a	108	0	0	0	0
58	b	1	0	0	0	0
58	c	1	0	0	0	0
All	All	144415	0	96305	1820	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 8.

All (1820) 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)
11:F:22:LEU:HA	11:F:25:LYS:HE3	1.52	0.90
35:f:21:ILE:HD12	35:f:181:HIS:HB3	1.58	0.86
30:a:669:A:H62	30:a:1328:A:H2	1.23	0.84
34:e:133:VAL:HG23	34:e:141:LYS:HD3	1.60	0.81
9:D:90:GLU:HG3	9:D:186:ILE:HG12	1.65	0.79
30:a:1710:A:H61	30:a:1726:U:H5'	1.48	0.79
30:a:6:G:H1	30:a:3076:U:H3	1.30	0.78
30:a:2239:G:H1	30:a:2794:C:H5	1.31	0.78
38:j:108:GLU:HB3	38:j:110:LYS:HE2	1.66	0.78
30:a:1327:G:N7	39:k:20:ARG:NH2	2.33	0.76
18:M:36:VAL:HG12	18:M:76:ILE:HD13	1.66	0.76
9:D:172:LYS:HD2	21:P:115:ALA:HB1	1.68	0.75
6:A:78:G:H22	6:A:95:U:H3	1.32	0.75
6:A:1023:C:H2'	6:A:1024:G:H8	1.50	0.75
30:a:1638:U:O2'	30:a:1640:G:N2	2.20	0.74
33:d:4:GLU:OE1	33:d:4:GLU:N	2.21	0.74
13:H:101:LEU:HD22	13:H:104:LEU:HB2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1166:G:N2	30:a:1169:A:OP2	2.20	0.74
6:A:1428:G:H8	6:A:1447:A:H62	1.36	0.73
13:H:41:LYS:NZ	13:H:48:ASP:OD1	2.22	0.73
34:e:153:LEU:H	34:e:154:ARG:NE	1.85	0.73
6:A:1089:G:O2'	7:B:109:LYS:NZ	2.20	0.73
22:Q:59:GLU:OE1	22:Q:59:GLU:N	2.20	0.73
27:V:3:LYS:NZ	30:a:1217:G:OP2	2.21	0.73
9:D:102:LEU:HD11	9:D:173:GLY:HA2	1.70	0.73
49:u:10:GLU:N	49:u:10:GLU:OE2	2.22	0.73
6:A:1215:G:OP2	19:N:114:ARG:NH2	2.22	0.73
40:l:60:ARG:HD3	40:l:60:ARG:H	1.52	0.73
30:a:1617:G:HO2'	30:a:1698:G:HO2'	1.32	0.72
30:a:1647:G:H5''	30:a:1648:C:H5'	1.71	0.72
30:a:2042:A:H61	30:a:2066:G:H1	1.37	0.72
30:a:1775:G:N2	30:a:1776:G:N7	2.36	0.72
34:e:176:GLU:N	34:e:176:GLU:OE2	2.23	0.72
6:A:1105:C:H2'	6:A:1106:A:H8	1.55	0.72
30:a:2495:C:OP2	35:f:80:ARG:NH2	2.21	0.71
30:a:225:G:H22	30:a:242:U:H4'	1.55	0.71
30:a:1281:C:H5	30:a:1318:G:H1	1.38	0.71
12:G:129:PHE:O	12:G:133:MET:HG3	1.89	0.71
30:a:712:U:H4'	30:a:739:G:N7	2.06	0.71
6:A:655:G:H2'	6:A:656:G:C8	2.26	0.70
6:A:1409:G:H5'	38:j:48:PRO:HB3	1.72	0.70
30:a:1254:G:N1	30:a:1257:U:OP2	2.24	0.70
46:r:42:ARG:NH1	46:r:91:ALA:O	2.23	0.70
30:a:130:G:H22	30:a:154:G:H22	1.40	0.70
39:k:36:THR:HG22	39:k:37:LYS:HG2	1.72	0.70
47:s:68:VAL:HG22	47:s:77:LYS:HG3	1.72	0.70
41:m:88:GLU:OE1	41:m:88:GLU:N	2.24	0.70
6:A:1272:G:H2'	6:A:1273:A:H4'	1.74	0.69
30:a:1138:G:H21	30:a:1168:A:H1'	1.57	0.69
15:J:135:GLU:N	15:J:135:GLU:OE2	2.25	0.69
30:a:73:A:OP1	52:x:47:ARG:NH2	2.25	0.69
42:n:67:GLU:OE1	42:n:67:GLU:N	2.23	0.69
45:q:6:ARG:HB3	45:q:38:LEU:HD21	1.73	0.69
7:B:24:ASN:ND2	7:B:192:CYS:O	2.25	0.69
30:a:1148:U:O2	30:a:1156:A:N6	2.25	0.69
33:d:189:GLU:OE1	33:d:189:GLU:N	2.25	0.69
4:3:16:VAL:HG12	4:3:25:VAL:HG22	1.74	0.69
11:F:30:ILE:HD11	11:F:75:LEU:HD22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:9:G:N7	42:n:2:ALA:N	2.40	0.69
31:b:43:C:O2	35:f:101:ARG:NH1	2.25	0.69
34:e:155:LYS:HZ2	34:e:196:ILE:HG12	1.56	0.69
12:G:41:TRP:O	12:G:45:ASN:ND2	2.26	0.69
30:a:2706:G:H1	30:a:2721:C:H5	1.38	0.69
19:N:49:THR:H	19:N:52:GLN:HE21	1.41	0.69
30:a:2510:A:H2'	30:a:2511:G:C8	2.28	0.68
39:k:94:VAL:HG22	39:k:97:LEU:HD22	1.75	0.68
6:A:656:G:H2'	6:A:657:A:H8	1.58	0.68
6:A:1246:G:H8	6:A:1261:A:H62	1.41	0.68
34:e:153:LEU:H	34:e:154:ARG:HE	1.42	0.68
9:D:145:LYS:HE2	21:P:122:LYS:HD3	1.75	0.68
21:P:19:ARG:NH1	21:P:36:GLU:OE2	2.27	0.68
36:g:118:ASP:N	36:g:118:ASP:OD1	2.26	0.68
21:P:95:GLN:HB2	21:P:98:ARG:HH12	1.58	0.68
2:1:19:ARG:NH1	30:a:124:A:OP2	2.26	0.68
6:A:1237:G:H21	6:A:1356:C:H1'	1.58	0.68
40:l:65:TRP:HB2	40:l:105:GLU:HB2	1.75	0.68
48:t:11:ARG:NH2	48:t:85:ASP:OD2	2.27	0.68
6:A:1096:A:N1	12:G:176:THR:OG1	2.26	0.68
6:A:1243:G:OP1	6:A:1243:G:N2	2.27	0.68
30:a:1688:U:H2'	30:a:1689:G:O4'	1.93	0.67
6:A:874:G:OP2	28:X:10:LYS:NZ	2.27	0.67
13:H:55:LYS:HA	13:H:55:LYS:HE3	1.75	0.67
30:a:670:G:H1	39:k:34:ARG:HD2	1.59	0.67
30:a:2824:A:H5''	37:i:80:ARG:HD2	1.76	0.67
7:B:99:GLY:O	7:B:101:LEU:N	2.28	0.67
18:M:5:LYS:HB3	18:M:6:ILE:HD12	1.76	0.67
30:a:1698:G:H1	30:a:1915:G:H22	1.41	0.67
12:G:52:SER:HB2	12:G:114:LEU:HD11	1.77	0.67
41:m:35:VAL:HG22	41:m:112:VAL:HG22	1.75	0.67
31:b:87:G:H21	31:b:90:A:H2	1.41	0.67
30:a:392:G:H21	30:a:415:A:H62	1.41	0.67
41:m:30:GLU:HG3	41:m:75:ILE:HD11	1.76	0.67
3:2:25:ARG:HB3	39:k:61:PRO:HG2	1.77	0.67
30:a:291:U:H5'	30:a:308:U:C5	2.30	0.67
11:F:23:MET:HA	11:F:23:MET:HE3	1.77	0.66
17:L:74:LEU:HD23	17:L:104:THR:HB	1.77	0.66
18:M:85:ASP:O	18:M:89:ARG:HD2	1.95	0.66
33:d:47:GLU:N	33:d:47:GLU:OE2	2.28	0.66
19:N:47:GLU:N	19:N:47:GLU:OE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:e:159:VAL:HB	34:e:202:GLY:HA2	1.77	0.66
30:a:2649:C:O2	40:l:124:LYS:NZ	2.27	0.66
18:M:5:LYS:HB2	18:M:77:LEU:HA	1.77	0.66
18:M:78:GLU:HG2	18:M:80:THR:HB	1.76	0.66
25:T:28:LEU:HD22	25:T:58:LEU:HD23	1.77	0.66
30:a:142:G:H21	30:a:147:G:H1	1.44	0.66
42:n:69:GLU:OE1	42:n:69:GLU:N	2.26	0.66
33:d:108:SER:N	33:d:111:ASP:OD2	2.28	0.66
6:A:917:G:O6	14:I:3:ARG:NH2	2.29	0.66
30:a:2584:G:OP2	30:a:2584:G:N2	2.22	0.66
52:x:10:ARG:NH1	52:x:62:GLU:OE2	2.29	0.66
1:0:9:ARG:NH1	30:a:2467:C:OP2	2.29	0.66
30:a:1687:G:H2'	30:a:1688:U:H5	1.61	0.66
42:n:83:ARG:O	42:n:87:ILE:HG13	1.95	0.66
33:d:95:GLU:OE2	33:d:95:GLU:N	2.29	0.66
41:m:103:ARG:HG3	41:m:110:MET:HE3	1.77	0.65
53:y:2:MET:HE1	53:y:4:LYS:HG3	1.78	0.65
6:A:271:U:H2'	6:A:272:A:C8	2.30	0.65
35:f:10:MET:HE3	35:f:14:LYS:HB3	1.78	0.65
34:e:142:GLN:NE2	34:e:170:SER:O	2.28	0.65
30:a:71:U:OP1	47:s:5:LYS:NZ	2.28	0.65
36:g:127:VAL:HG23	36:g:133:PHE:HB3	1.78	0.65
16:K:87:ARG:HB2	16:K:112:GLU:HB2	1.79	0.65
30:a:1698:G:H22	30:a:1915:G:N2	1.95	0.65
6:A:728:U:H2'	6:A:729:U:C2	2.32	0.65
7:B:58:LYS:HE3	7:B:224:GLU:HG2	1.79	0.65
18:M:10:LEU:HD23	18:M:98:ILE:HD11	1.77	0.65
30:a:941:G:H2'	30:a:942:A:C8	2.32	0.65
14:I:27:VAL:O	14:I:31:LEU:HB2	1.97	0.65
39:k:94:VAL:HG23	39:k:96:ASP:H	1.62	0.65
30:a:379:A:O2'	30:a:380:G:O4'	2.14	0.65
30:a:1831:U:H5'	30:a:1832:C:H5'	1.77	0.65
8:C:21:A:H61	8:C:46:G:H2'	1.62	0.64
34:e:150:LEU:O	34:e:154:ARG:NH1	2.31	0.64
34:e:207:VAL:O	34:e:211:SER:HB3	1.97	0.64
6:A:696:G:H2'	6:A:697:A:C8	2.32	0.64
30:a:1623:C:H5	30:a:1731:G:H1	1.45	0.64
6:A:271:U:H2'	6:A:272:A:H8	1.62	0.64
6:A:659:U:H3	6:A:695:G:H22	1.45	0.64
6:A:984:A:N1	6:A:1025:G:O6	2.31	0.64
6:A:406:G:OP2	9:D:110:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:695:G:H2'	6:A:696:G:C8	2.32	0.64
21:P:46:PRO:HG2	21:P:96:PRO:HA	1.78	0.64
6:A:805:G:HO2'	13:H:2:THR:N	1.94	0.64
11:F:23:MET:O	11:F:27:LEU:HG	1.98	0.64
30:a:332:U:H3	30:a:449:G:H1	1.44	0.64
6:A:1204:C:H2'	6:A:1205:A:C8	2.33	0.64
18:M:34:ALA:HB1	18:M:76:ILE:HD11	1.80	0.64
26:U:11:VAL:HA	26:U:38:SER:HB2	1.79	0.64
21:P:45:ASP:HB3	21:P:46:PRO:HD3	1.80	0.64
41:m:33:ARG:NH1	54:z:60:VAL:O	2.31	0.64
49:u:107:LEU:O	49:u:108:ARG:NH1	2.29	0.64
30:a:2287:G:H1	30:a:2366:U:H3	1.46	0.64
30:a:970:U:H3	30:a:975:G:H1	1.44	0.63
30:a:1143:U:H3	30:a:1171:A:H8	1.42	0.63
12:G:119:ILE:O	12:G:123:LEU:HG	1.97	0.63
9:D:169:ARG:HD2	21:P:116:PRO:HD3	1.80	0.63
31:b:16:G:OP1	42:n:8:ARG:NH2	2.30	0.63
14:I:36:LYS:O	14:I:40:GLN:HG2	1.97	0.63
30:a:179:G:N2	30:a:180:U:O4	2.29	0.63
36:g:9:ILE:HB	36:g:51:ILE:HB	1.81	0.63
21:P:68:GLU:N	21:P:68:GLU:OE2	2.32	0.63
30:a:875:U:O4	34:e:69:ARG:NH1	2.31	0.63
34:e:127:PHE:HB2	34:e:197:VAL:HG12	1.79	0.63
36:g:17:VAL:HG12	36:g:26:VAL:HG22	1.79	0.63
11:F:27:LEU:HB3	11:F:37:VAL:HG21	1.79	0.63
6:A:988:G:N2	6:A:1022:U:O2	2.32	0.63
6:A:1270:C:OP2	6:A:1271:G:O2'	2.16	0.63
11:F:33:GLU:OE1	11:F:33:GLU:N	2.32	0.63
6:A:60:U:H2'	6:A:61:G:H8	1.64	0.63
6:A:195:G:O2'	22:Q:8:ARG:NH2	2.32	0.63
6:A:438:C:H4'	9:D:148:PRO:HG2	1.80	0.63
30:a:1489:C:H2'	30:a:1490:A:C8	2.34	0.63
6:A:1342:G:H2'	6:A:1343:A:C8	2.33	0.62
19:N:88:GLN:HG2	19:N:98:VAL:HB	1.81	0.62
30:a:2288:G:O2'	30:a:2289:U:OP1	2.17	0.62
33:d:71:ALA:O	33:d:75:GLU:HG3	1.98	0.62
30:a:1105:G:N2	30:a:1106:U:O4	2.30	0.62
18:M:77:LEU:HD23	18:M:77:LEU:H	1.62	0.62
30:a:1981:U:OP2	32:c:270:ARG:NH2	2.31	0.62
30:a:3073:G:H4'	30:a:3074:A:H5'	1.80	0.62
30:a:1687:G:H2'	30:a:1688:U:C5	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2720:C:O2'	30:a:2721:C:O2	2.10	0.62
34:e:160:LEU:HB2	34:e:164:ASP:HB2	1.80	0.62
6:A:822:C:H2'	6:A:823:A:C8	2.34	0.62
32:c:223:GLY:HA2	32:c:226:MET:HG3	1.81	0.62
47:s:7:ARG:NH2	47:s:43:GLU:OE2	2.33	0.62
52:x:34:GLN:HG2	52:x:39:GLN:HB2	1.81	0.62
30:a:2291:U:O2	30:a:2361:C:N4	2.33	0.62
14:I:118:GLU:OE1	14:I:118:GLU:N	2.32	0.61
25:T:48:THR:O	25:T:52:ARG:HG2	1.99	0.61
35:f:59:MET:HE2	35:f:76:VAL:HG13	1.82	0.61
36:g:98:LEU:HG	36:g:106:GLU:HB3	1.81	0.61
49:u:102:ASP:HA	49:u:129:GLN:HA	1.82	0.61
5:4:10:ARG:HH12	5:4:30:SER:HA	1.63	0.61
11:F:34:LYS:HD2	11:F:34:LYS:O	2.00	0.61
7:B:214:LEU:O	7:B:218:ILE:HG12	2.00	0.61
41:m:69:THR:HG22	41:m:70:ILE:H	1.66	0.61
41:m:69:THR:O	41:m:71:THR:N	2.33	0.61
22:Q:35:ARG:NH2	22:Q:46:THR:OG1	2.34	0.61
30:a:153:U:H2'	30:a:154:G:C8	2.36	0.61
33:d:186:VAL:HG22	33:d:193:MET:HG2	1.83	0.61
53:y:22:GLU:HG3	53:y:25:ARG:HH21	1.65	0.61
30:a:1092:A:N3	30:a:1237:C:O2'	2.34	0.61
34:e:159:VAL:HG22	34:e:160:LEU:H	1.64	0.61
53:y:23:THR:HG23	53:y:47:MET:HG2	1.81	0.61
6:A:1204:C:H2'	6:A:1205:A:H8	1.65	0.61
12:G:76:ILE:HA	12:G:83:ALA:HB2	1.83	0.61
36:g:33:LEU:HB3	36:g:76:MET:HE2	1.82	0.61
40:l:43:THR:HG22	40:l:94:ILE:HG22	1.82	0.61
6:A:348:G:OP1	43:o:39:ARG:NH1	2.33	0.61
6:A:358:A:N3	6:A:370:U:O2'	2.33	0.61
22:Q:18:LEU:HD13	22:Q:65:ARG:HH21	1.66	0.60
30:a:1716:U:O2'	30:a:1721:G:N2	2.34	0.60
46:r:23:ILE:HG12	46:r:121:THR:HG23	1.82	0.60
49:u:161:GLU:N	49:u:161:GLU:OE2	2.33	0.60
15:J:71:LYS:HA	15:J:71:LYS:HE3	1.82	0.60
23:R:29:LEU:O	23:R:33:ILE:HG13	2.01	0.60
30:a:198:A:H2'	30:a:199:G:C8	2.36	0.60
6:A:1384:C:OP2	10:E:52:ARG:NH2	2.34	0.60
18:M:11:ARG:HE	18:M:71:LYS:HG3	1.66	0.60
30:a:1982:G:OP1	32:c:258:ARG:NH1	2.34	0.60
39:k:24:GLY:O	39:k:29:GLY:HA3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:95:G:OP1	49:u:25:ARG:NH2	2.30	0.60
20:O:5:GLU:H	20:O:5:GLU:CD	2.09	0.60
30:a:130:G:N2	30:a:154:G:H22	1.99	0.60
18:M:52:ILE:HB	24:S:41:ARG:HD2	1.84	0.60
34:e:152:GLU:HB3	34:e:176:GLU:HG3	1.82	0.60
30:a:949:G:H21	30:a:951:A:H62	1.49	0.60
6:A:148:G:H2'	6:A:149:G:C8	2.36	0.60
6:A:930:A:H2'	6:A:931:G:C8	2.37	0.60
24:S:27:CYS:SG	24:S:28:GLY:N	2.74	0.60
30:a:1647:G:H4'	30:a:1729:G:H21	1.67	0.60
40:l:59:LYS:HB3	40:l:60:ARG:HD3	1.83	0.60
6:A:1341:A:H2'	6:A:1342:G:H8	1.65	0.60
7:B:67:ILE:HD12	7:B:161:ALA:HB3	1.82	0.60
30:a:132:A:N3	30:a:1598:U:O2'	2.33	0.60
30:a:288:G:N3	30:a:310:C:N4	2.49	0.60
6:A:25:G:H2'	6:A:26:G:C8	2.36	0.59
19:N:108:ARG:NH2	19:N:113:LYS:O	2.35	0.59
30:a:384:A:N3	30:a:404:C:O2'	2.32	0.59
6:A:183:G:H2'	6:A:184:G:H2'	1.84	0.59
6:A:1006:U:H2'	6:A:1007:G:H8	1.67	0.59
6:A:1359:U:OP1	15:J:115:THR:OG1	2.20	0.59
12:G:168:ARG:NH2	12:G:170:GLY:O	2.35	0.59
30:a:1695:U:H3'	30:a:1696:G:C8	2.37	0.59
6:A:656:G:H2'	6:A:657:A:C8	2.37	0.59
15:J:84:LYS:O	15:J:84:LYS:NZ	2.27	0.59
19:N:106:ASN:O	19:N:108:ARG:HD2	2.02	0.59
21:P:56:VAL:HG21	21:P:74:LEU:HD21	1.83	0.59
9:D:3:ARG:HD2	9:D:110:ARG:HE	1.66	0.59
16:K:23:VAL:O	16:K:86:LYS:N	2.35	0.59
30:a:1047:U:O2'	30:a:2455:A:N3	2.34	0.59
30:a:1440:G:OP1	51:w:2:ALA:N	2.36	0.59
14:I:38:VAL:O	14:I:42:ILE:HG13	2.01	0.59
30:a:3016:U:H2'	30:a:3017:A:C8	2.38	0.59
47:s:72:ARG:O	47:s:73:THR:OG1	2.17	0.59
6:A:1115:A:H2'	6:A:1116:G:H8	1.68	0.59
11:F:47:ARG:NH1	11:F:56:SER:OG	2.36	0.59
30:a:2801:C:OP1	33:d:163:LYS:NZ	2.35	0.59
52:x:41:GLU:H	52:x:41:GLU:CD	2.09	0.59
7:B:61:VAL:HG11	7:B:225:GLY:HA3	1.85	0.59
30:a:287:U:O2'	30:a:311:A:N6	2.34	0.59
31:b:30:C:OP1	42:n:14:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:m:30:GLU:HG3	41:m:75:ILE:CD1	2.32	0.59
49:u:102:ASP:OD1	49:u:102:ASP:N	2.26	0.59
5:4:42:HIS:HB3	5:4:45:TYR:HD2	1.68	0.59
48:t:67:GLU:OE1	48:t:67:GLU:N	2.35	0.59
1:0:45:ARG:HH22	30:a:2583:U:H5'	1.66	0.58
9:D:53:LYS:NZ	9:D:64:GLU:OE1	2.35	0.58
6:A:1422:G:H2'	6:A:1423:C:C6	2.37	0.58
9:D:49:GLN:HB3	9:D:198:LEU:HB2	1.85	0.58
10:E:108:VAL:HG23	10:E:119:LEU:HB2	1.85	0.58
30:a:660:G:O2'	30:a:1331:A:OP1	2.21	0.58
30:a:799:U:O2'	30:a:801:A:N7	2.29	0.58
32:c:166:VAL:HG21	32:c:182:MET:HE1	1.85	0.58
35:f:127:ASN:HD22	35:f:127:ASN:H	1.51	0.58
6:A:977:G:O2'	6:A:978:A:N7	2.36	0.58
9:D:87:GLN:O	9:D:91:SER:OG	2.21	0.58
34:e:157:LEU:HD11	34:e:185:LEU:HD13	1.85	0.58
30:a:838:U:H2'	30:a:839:G:H8	1.67	0.58
23:R:47:LEU:HD22	23:R:51:ASP:HB3	1.84	0.58
30:a:480:A:H1'	30:a:500:G:O4'	2.03	0.58
35:f:119:ARG:NH1	35:f:146:MET:O	2.31	0.58
36:g:107:PHE:HB2	36:g:115:VAL:HG13	1.86	0.58
6:A:183:G:H21	6:A:226:G:H4'	1.67	0.58
6:A:1024:G:H2'	6:A:1025:G:C8	2.38	0.58
34:e:15:LYS:H	34:e:15:LYS:HE2	1.68	0.58
44:p:93:LYS:HG2	44:p:94:MET:HE2	1.84	0.58
6:A:646:G:H22	6:A:723:G:H1	1.51	0.58
6:A:718:U:H2'	6:A:719:C:C6	2.39	0.58
6:A:1274:A:H2'	6:A:1275:A:C8	2.38	0.58
49:u:71:MET:HE2	49:u:94:THR:HG21	1.86	0.58
6:A:980:A:H2'	6:A:981:U:C6	2.39	0.58
6:A:1341:A:H2'	6:A:1342:G:C8	2.38	0.58
30:a:279:A:HO2'	30:a:456:C:HO2'	1.50	0.58
41:m:7:GLY:O	41:m:9:ARG:NH1	2.36	0.58
15:J:97:ALA:HB2	15:J:141:LEU:HD11	1.84	0.58
20:O:87:ARG:HH21	30:a:799:U:H3'	1.69	0.58
30:a:204:A:N6	30:a:2612:A:O2'	2.36	0.58
30:a:1489:C:H2'	30:a:1490:A:H8	1.66	0.58
30:a:2052:G:N2	30:a:2055:U:OP2	2.36	0.58
50:v:38:VAL:HG12	50:v:59:LEU:HB2	1.86	0.58
22:Q:8:ARG:O	22:Q:10:THR:N	2.37	0.57
36:g:124:THR:HG23	36:g:136:GLN:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:150:ILE:HA	36:g:153:ILE:HD12	1.86	0.57
9:D:139:ASP:OD2	9:D:140:VAL:N	2.37	0.57
30:a:2036:A:H2'	30:a:2037:A:C8	2.39	0.57
6:A:265:G:OP1	25:T:74:ASN:ND2	2.26	0.57
6:A:384:A:H2'	6:A:385:A:H8	1.69	0.57
11:F:16:GLU:O	11:F:19:VAL:HG22	2.05	0.57
25:T:15:GLU:OE2	25:T:18:ARG:NH2	2.36	0.57
30:a:2288:G:N2	30:a:2366:U:O2	2.36	0.57
34:e:155:LYS:NZ	34:e:196:ILE:HG12	2.19	0.57
44:p:89:GLU:OE2	45:q:6:ARG:NH2	2.36	0.57
6:A:1309:G:H2'	6:A:1310:A:C8	2.39	0.57
20:O:76:TYR:O	20:O:80:ILE:HG12	2.03	0.57
30:a:82:G:N2	30:a:102:A:OP2	2.35	0.57
30:a:1118:U:H5''	36:g:60:ARG:HE	1.69	0.57
38:j:69:HIS:ND1	38:j:105:GLU:OE1	2.37	0.57
7:B:66:GLN:HB2	7:B:160:GLN:HG2	1.86	0.57
12:G:179:ALA:HB1	12:G:202:TYR:HE1	1.69	0.57
30:a:903:G:N1	30:a:1265:U:OP2	2.30	0.57
44:p:69:SER:OG	44:p:74:MET:O	2.21	0.57
6:A:1057:G:H21	7:B:106:THR:HG21	1.69	0.57
30:a:106:G:H4'	30:a:379:A:H5''	1.86	0.57
30:a:1727:G:H2'	30:a:1728:A:C8	2.39	0.57
35:f:113:LEU:HA	35:f:117:LEU:HD21	1.87	0.57
6:A:618:U:O3'	22:Q:11:ARG:NH2	2.37	0.57
30:a:1224:U:OP2	37:i:68:LYS:NZ	2.37	0.57
30:a:2843:G:O6	36:g:177:LYS:NZ	2.31	0.57
32:c:147:LEU:HD13	32:c:155:MET:HE2	1.87	0.57
6:A:1023:C:H2'	6:A:1024:G:C8	2.36	0.57
11:F:21:SER:HA	11:F:24:GLU:HG3	1.86	0.57
18:M:80:THR:HG23	18:M:83:THR:OG1	2.04	0.57
5:4:44:PHE:HE2	35:f:185:PRO:HB3	1.70	0.57
6:A:668:G:O2'	6:A:685:G:N2	2.38	0.57
6:A:1056:C:H2'	6:A:1057:G:H8	1.70	0.57
30:a:392:G:N1	30:a:395:A:OP2	2.35	0.57
30:a:2208:G:H2'	30:a:2209:A:C8	2.40	0.57
52:x:19:ASN:O	52:x:23:GLU:HG3	2.04	0.57
6:A:21:U:H2'	6:A:22:C:C6	2.40	0.56
34:e:160:LEU:C	34:e:162:ARG:H	2.13	0.56
43:o:3:ASN:O	43:o:7:GLU:HG3	2.04	0.56
9:D:26:PHE:O	9:D:29:ARG:NE	2.28	0.56
34:e:153:LEU:HB3	34:e:194:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:521:A:H2'	6:A:522:G:H8	1.70	0.56
6:A:739:U:H2'	6:A:740:G:O4'	2.06	0.56
6:A:1154:C:H3'	6:A:1155:A:H8	1.69	0.56
6:A:1441:U:H2'	6:A:1442:G:C8	2.40	0.56
9:D:69:ARG:O	9:D:73:GLU:HG3	2.06	0.56
9:D:148:PRO:O	9:D:152:ILE:HG12	2.05	0.56
30:a:63:A:H2'	30:a:64:C:C6	2.40	0.56
30:a:142:G:H22	30:a:147:G:H22	1.53	0.56
7:B:174:ILE:O	7:B:178:ARG:HG2	2.06	0.56
30:a:1481:C:H2'	30:a:1482:G:H8	1.70	0.56
30:a:1711:G:N1	30:a:1725:G:O2'	2.30	0.56
32:c:133:LEU:HD12	32:c:136:ILE:HD12	1.88	0.56
6:A:12:A:N6	9:D:197:GLU:O	2.39	0.56
15:J:69:GLN:NE2	15:J:104:ASP:OD1	2.39	0.56
52:x:35:SER:HB2	52:x:40:LEU:HD22	1.87	0.56
6:A:454:A:H5''	6:A:455:G:H21	1.70	0.56
6:A:751:G:H4'	6:A:1500:A:H4'	1.87	0.56
31:b:40:U:N3	31:b:44:G:OP2	2.32	0.56
46:r:54:LYS:HE3	46:r:65:ARG:HD2	1.88	0.56
6:A:317:A:N7	6:A:330:U:H5	2.03	0.56
34:e:153:LEU:H	34:e:154:ARG:CZ	2.19	0.56
43:o:2:SER:OG	43:o:3:ASN:N	2.39	0.56
6:A:1189:C:OP1	24:S:2:ALA:N	2.38	0.56
6:A:1500:A:H2'	6:A:1501:C:C6	2.41	0.56
6:A:1507:G:N7	28:X:15:LYS:NZ	2.44	0.56
7:B:213:LEU:O	7:B:217:ILE:HG23	2.06	0.56
27:V:21:ARG:NH2	30:a:1065:C:N3	2.54	0.56
30:a:1255:U:H4'	30:a:1256:G:N2	2.21	0.56
35:f:10:MET:HE1	35:f:15:LYS:HB3	1.87	0.56
6:A:697:A:H2'	6:A:698:A:C8	2.40	0.56
30:a:917:U:H2'	30:a:918:G:H8	1.70	0.56
6:A:1383:A:H4'	6:A:1384:C:H5''	1.88	0.55
19:N:12:ASP:O	19:N:44:ARG:NH2	2.38	0.55
30:a:1175:C:H2'	30:a:1176:G:O4'	2.07	0.55
36:g:57:ASP:OD2	36:g:59:GLU:N	2.39	0.55
38:j:35:LEU:HD21	38:j:65:THR:H	1.71	0.55
48:t:120:GLU:OE1	48:t:120:GLU:N	2.39	0.55
9:D:182:THR:O	9:D:186:ILE:HD12	2.05	0.55
30:a:1835:G:H5'	41:m:39:THR:HG21	1.88	0.55
6:A:1040:A:O2'	12:G:160:GLU:O	2.24	0.55
6:A:1309:G:H2'	6:A:1310:A:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:60:THR:HG22	7:B:65:GLY:HA2	1.89	0.55
30:a:2428:G:H2'	30:a:2429:A:C8	2.42	0.55
6:A:1342:G:H2'	6:A:1343:A:H8	1.69	0.55
9:D:14:ARG:HA	9:D:32:PRO:HB3	1.88	0.55
10:E:133:SER:HB3	10:E:160:VAL:HG23	1.88	0.55
14:I:90:GLU:H	14:I:90:GLU:CD	2.15	0.55
19:N:7:VAL:HG11	19:N:22:ILE:HG12	1.89	0.55
30:a:1901:U:H2'	30:a:1902:C:C6	2.41	0.55
30:a:2042:A:N6	30:a:2066:G:H1	2.03	0.55
34:e:11:ASP:HB2	34:e:17:ALA:HB3	1.87	0.55
39:k:56:ILE:HD12	39:k:57:HIS:N	2.21	0.55
54:z:31:ALA:O	54:z:54:ARG:NH1	2.39	0.55
7:B:100:MET:HA	7:B:107:ILE:HG13	1.88	0.55
7:B:191:ASN:ND2	7:B:191:ASN:O	2.40	0.55
9:D:80:LYS:HE2	10:E:124:PRO:HB2	1.89	0.55
12:G:11:ARG:NH1	12:G:176:THR:O	2.39	0.55
30:a:83:A:H62	30:a:101:G:H8	1.53	0.55
30:a:373:G:N3	30:a:438:G:N2	2.55	0.55
6:A:521:A:H2'	6:A:522:G:C8	2.40	0.55
6:A:829:C:H5'	23:R:17:HIS:CE1	2.42	0.55
30:a:994:A:H2'	30:a:995:A:C8	2.42	0.55
30:a:2425:U:H2'	30:a:2426:U:C6	2.41	0.55
30:a:2612:A:H2'	30:a:2612:A:N3	2.21	0.55
6:A:1080:U:OP1	6:A:1093:G:N2	2.33	0.55
25:T:36:ARG:O	25:T:40:GLU:HG3	2.07	0.55
6:A:208:U:H5''	25:T:52:ARG:NH2	2.21	0.55
6:A:1460:G:H2'	6:A:1461:G:C8	2.41	0.55
24:S:47:MET:HG2	24:S:52:GLN:HB2	1.89	0.55
30:a:263:A:H2'	30:a:264:A:C8	2.42	0.55
33:d:105:ASP:N	33:d:105:ASP:OD2	2.38	0.55
40:l:60:ARG:HD3	40:l:60:ARG:N	2.19	0.55
6:A:326:G:N1	6:A:329:A:OP2	2.40	0.55
6:A:1162:A:H2'	6:A:1163:G:C8	2.42	0.55
30:a:827:U:H2'	30:a:828:C:C6	2.42	0.55
39:k:56:ILE:HD12	39:k:57:HIS:H	1.72	0.55
11:F:18:GLN:O	11:F:22:LEU:HG	2.06	0.54
30:a:63:A:H2'	30:a:64:C:H6	1.72	0.54
30:a:130:G:H22	30:a:154:G:N2	2.04	0.54
30:a:1143:U:H4'	30:a:1144:U:H5'	1.89	0.54
30:a:2382:C:OP2	51:w:37:ARG:NH1	2.40	0.54
6:A:9:U:O2'	6:A:10:G:O5'	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:208:U:H4'	25:T:52:ARG:HE	1.72	0.54
6:A:527:C:H5'	9:D:64:GLU:HB2	1.90	0.54
6:A:728:U:H2'	6:A:729:U:N3	2.21	0.54
17:L:33:VAL:HG22	17:L:79:MET:HE1	1.89	0.54
18:M:40:VAL:HG23	18:M:73:LEU:HB3	1.88	0.54
30:a:1078:C:O2	37:i:3:THR:OG1	2.25	0.54
33:d:23:GLU:OE2	33:d:24:HIS:ND1	2.40	0.54
6:A:140:U:O2	6:A:226:G:O6	2.26	0.54
30:a:1985:A:H2'	30:a:1986:A:C8	2.41	0.54
30:a:2445:C:N4	50:v:15:ASP:OD1	2.40	0.54
34:e:11:ASP:OD2	34:e:200:GLN:NE2	2.39	0.54
6:A:495:A:H2'	6:A:496:C:C6	2.42	0.54
30:a:1159:C:H2'	30:a:1160:A:C4	2.42	0.54
30:a:1490:A:H2	30:a:1772:G:H22	1.56	0.54
30:a:1708:G:H22	30:a:1729:G:H1	1.55	0.54
6:A:1091:G:O2'	12:G:168:ARG:NH2	2.40	0.54
15:J:84:LYS:HZ3	15:J:88:GLN:H	1.55	0.54
30:a:1418:A:O2'	30:a:1420:U:OP1	2.26	0.54
35:f:144:GLN:HG2	35:f:159:ARG:HG3	1.88	0.54
49:u:38:HIS:ND1	49:u:39:ASP:O	2.41	0.54
6:A:987:G:H1	6:A:1022:U:H3	1.56	0.54
30:a:1698:G:H1	30:a:1915:G:N2	2.05	0.54
30:a:2650:G:O2'	30:a:2663:G:N2	2.39	0.54
45:q:49:ASP:OD1	45:q:49:ASP:N	2.39	0.54
6:A:277:G:H5'	22:Q:23:LYS:HD3	1.89	0.54
6:A:418:G:H2'	6:A:419:G:H8	1.73	0.54
6:A:996:C:H2'	6:A:997:A:C8	2.43	0.54
30:a:374:C:H2'	30:a:375:G:C8	2.42	0.54
30:a:565:G:N1	30:a:568:A:OP2	2.37	0.54
1:O:24:TYR:OH	30:a:2529:C:O2'	2.24	0.54
23:R:73:THR:OG1	23:R:74:ALA:N	2.36	0.54
15:J:84:LYS:HZ3	15:J:88:GLN:N	2.05	0.54
30:a:2773:C:H2'	30:a:2774:G:C8	2.43	0.54
40:l:54:MET:SD	40:l:118:MET:HG2	2.48	0.54
42:n:86:THR:O	42:n:90:GLU:HG2	2.07	0.54
6:A:506:G:H2'	6:A:507:C:C6	2.43	0.54
9:D:171:ASN:C	21:P:119:ALA:HB1	2.32	0.54
30:a:1156:A:H2'	30:a:1157:G:C8	2.41	0.54
30:a:1350:G:N2	30:a:1378:U:O4	2.41	0.54
32:c:119:SER:HB2	32:c:130:ASN:HB3	1.90	0.54
34:e:167:ASP:O	34:e:171:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:61:GLU:OE1	36:g:62:ASN:ND2	2.41	0.54
6:A:721:C:OP1	11:F:2:ARG:NH2	2.41	0.53
6:A:1040:A:H2	6:A:1186:C:H42	1.56	0.53
13:H:118:ASP:OD2	13:H:118:ASP:N	2.41	0.53
30:a:1090:C:OP1	37:i:37:ARG:NH1	2.39	0.53
36:g:3:ARG:NH1	36:g:3:ARG:O	2.42	0.53
11:F:82:ASP:HB3	11:F:85:ILE:HD12	1.90	0.53
16:K:94:GLY:O	16:K:99:ARG:NH2	2.40	0.53
20:O:45:LYS:O	20:O:51:ARG:NH2	2.35	0.53
33:d:90:THR:OG1	33:d:92:ASP:OD2	2.27	0.53
34:e:154:ARG:HE	34:e:154:ARG:N	2.06	0.53
17:L:50:ARG:NH1	17:L:89:ASP:OD2	2.40	0.53
30:a:1042:A:H2'	30:a:1043:A:C8	2.43	0.53
30:a:1253:U:H2'	30:a:1254:G:C8	2.43	0.53
30:a:2291:U:O2'	30:a:2362:U:O4	2.23	0.53
30:a:2486:G:O2'	35:f:162:ASP:OD1	2.26	0.53
30:a:2961:U:H4'	30:a:2962:A:O5'	2.07	0.53
6:A:183:G:N2	6:A:226:G:O5'	2.41	0.53
6:A:463:G:O2'	6:A:465:C:N4	2.41	0.53
30:a:960:U:H4'	49:u:172:VAL:HG11	1.90	0.53
30:a:1152:A:H4'	30:a:1153:A:H8	1.73	0.53
6:A:9:U:O4	9:D:78:GLN:NE2	2.42	0.53
6:A:483:C:H2'	6:A:484:A:H8	1.73	0.53
6:A:1047:U:H2'	6:A:1048:C:C6	2.43	0.53
6:A:1503:2MG:N1	6:A:1506:MA6:OP2	2.41	0.53
18:M:11:ARG:NE	18:M:71:LYS:HG3	2.23	0.53
30:a:622:U:H2'	30:a:623:C:C6	2.44	0.53
30:a:1111:A:N3	30:a:2668:C:O2'	2.36	0.53
30:a:2473:U:H2'	30:a:2474:U:C6	2.43	0.53
6:A:989:G:O6	6:A:1009:G:O2'	2.23	0.53
14:I:114:LYS:O	14:I:119:ARG:NH1	2.41	0.53
18:M:63:GLU:OE2	24:S:58:LYS:NZ	2.37	0.53
6:A:42:G:H22	6:A:399:A:H5'	1.73	0.53
18:M:30:THR:HA	18:M:33:GLY:O	2.09	0.53
30:a:898:U:H2'	30:a:899:C:C6	2.44	0.53
34:e:133:VAL:HG21	34:e:138:PRO:HD2	1.89	0.53
40:l:31:ASP:H	40:l:107:SER:HB3	1.74	0.53
6:A:537:C:H2'	6:A:538:C:C6	2.44	0.53
6:A:537:C:H2'	6:A:538:C:H6	1.74	0.53
6:A:1412:A:H2'	6:A:1413:A:O4'	2.08	0.53
12:G:148:ILE:HD12	12:G:201:ILE:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:87:ARG:NH2	30:a:799:U:O5'	2.42	0.53
30:a:552:G:N2	30:a:555:A:OP2	2.32	0.53
30:a:1903:G:H22	30:a:1922:U:H5	1.57	0.53
30:a:2197:A:H2'	30:a:2198:A:C8	2.43	0.53
31:b:48:C:H2'	31:b:49:C:H6	1.73	0.53
48:t:29:VAL:HG13	48:t:36:VAL:HG12	1.91	0.53
46:r:78:THR:OG1	46:r:79:GLU:OE1	2.23	0.53
6:A:1283:U:H1'	6:A:1284:C:H5	1.73	0.53
30:a:2290:U:H3'	30:a:2291:U:C6	2.44	0.53
38:j:3:GLN:HE21	38:j:32:TYR:HE1	1.54	0.53
45:q:60:ALA:HB1	45:q:95:VAL:HG13	1.91	0.53
6:A:483:C:H2'	6:A:484:A:C8	2.43	0.52
6:A:1026:U:H2'	6:A:1027:U:C6	2.44	0.52
9:D:197:GLU:OE1	10:E:128:VAL:N	2.33	0.52
26:U:41:THR:O	26:U:44:MET:HG2	2.09	0.52
30:a:1142:G:N2	30:a:1163:C:O2	2.43	0.52
48:t:94:ARG:NH1	48:t:112:SER:OG	2.36	0.52
6:A:384:A:H2'	6:A:385:A:C8	2.44	0.52
6:A:512:G:C2	29:Y:22:U:H5''	2.44	0.52
6:A:1300:C:H2'	6:A:1301:U:C6	2.44	0.52
20:O:68:ILE:HG22	20:O:76:TYR:HB2	1.91	0.52
30:a:2180:C:H5'	33:d:128:MET:HE1	1.91	0.52
12:G:118:GLY:O	12:G:122:GLN:HG3	2.10	0.52
30:a:374:C:O2'	30:a:375:G:O4'	2.19	0.52
30:a:1145:G:N2	30:a:1160:A:N1	2.56	0.52
30:a:2509:A:H2'	30:a:2510:A:C8	2.44	0.52
42:n:38:MET:HE2	42:n:100:VAL:HG21	1.92	0.52
6:A:382:G:N2	6:A:385:A:OP2	2.39	0.52
30:a:130:G:H1	30:a:154:G:H1	1.56	0.52
30:a:1391:C:H2'	30:a:1392:A:H8	1.74	0.52
30:a:2502:U:O4	30:a:2515:A:O2'	2.22	0.52
35:f:127:ASN:H	35:f:127:ASN:ND2	2.07	0.52
6:A:1242:U:OP2	6:A:1265:A:N6	2.43	0.52
9:D:163:PRO:HB2	9:D:165:TRP:CD1	2.45	0.52
9:D:179:GLN:OE1	9:D:179:GLN:N	2.43	0.52
21:P:112:ALA:O	21:P:116:PRO:HD2	2.10	0.52
30:a:1491:C:H2'	30:a:1492:C:H6	1.74	0.52
2:l:7:PRO:HB2	30:a:1385:G:H4'	1.92	0.52
6:A:1517:G:H2'	6:A:1518:A:O4'	2.10	0.52
30:a:4:A:H2'	30:a:5:A:C8	2.45	0.52
30:a:2256:U:H2'	30:a:2257:U:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2982:U:OP2	30:a:2983:C:N4	2.43	0.52
51:w:3:ALA:HB1	51:w:12:PRO:HG3	1.90	0.52
25:T:31:TYR:CE2	25:T:57:GLN:HG3	2.45	0.52
30:a:917:U:H2'	30:a:918:G:C8	2.45	0.52
30:a:1147:C:H2'	30:a:1148:U:O4'	2.10	0.52
39:k:68:ASN:HB3	39:k:71:ARG:HB2	1.92	0.52
9:D:147:LEU:HB2	9:D:150:ILE:HG22	1.92	0.52
16:K:112:GLU:H	16:K:112:GLU:CD	2.15	0.52
17:L:54:ARG:HH21	17:L:62:GLU:HB3	1.74	0.52
27:V:12:ARG:NH2	31:b:89:G:OP1	2.39	0.52
30:a:3016:U:H2'	30:a:3017:A:H8	1.75	0.52
21:P:113:ASP:OD1	21:P:114:GLU:N	2.43	0.52
30:a:3055:U:H4'	43:o:2:SER:HA	1.91	0.52
52:x:49:VAL:O	52:x:53:ILE:HG13	2.10	0.52
11:F:15:GLU:OE1	11:F:15:GLU:N	2.43	0.51
30:a:26:G:N2	30:a:600:G:H1'	2.26	0.51
30:a:1043:A:H61	40:l:83:MET:HE2	1.76	0.51
30:a:1095:U:H5'	30:a:1096:G:H5''	1.92	0.51
30:a:1492:C:H2'	30:a:1493:G:C8	2.45	0.51
30:a:2915:U:H2'	30:a:2916:U:C6	2.44	0.51
33:d:192:ILE:HG21	43:o:8:ILE:HD11	1.93	0.51
7:B:110:ARG:HH21	7:B:145:LEU:HD11	1.75	0.51
54:z:35:CYS:HB2	54:z:48:CYS:HB3	1.91	0.51
30:a:1145:G:H2'	30:a:1146:G:H8	1.76	0.51
30:a:2252:G:H2'	30:a:2253:A:C8	2.46	0.51
6:A:1236:A:H4'	15:J:111:GLY:HA2	1.91	0.51
17:L:54:ARG:NH1	17:L:64:THR:OG1	2.44	0.51
30:a:599:U:H4'	30:a:1312:G:H4'	1.91	0.51
30:a:881:A:H2'	30:a:882:C:C6	2.46	0.51
30:a:1156:A:H1'	30:a:2656:U:H4'	1.92	0.51
30:a:1862:A:H2'	30:a:1863:A:C8	2.45	0.51
30:a:2053:U:H3'	30:a:2054:A:H8	1.74	0.51
30:a:3037:G:N2	30:a:3040:A:OP2	2.31	0.51
39:k:94:VAL:HG22	39:k:97:LEU:CD2	2.41	0.51
6:A:339:G:H2'	6:A:340:A:C8	2.46	0.51
6:A:936:C:H2'	6:A:937:G:H8	1.76	0.51
12:G:47:GLU:OE1	12:G:47:GLU:HA	2.09	0.51
12:G:133:MET:HE2	12:G:167:TYR:HD1	1.75	0.51
14:I:65:ALA:O	14:I:69:ILE:HD12	2.11	0.51
30:a:503:C:H2'	30:a:504:A:H8	1.75	0.51
30:a:1404:G:H2'	30:a:1406:C:C5	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:60:U:H2'	6:A:61:G:C8	2.45	0.51
30:a:336:G:O2'	30:a:357:G:N7	2.44	0.51
30:a:503:C:H2'	30:a:504:A:C8	2.45	0.51
30:a:725:U:H2'	30:a:726:C:C6	2.45	0.51
30:a:1189:G:H2'	30:a:1190:G:H8	1.75	0.51
30:a:1851:G:O2'	30:a:2174:U:O4	2.26	0.51
32:c:172:TYR:HB3	32:c:184:MET:HG2	1.92	0.51
40:l:51:ARG:HD3	40:l:66:ILE:HD11	1.91	0.51
6:A:110:C:O2'	21:P:26:ARG:O	2.28	0.51
15:J:44:MET:H	15:J:44:MET:HE3	1.75	0.51
30:a:263:A:H2'	30:a:264:A:H8	1.74	0.51
30:a:1083:A:H2'	30:a:1084:A:C8	2.45	0.51
30:a:2880:U:H2'	30:a:2881:U:C6	2.45	0.51
43:o:16:ASP:OD1	43:o:16:ASP:N	2.34	0.51
54:z:45:CYS:HB3	54:z:48:CYS:SG	2.51	0.51
6:A:443:G:H1'	6:A:479:G:N2	2.26	0.51
6:A:930:A:H2'	6:A:931:G:H8	1.75	0.51
21:P:81:GLN:OE1	21:P:81:GLN:N	2.44	0.51
30:a:1224:U:OP2	37:i:65:THR:OG1	2.27	0.51
30:a:1861:A:H2'	30:a:1862:A:H8	1.75	0.51
30:a:2253:A:H2'	30:a:2254:C:C6	2.46	0.51
40:l:57:TYR:HD1	40:l:117:ALA:HB2	1.76	0.51
3:2:7:HIS:NE2	30:a:258:A:OP1	2.40	0.51
6:A:1137:G:O2'	6:A:1138:U:H5''	2.11	0.51
6:A:1378:U:H2'	6:A:1379:G:C8	2.46	0.51
14:I:115:THR:O	14:I:119:ARG:HB2	2.11	0.51
30:a:279:A:H62	30:a:319:G:H21	1.58	0.51
30:a:2247:C:H2'	30:a:2248:C:C6	2.46	0.51
36:g:95:TYR:HA	36:g:108:ASN:O	2.11	0.51
38:j:92:GLU:HG3	38:j:93:PRO:HD2	1.92	0.51
49:u:160:PRO:O	49:u:163:THR:OG1	2.25	0.51
6:A:1418:C:H2'	6:A:1419:G:O4'	2.10	0.51
14:I:136:LYS:HA	14:I:139:GLU:OE1	2.11	0.51
19:N:69:ASP:OD2	19:N:70:LEU:N	2.44	0.51
24:S:24:CYS:HB3	24:S:29:ARG:H	1.76	0.51
26:U:44:MET:C	26:U:47:HIS:HD1	2.19	0.51
30:a:669:A:N1	30:a:894:G:O2'	2.38	0.51
30:a:1612:G:H2'	30:a:1613:U:C6	2.46	0.51
6:A:561:U:H2'	6:A:562:C:C6	2.46	0.50
6:A:938:G:H2'	6:A:939:A:C8	2.45	0.50
30:a:723:A:H5''	39:k:114:THR:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:806:U:H2'	30:a:807:C:C6	2.47	0.50
36:g:106:GLU:OE1	36:g:114:PRO:HB2	2.10	0.50
38:j:63:VAL:HG12	38:j:106:LEU:HD21	1.93	0.50
22:Q:14:VAL:O	22:Q:15:ARG:NH1	2.43	0.50
30:a:1491:C:H2'	30:a:1492:C:C6	2.45	0.50
32:c:9:THR:HG22	32:c:10:THR:HG23	1.93	0.50
47:s:20:GLU:H	47:s:20:GLU:CD	2.18	0.50
6:A:1356:C:H2'	6:A:1357:G:C8	2.45	0.50
6:A:1399:C:H2'	6:A:1400:A:C8	2.47	0.50
9:D:99:ARG:HH22	9:D:187:VAL:HG22	1.77	0.50
18:M:42:LEU:HG	18:M:71:LYS:HD3	1.92	0.50
30:a:303:G:H2'	30:a:304:G:O4'	2.11	0.50
30:a:788:U:H2'	30:a:789:G:O4'	2.12	0.50
30:a:1199:U:H2'	30:a:1200:U:C6	2.46	0.50
30:a:1754:A:H2'	30:a:1755:A:C8	2.46	0.50
30:a:2651:A:H2'	30:a:2652:G:O4'	2.12	0.50
43:o:15:ASP:OD2	43:o:15:ASP:N	2.43	0.50
43:o:62:ARG:HG3	43:o:71:GLU:HG3	1.93	0.50
6:A:79:C:H2'	6:A:80:C:C6	2.46	0.50
30:a:339:U:H3'	30:a:340:C:H6	1.76	0.50
30:a:670:G:H5'	34:e:93:HIS:CD2	2.47	0.50
30:a:729:A:N1	30:a:2551:A:O2'	2.44	0.50
30:a:2009:C:O2'	30:a:2154:U:OP2	2.29	0.50
30:a:2473:U:OP1	30:a:2562:U:O2'	2.30	0.50
48:t:35:ARG:HB3	48:t:69:PRO:HB2	1.93	0.50
6:A:208:U:H5''	25:T:52:ARG:HH21	1.76	0.50
6:A:718:U:H2'	6:A:719:C:H6	1.76	0.50
6:A:1241:G:O2'	6:A:1244:G:N3	2.38	0.50
20:O:87:ARG:HH11	20:O:87:ARG:C	2.20	0.50
25:T:8:ILE:O	25:T:11:VAL:HG22	2.11	0.50
26:U:3:ARG:HH11	26:U:10:PHE:HB2	1.76	0.50
29:Y:21:U:H2'	29:Y:22:U:H4'	1.93	0.50
30:a:453:U:O2	30:a:455:C:N4	2.40	0.50
31:b:25:A:H2'	31:b:26:A:C8	2.46	0.50
6:A:1138:U:OP1	18:M:70:HIS:ND1	2.37	0.50
11:F:45:LYS:HG2	11:F:57:GLU:HG2	1.94	0.50
30:a:1174:G:H2'	30:a:1175:C:C6	2.47	0.50
30:a:2579:A:H2'	30:a:2580:C:C6	2.47	0.50
50:v:84:GLU:OE1	50:v:84:GLU:N	2.33	0.50
10:E:155:ASN:O	10:E:159:VAL:HG23	2.11	0.50
30:a:291:U:H5'	30:a:308:U:H5	1.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2268:U:H2'	30:a:2269:G:C8	2.47	0.50
35:f:117:LEU:H	35:f:117:LEU:HD23	1.77	0.50
5:4:65:TYR:HE2	26:U:5:LEU:HD12	1.76	0.50
6:A:1169:U:O2'	6:A:1170:G:OP1	2.28	0.50
12:G:55:GLU:HB3	12:G:66:PHE:HB2	1.94	0.50
12:G:125:ALA:O	12:G:126:ARG:HG2	2.11	0.50
38:j:7:ARG:HD3	38:j:18:GLU:OE2	2.12	0.50
2:1:25:ARG:NH2	30:a:218:G:OP1	2.42	0.50
6:A:996:C:H2'	6:A:997:A:H8	1.75	0.50
6:A:1282:C:H4'	6:A:1288:U:O4	2.12	0.50
7:B:30:PHE:CZ	7:B:41:ILE:HG23	2.47	0.50
30:a:1912:U:H3'	30:a:1913:G:H3'	1.93	0.50
30:a:1980:G:HO2'	32:c:257:THR:HG1	1.60	0.50
30:a:2971:C:H1'	30:a:3071:A:H2	1.77	0.50
36:g:157:GLU:OE2	36:g:160:LYS:N	2.45	0.50
6:A:992:U:H2'	6:A:993:G:C8	2.46	0.49
30:a:1165:U:H3'	30:a:1166:G:H8	1.76	0.49
14:I:31:LEU:O	14:I:31:LEU:HD13	2.11	0.49
15:J:109:ILE:HD12	15:J:121:LEU:HD21	1.94	0.49
20:O:10:ILE:HG21	20:O:20:THR:HG22	1.95	0.49
25:T:15:GLU:O	25:T:19:GLN:HG2	2.12	0.49
30:a:2403:A:O2'	32:c:188:ARG:NH2	2.44	0.49
30:a:2773:C:H2'	30:a:2774:G:H8	1.76	0.49
47:s:54:VAL:HG13	47:s:92:ASP:HB3	1.94	0.49
51:w:16:HIS:HA	51:w:25:THR:O	2.11	0.49
6:A:503:G:H4'	17:L:70:VAL:HG22	1.93	0.49
6:A:1271:G:H4'	6:A:1272:G:O5'	2.12	0.49
20:O:6:LYS:O	20:O:10:ILE:HG13	2.12	0.49
20:O:38:THR:O	20:O:42:LYS:HG2	2.12	0.49
26:U:3:ARG:HH21	26:U:7:LYS:HG2	1.78	0.49
30:a:2977:A:H2'	30:a:2978:G:O4'	2.11	0.49
30:a:2986:G:H2'	30:a:2987:G:C8	2.47	0.49
10:E:116:VAL:HB	10:E:151:LEU:O	2.12	0.49
30:a:709:U:H2'	30:a:710:C:C6	2.47	0.49
30:a:1650:A:H2'	30:a:1651:A:C8	2.47	0.49
42:n:64:SER:OG	42:n:65:THR:N	2.45	0.49
6:A:299:G:N2	6:A:302:A:OP2	2.32	0.49
6:A:827:C:H3'	6:A:828:A:C8	2.47	0.49
6:A:1202:U:H2'	6:A:1203:C:H6	1.76	0.49
6:A:1225:A:H62	6:A:1285:A:N6	2.11	0.49
10:E:117:VAL:HG11	10:E:163:THR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:71:LYS:HB3	15:J:106:ILE:HD13	1.94	0.49
18:M:10:LEU:HD12	18:M:72:ARG:HB3	1.94	0.49
30:a:373:G:N2	30:a:374:C:O4'	2.45	0.49
30:a:692:A:H2'	30:a:693:A:C8	2.48	0.49
30:a:1995:A:H2'	30:a:1996:C:C6	2.48	0.49
30:a:2494:U:H5'	35:f:94:ILE:HD11	1.94	0.49
30:a:2513:G:O2'	30:a:2518:A:N1	2.42	0.49
7:B:73:LYS:HZ3	7:B:166:ASP:HB2	1.77	0.49
9:D:56:ALA:HB2	9:D:190:VAL:HG21	1.94	0.49
25:T:7:GLN:O	25:T:11:VAL:HG13	2.13	0.49
30:a:2527:G:N3	30:a:2563:C:H2'	2.27	0.49
30:a:2800:G:H21	33:d:161:VAL:HG21	1.77	0.49
30:a:2859:U:H2'	30:a:2860:G:C8	2.48	0.49
6:A:678:A:H2'	6:A:679:U:H6	1.76	0.49
6:A:821:C:H2'	6:A:822:C:H6	1.78	0.49
20:O:5:GLU:CD	20:O:5:GLU:N	2.70	0.49
30:a:115:C:O2'	30:a:125:A:N3	2.41	0.49
30:a:1716:U:H2'	30:a:1717:G:C8	2.48	0.49
35:f:171:THR:HG22	35:f:173:GLU:H	1.76	0.49
1:0:43:CYS:HB3	1:0:46:CYS:HB2	1.94	0.49
6:A:710:A:H2'	6:A:711:A:C8	2.48	0.49
3:2:26:LYS:HD3	3:2:48:THR:HB	1.93	0.49
12:G:82:GLU:O	12:G:86:VAL:HG13	2.13	0.49
18:M:51:VAL:CG1	24:S:41:ARG:HG3	2.43	0.49
30:a:450:G:C2	30:a:451:G:C8	3.01	0.49
30:a:2630:A:O2'	30:a:2631:H2U:H52	2.13	0.49
31:b:48:C:H2'	31:b:49:C:C6	2.47	0.49
6:A:1304:A:H1'	26:U:37:ARG:HH11	1.78	0.49
22:Q:1:MET:SD	22:Q:2:SER:N	2.85	0.49
30:a:203:A:C2	39:k:49:PHE:HZ	2.31	0.49
30:a:373:G:N2	30:a:437:G:H1	2.11	0.49
52:x:52:ASP:O	52:x:56:VAL:HG23	2.13	0.49
6:A:998:G:N2	6:A:1001:A:OP2	2.35	0.48
6:A:1346:A:H2'	6:A:1347:G:C8	2.48	0.48
30:a:682:U:H2'	30:a:683:G:C8	2.48	0.48
30:a:1628:C:O2'	30:a:1727:G:N3	2.38	0.48
49:u:122:GLU:HG3	49:u:172:VAL:HG23	1.94	0.48
53:y:12:SER:HB3	53:y:32:ILE:HD11	1.95	0.48
6:A:12:A:N6	9:D:201:LYS:HB3	2.28	0.48
6:A:821:C:H2'	6:A:822:C:C6	2.48	0.48
6:A:982:G:H2'	6:A:983:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1003:G:H2'	6:A:1004:G:H5'	1.95	0.48
6:A:1503:2MG:HM21	6:A:1506:MA6:N7	2.28	0.48
7:B:176:GLU:O	7:B:180:LEU:HG	2.13	0.48
10:E:178:ARG:HG2	10:E:178:ARG:HH11	1.78	0.48
14:I:21:PRO:O	14:I:24:SER:OG	2.26	0.48
40:l:54:MET:HE1	40:l:104:PHE:HB3	1.95	0.48
5:4:44:PHE:CE2	35:f:185:PRO:HB3	2.48	0.48
6:A:78:G:H2'	6:A:79:C:C6	2.49	0.48
30:a:272:A:N6	30:a:516:U:O2'	2.37	0.48
30:a:445:U:H2'	30:a:446:G:C8	2.48	0.48
30:a:2474:U:H2'	30:a:2475:C:C6	2.47	0.48
48:t:81:ILE:HD12	48:t:82:ASP:N	2.27	0.48
53:y:2:MET:HA	53:y:40:ASP:HB3	1.95	0.48
5:4:61:PHE:O	5:4:65:TYR:HB2	2.12	0.48
6:A:1333:G:N7	15:J:55:LYS:HE2	2.29	0.48
30:a:491:A:H2'	30:a:492:U:O4'	2.13	0.48
30:a:1624:A:H2'	30:a:1626:C:C5	2.48	0.48
30:a:1686:C:H2'	30:a:1687:G:O4'	2.13	0.48
30:a:1973:C:H2'	30:a:1974:A:C5	2.49	0.48
30:a:2644:U:H2'	30:a:2645:U:C6	2.48	0.48
30:a:2779:G:H2'	30:a:2780:A:C8	2.48	0.48
33:d:23:GLU:OE1	33:d:23:GLU:N	2.45	0.48
6:A:508:C:OP2	17:L:88:LYS:NZ	2.43	0.48
6:A:904:U:H2'	6:A:905:U:C6	2.49	0.48
6:A:1105:C:H2'	6:A:1106:A:C8	2.42	0.48
7:B:155:MET:HE1	7:B:159:PRO:HG3	1.96	0.48
13:H:101:LEU:HD12	13:H:135:TRP:CD1	2.48	0.48
30:a:663:C:H2'	30:a:664:C:C6	2.48	0.48
30:a:1418:A:OP1	47:s:41:LYS:NZ	2.27	0.48
30:a:1894:U:H2'	30:a:1895:G:O4'	2.13	0.48
30:a:2571:G:H5''	30:a:2572:U:O4'	2.13	0.48
30:a:2838:U:O2	30:a:2847:A:N7	2.47	0.48
30:a:2980:G:H2'	30:a:2981:U:C2	2.49	0.48
34:e:155:LYS:HZ2	34:e:155:LYS:HB3	1.78	0.48
38:j:73:ASP:OD1	38:j:75:SER:OG	2.22	0.48
6:A:113:G:H1'	6:A:356:G:H5'	1.96	0.48
6:A:148:G:H2'	6:A:149:G:H8	1.78	0.48
30:a:714:G:H2'	30:a:715:C:C6	2.48	0.48
30:a:1615:A:H2'	30:a:1616:G:C8	2.48	0.48
39:k:99:SER:OG	39:k:105:ASP:HB3	2.14	0.48
6:A:266:U:O2'	22:Q:73:PRO:O	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:116:PRO:HA	21:P:119:ALA:HB3	1.94	0.48
30:a:1111:A:H2'	30:a:1112:A:C8	2.49	0.48
30:a:1306:U:O2'	30:a:1307:G:OP1	2.24	0.48
30:a:1337:G:OP1	46:r:100:ARG:NH1	2.47	0.48
30:a:1812:G:H2'	30:a:1813:U:C6	2.48	0.48
30:a:2455:A:H2'	30:a:2456:A:C8	2.48	0.48
34:e:119:ASP:OD2	39:k:2:ALA:N	2.47	0.48
16:K:56:VAL:HG21	16:K:71:MET:HB3	1.96	0.48
19:N:15:LEU:HD23	19:N:34:LEU:HD11	1.95	0.48
26:U:84:VAL:C	26:U:85:LYS:HE2	2.39	0.48
30:a:2263:U:H2'	30:a:2264:A:H8	1.79	0.48
35:f:156:ASP:OD1	35:f:156:ASP:N	2.41	0.48
41:m:36:THR:O	41:m:40:LYS:HB2	2.14	0.48
1:0:47:ARG:HG2	1:0:47:ARG:HH11	1.78	0.48
6:A:1265:A:O2'	6:A:1268:C:N4	2.46	0.48
23:R:68:LEU:HD23	23:R:69:PRO:HD2	1.96	0.48
30:a:286:G:N7	30:a:313:G:N2	2.61	0.48
30:a:727:C:O2'	30:a:2532:U:OP1	2.25	0.48
30:a:1600:C:O2'	30:a:2393:G:N1	2.46	0.48
30:a:2366:U:H2'	30:a:2367:G:C8	2.49	0.48
35:f:143:GLU:OE2	35:f:146:MET:N	2.46	0.48
6:A:392:U:H2'	6:A:393:G:C8	2.48	0.48
6:A:772:A:OP1	8:C:38:A:O2'	2.32	0.48
6:A:1434:A:P	6:A:1435:C:H41	2.37	0.48
12:G:69:ALA:O	12:G:105:VAL:HG23	2.14	0.48
30:a:2423:A:H2'	30:a:2424:G:C8	2.49	0.48
30:a:2710:U:H2'	30:a:2712:G:H5''	1.95	0.48
34:e:156:VAL:HG12	34:e:158:VAL:HG13	1.96	0.48
45:q:89:ARG:HA	45:q:89:ARG:HD2	1.70	0.48
47:s:8:ASP:OD2	47:s:10:ARG:NH1	2.47	0.48
6:A:1361:A:O2'	14:I:31:LEU:HD12	2.13	0.47
15:J:163:LYS:HB2	15:J:166:LYS:HB3	1.96	0.47
30:a:1724:G:H3'	30:a:1725:G:C8	2.49	0.47
30:a:1861:A:H2'	30:a:1862:A:C8	2.48	0.47
30:a:2072:A:H2'	30:a:2073:A:C8	2.49	0.47
30:a:2415:U:H2'	30:a:2416:G:C8	2.49	0.47
33:d:92:ASP:OD2	33:d:92:ASP:N	2.47	0.47
35:f:78:LYS:HB3	35:f:91:GLY:HA2	1.95	0.47
36:g:123:ILE:HD11	36:g:142:VAL:HG11	1.96	0.47
37:i:4:TYR:CG	44:p:100:VAL:HG11	2.48	0.47
11:F:26:TYR:O	11:F:29:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:334:G:H2'	30:a:334:G:N3	2.29	0.47
30:a:433:G:H2'	30:a:435:G:O4'	2.14	0.47
30:a:1437:G:H2'	30:a:1438:C:C6	2.48	0.47
30:a:1984:G:H3'	30:a:1985:A:H5'	1.96	0.47
30:a:2135:A:N3	30:a:2742:C:O2'	2.44	0.47
30:a:2429:A:H2'	30:a:2430:C:H6	1.79	0.47
34:e:159:VAL:HG13	34:e:160:LEU:N	2.30	0.47
42:n:37:ARG:NH2	42:n:54:ASP:OD1	2.45	0.47
42:n:42:ARG:HB2	42:n:113:ILE:HD11	1.96	0.47
42:n:80:LYS:O	42:n:84:VAL:HG23	2.15	0.47
6:A:1288:U:C6	19:N:17:VAL:HG11	2.49	0.47
16:K:77:GLY:O	16:K:81:MET:HG2	2.13	0.47
35:f:59:MET:HE1	35:f:96:CYS:HB3	1.94	0.47
52:x:12:LEU:O	52:x:63:ARG:NH2	2.39	0.47
6:A:906:G:H2'	6:A:907:A:C8	2.49	0.47
6:A:1210:U:O2'	6:A:1308:C:OP1	2.23	0.47
11:F:7:MET:SD	23:R:65:LEU:HD21	2.54	0.47
12:G:141:MET:HE3	12:G:141:MET:O	2.15	0.47
16:K:87:ARG:HD2	16:K:87:ARG:O	2.13	0.47
18:M:11:ARG:HB2	18:M:97:ASP:OD2	2.14	0.47
27:V:20:LYS:NZ	30:a:1069:C:OP1	2.47	0.47
30:a:361:G:N2	30:a:443:G:H22	2.11	0.47
30:a:390:C:H2'	30:a:391:U:C6	2.49	0.47
30:a:1977:U:H2'	30:a:1978:C:H6	1.79	0.47
39:k:88:LYS:HD2	39:k:88:LYS:C	2.40	0.47
30:a:373:G:N2	30:a:437:G:H22	2.12	0.47
30:a:377:G:H2'	30:a:378:A:O4'	2.15	0.47
30:a:407:A:OP2	34:e:173:ASN:HB2	2.14	0.47
30:a:682:U:H2'	30:a:683:G:H8	1.79	0.47
30:a:938:U:H2'	30:a:939:U:C6	2.49	0.47
30:a:1192:C:H2'	30:a:1193:A:O4'	2.14	0.47
30:a:1395:G:H2'	30:a:1396:U:C6	2.49	0.47
30:a:1962:U:OP2	30:a:1967:A:N6	2.35	0.47
30:a:1977:U:H2'	30:a:1978:C:C6	2.48	0.47
30:a:2887:A:O2'	30:a:3032:G:OP1	2.31	0.47
31:b:5:C:OP1	31:b:61:C:O2'	2.32	0.47
6:A:495:A:H2'	6:A:496:C:H6	1.80	0.47
9:D:87:GLN:NE2	9:D:181:PRO:O	2.46	0.47
30:a:361:G:N2	30:a:444:G:N3	2.62	0.47
30:a:431:A:H2'	30:a:432:A:O4'	2.15	0.47
30:a:1151:G:O2'	30:a:1179:A:O2'	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1391:C:H2'	30:a:1392:A:C8	2.49	0.47
30:a:1691:A:O2'	30:a:1692:G:H8	1.97	0.47
32:c:136:ILE:HD13	32:c:142:VAL:HG11	1.96	0.47
48:t:78:VAL:HG22	48:t:85:ASP:OD1	2.15	0.47
49:u:96:ARG:NH1	49:u:96:ARG:HB2	2.29	0.47
5:4:45:TYR:CE1	35:f:185:PRO:HG3	2.49	0.47
6:A:10:G:H4'	6:A:300:A:H4'	1.96	0.47
6:A:920:C:C2	6:A:921:A:C8	3.03	0.47
6:A:1050:U:H4'	6:A:1051:C:O5'	2.13	0.47
12:G:101:ASN:N	12:G:101:ASN:OD1	2.48	0.47
12:G:179:ALA:HB1	12:G:202:TYR:CE1	2.50	0.47
14:I:57:ASP:OD1	14:I:60:GLN:N	2.44	0.47
30:a:361:G:H1	30:a:443:G:H1	1.60	0.47
30:a:436:U:H2'	30:a:437:G:C8	2.50	0.47
30:a:1753:A:H2'	30:a:1754:A:C8	2.50	0.47
30:a:2925:C:O2'	36:g:152:LYS:HE2	2.14	0.47
32:c:147:LEU:HD12	32:c:183:ARG:NH2	2.30	0.47
39:k:79:LEU:HD13	39:k:117:LEU:HB2	1.96	0.47
39:k:80:ASP:OD1	39:k:80:ASP:N	2.48	0.47
39:k:94:VAL:H	39:k:97:LEU:HD23	1.80	0.47
6:A:139:U:H2'	6:A:140:U:C6	2.50	0.47
6:A:339:G:H2'	6:A:340:A:H8	1.80	0.47
6:A:861:C:OP1	13:H:85:LYS:HE3	2.14	0.47
30:a:686:G:O2'	30:a:740:A:N1	2.48	0.47
35:f:117:LEU:HG	35:f:118:PRO:HD3	1.95	0.47
6:A:1237:G:H4'	15:J:56:GLU:OE2	2.15	0.47
6:A:1271:G:H5'	6:A:1272:G:C4	2.50	0.47
6:A:1300:C:H2'	6:A:1301:U:H6	1.80	0.47
9:D:171:ASN:N	9:D:171:ASN:OD1	2.46	0.47
10:E:103:THR:OG1	10:E:145:ASP:O	2.24	0.47
11:F:52:ILE:HG22	11:F:53:GLN:NE2	2.29	0.47
28:X:3:SER:C	28:X:5:ILE:H	2.22	0.47
30:a:51:A:H2'	30:a:52:A:C8	2.50	0.47
30:a:337:G:H2'	30:a:338:U:O4'	2.14	0.47
30:a:418:G:O2'	30:a:419:U:OP1	2.29	0.47
30:a:442:U:H3'	30:a:443:G:H8	1.80	0.47
30:a:2739:G:H2'	30:a:2740:C:C6	2.50	0.47
30:a:3012:U:OP1	33:d:64:LYS:NZ	2.48	0.47
35:f:33:ASN:OD1	35:f:35:MET:HG2	2.15	0.47
35:f:60:ASP:O	35:f:63:ILE:HG13	2.14	0.47
40:l:118:MET:O	40:l:122:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:o:104:ARG:HB3	43:o:104:ARG:NH1	2.30	0.47
6:A:256:G:OP1	22:Q:77:THR:OG1	2.29	0.47
9:D:28:ARG:HB3	9:D:31:TYR:CZ	2.50	0.47
9:D:141:ARG:HH21	9:D:144:SER:HB2	1.80	0.47
18:M:66:GLU:HB3	24:S:59:SER:HB3	1.97	0.47
30:a:166:A:N3	30:a:2390:C:O2'	2.46	0.47
30:a:344:U:H2'	30:a:345:G:H21	1.79	0.47
30:a:1280:U:O2	39:k:6:HIS:HB3	2.15	0.47
30:a:1361:G:N2	30:a:1404:G:H5''	2.30	0.47
36:g:107:PHE:HB2	36:g:115:VAL:CG1	2.45	0.47
7:B:118:GLU:HA	7:B:142:LYS:HE3	1.97	0.46
18:M:82:LYS:H	18:M:82:LYS:HG3	1.56	0.46
19:N:50:ASP:O	19:N:54:VAL:HG12	2.14	0.46
30:a:568:A:H1'	30:a:569:A:H5''	1.97	0.46
30:a:1717:G:H1'	30:a:1718:G:O4'	2.14	0.46
30:a:2501:G:O2'	30:a:2502:U:O4'	2.28	0.46
30:a:2510:A:H2'	30:a:2511:G:H8	1.74	0.46
30:a:2730:G:N3	38:j:23:ARG:NH2	2.63	0.46
30:a:2807:G:H2'	30:a:2808:C:C6	2.50	0.46
30:a:2830:G:H2'	30:a:2831:U:C6	2.50	0.46
41:m:87:MET:HE1	41:m:116:ILE:HB	1.97	0.46
6:A:362:G:H2'	6:A:363:G:C8	2.50	0.46
6:A:411:G:H2'	6:A:412:G:O4'	2.16	0.46
6:A:1108:U:H4'	18:M:38:GLY:HA3	1.96	0.46
8:C:43:A:H2'	8:C:44:A:C8	2.49	0.46
16:K:52:SER:H	16:K:55:THR:HB	1.79	0.46
30:a:15:U:H5''	54:z:14:ARG:HB3	1.96	0.46
30:a:1906:C:H2'	30:a:1907:A:O4'	2.13	0.46
30:a:2041:G:N7	30:a:2067:A:O2'	2.48	0.46
30:a:2486:G:H22	30:a:2494:U:H3	1.62	0.46
46:r:50:VAL:HG21	46:r:72:MET:HE2	1.97	0.46
6:A:325:U:H2'	6:A:326:G:O4'	2.14	0.46
6:A:467:G:H1'	6:A:468:U:OP2	2.16	0.46
6:A:634:U:O4	6:A:734:G:O2'	2.24	0.46
6:A:929:G:C2	6:A:930:A:C8	3.03	0.46
6:A:994:C:H2'	6:A:995:U:O4'	2.16	0.46
9:D:138:ILE:HB	9:D:175:ILE:HB	1.97	0.46
9:D:157:PHE:CE1	9:D:170:PRO:HG3	2.51	0.46
19:N:33:THR:O	19:N:37:THR:HG22	2.15	0.46
19:N:67:GLU:O	19:N:71:ARG:HG2	2.14	0.46
30:a:637:U:H2'	30:a:638:G:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1148:U:H3'	30:a:1149:U:H5''	1.96	0.46
30:a:2053:U:H3'	30:a:2054:A:C8	2.50	0.46
30:a:2511:G:H2'	30:a:2512:U:C6	2.50	0.46
33:d:214:LYS:O	33:d:216:ALA:N	2.47	0.46
43:o:13:MET:HE3	43:o:13:MET:HB2	1.75	0.46
49:u:153:TYR:CZ	49:u:155:GLY:HA3	2.51	0.46
6:A:66:U:H2'	6:A:67:C:C6	2.51	0.46
6:A:865:G:OP2	17:L:9:ARG:NH2	2.48	0.46
6:A:1273:A:H2	6:A:1339:G:H1'	1.79	0.46
7:B:14:VAL:O	7:B:204:ASN:HB2	2.15	0.46
30:a:101:G:O6	48:t:111:ARG:NH1	2.49	0.46
30:a:288:G:O2'	30:a:289:U:H5'	2.15	0.46
30:a:1030:A:H2'	30:a:1031:C:C6	2.50	0.46
36:g:119:ALA:HB2	36:g:125:PHE:CE2	2.50	0.46
38:j:120:GLU:HG2	43:o:66:PHE:HE2	1.80	0.46
6:A:38:C:H2'	6:A:39:G:H8	1.81	0.46
7:B:47:LEU:O	7:B:50:ILE:HG22	2.15	0.46
10:E:84:ALA:O	10:E:88:GLU:HG2	2.16	0.46
30:a:57:G:H5'	47:s:79:PRO:HB3	1.97	0.46
30:a:1149:U:O4	30:a:1152:A:H5''	2.16	0.46
30:a:1675:A:H2'	30:a:1676:A:C8	2.51	0.46
30:a:1714:C:H2'	30:a:1715:A:O4'	2.16	0.46
31:b:3:U:H2'	31:b:4:C:C6	2.50	0.46
31:b:13:A:N1	31:b:69:G:O2'	2.48	0.46
31:b:29:A:H2'	31:b:30:C:C6	2.50	0.46
36:g:106:GLU:HA	36:g:106:GLU:OE2	2.15	0.46
9:D:15:LEU:O	9:D:55:LYS:NZ	2.48	0.46
12:G:45:ASN:O	12:G:48:ARG:NH1	2.45	0.46
16:K:86:LYS:HA	16:K:86:LYS:HD2	1.63	0.46
19:N:39:ILE:HD12	19:N:56:LEU:HD11	1.98	0.46
26:U:42:PRO:HA	26:U:45:ILE:HG23	1.97	0.46
30:a:352:G:H2'	30:a:353:A:C4	2.51	0.46
30:a:1912:U:H4'	30:a:1914:C:C6	2.50	0.46
30:a:2706:G:H22	30:a:2721:C:H5	1.62	0.46
34:e:56:THR:O	34:e:60:VAL:HG23	2.16	0.46
35:f:63:ILE:HA	35:f:66:ILE:HG22	1.98	0.46
36:g:23:TYR:HE1	36:g:34:ASN:HB2	1.81	0.46
43:o:111:LYS:HB2	43:o:111:LYS:HE2	1.77	0.46
5:4:25:ARG:O	35:f:111:ARG:NH1	2.49	0.46
6:A:988:G:C6	6:A:1010:C:N4	2.84	0.46
12:G:155:ARG:HG2	12:G:159:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:87:ARG:O	20:O:87:ARG:NH1	2.46	0.46
30:a:1624:A:H2'	30:a:1626:C:H5	1.81	0.46
42:n:34:GLU:OE1	42:n:34:GLU:N	2.30	0.46
46:r:97:ILE:O	46:r:117:SER:OG	2.34	0.46
6:A:733:U:H2'	6:A:734:G:O4'	2.16	0.46
6:A:823:A:H2'	6:A:824:U:C6	2.51	0.46
6:A:1516:G:N7	28:X:7:LYS:HE3	2.31	0.46
14:I:111:ARG:HB2	14:I:119:ARG:HG2	1.97	0.46
21:P:95:GLN:CB	21:P:98:ARG:HH12	2.26	0.46
27:V:21:ARG:HG3	27:V:22:PRO:HD2	1.97	0.46
30:a:720:G:H2'	30:a:721:C:C6	2.51	0.46
30:a:1145:G:H2'	30:a:1146:G:C8	2.50	0.46
6:A:69:A:C2	6:A:220:G:H8	2.34	0.46
6:A:265:G:H2'	6:A:266:U:C6	2.51	0.46
6:A:658:A:H1'	16:K:123:PRO:HB3	1.97	0.46
15:J:46:ALA:HB3	15:J:132:VAL:HG13	1.98	0.46
16:K:29:ILE:HG12	16:K:38:ILE:HG23	1.97	0.46
18:M:6:ILE:HG23	18:M:102:LEU:HA	1.98	0.46
23:R:65:LEU:HD23	23:R:67:LEU:HD21	1.98	0.46
30:a:142:G:N2	30:a:147:G:H22	2.13	0.46
30:a:373:G:N3	30:a:373:G:H2'	2.30	0.46
30:a:826:U:H2'	30:a:827:U:C6	2.51	0.46
30:a:2977:A:H2	30:a:2982:U:H5	1.64	0.46
42:n:88:ILE:HD12	42:n:88:ILE:HA	1.82	0.46
6:A:179:G:C2	6:A:180:A:C8	3.04	0.46
6:A:992:U:O2	6:A:1007:G:O6	2.34	0.46
12:G:23:TYR:CZ	18:M:11:ARG:HB3	2.51	0.46
21:P:23:MET:HG2	21:P:33:ALA:HA	1.98	0.46
26:U:66:MET:HE3	26:U:74:PHE:CE2	2.51	0.46
30:a:653:G:H2'	30:a:2213:A:N7	2.31	0.46
36:g:103:LYS:HB3	36:g:119:ALA:HB3	1.97	0.46
40:l:78:PRO:O	40:l:81:SER:OG	2.33	0.46
41:m:33:ARG:HB3	41:m:114:GLU:HB2	1.97	0.46
52:x:45:ARG:O	52:x:49:VAL:HG23	2.16	0.46
6:A:641:A:H2'	6:A:642:G:H8	1.81	0.45
6:A:729:U:H2'	6:A:730:U:C6	2.51	0.45
6:A:1422:G:H2'	6:A:1423:C:H6	1.81	0.45
8:C:62:C:H2'	8:C:63:G:H8	1.81	0.45
12:G:91:GLU:OE1	12:G:98:ILE:N	2.49	0.45
16:K:99:ARG:NH1	16:K:118:ASP:OD2	2.46	0.45
21:P:44:ALA:O	21:P:45:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2993:U:H2'	30:a:2994:C:H6	1.82	0.45
49:u:33:MET:HG2	49:u:41:ILE:HB	1.98	0.45
53:y:47:MET:O	53:y:51:VAL:HG22	2.15	0.45
6:A:1134:U:H2'	6:A:1135:C:O4'	2.16	0.45
7:B:74:LYS:H	7:B:74:LYS:HD2	1.82	0.45
9:D:174:ARG:C	9:D:175:ILE:HD12	2.41	0.45
30:a:354:U:H2'	30:a:355:U:O4'	2.16	0.45
30:a:1305:G:O3'	30:a:1306:U:H3'	2.15	0.45
30:a:1912:U:H5''	30:a:1913:G:H3'	1.98	0.45
30:a:2818:U:H4'	33:d:87:GLU:OE2	2.16	0.45
6:A:798:A:OP1	6:A:1513:G:O2'	2.32	0.45
6:A:848:A:H2'	6:A:849:A:C8	2.51	0.45
6:A:1202:U:H2'	6:A:1203:C:C6	2.51	0.45
10:E:167:LEU:O	10:E:170:LEU:HB2	2.16	0.45
12:G:87:ARG:O	12:G:91:GLU:HG2	2.16	0.45
12:G:155:ARG:HH21	12:G:192:PHE:HB2	1.82	0.45
13:H:10:MET:SD	13:H:33:LYS:HG2	2.57	0.45
15:J:63:ILE:HG13	15:J:103:TYR:CE1	2.51	0.45
15:J:78:GLU:N	15:J:78:GLU:OE2	2.50	0.45
17:L:87:VAL:HG11	17:L:90:LEU:HD12	1.98	0.45
18:M:78:GLU:O	18:M:80:THR:HG22	2.16	0.45
20:O:23:PRO:HB2	20:O:68:ILE:HD11	1.97	0.45
25:T:59:ASP:OD2	25:T:76:LYS:HD2	2.16	0.45
30:a:548:U:H2'	30:a:549:A:H8	1.81	0.45
30:a:654:A:O2'	45:q:79:LYS:HE3	2.16	0.45
30:a:993:A:H2'	30:a:996:C:H5	1.81	0.45
30:a:1755:A:H2'	30:a:1756:G:H8	1.81	0.45
30:a:1974:A:N6	30:a:2011:G:O2'	2.42	0.45
30:a:2697:C:H2'	30:a:2698:G:H8	1.81	0.45
30:a:2995:C:O2'	54:z:42:HIS:ND1	2.41	0.45
42:n:48:PHE:HD1	42:n:64:SER:HB2	1.81	0.45
6:A:234:A:H2'	6:A:235:C:C6	2.51	0.45
10:E:100:VAL:O	10:E:103:THR:HG22	2.17	0.45
18:M:15:HIS:HA	18:M:18:ILE:HG22	1.97	0.45
18:M:88:MET:N	18:M:88:MET:SD	2.90	0.45
20:O:74:GLU:OE2	20:O:74:GLU:N	2.32	0.45
30:a:1350:G:H3'	30:a:1351:U:H5''	1.96	0.45
30:a:2047:U:OP1	30:a:2592:G:O2'	2.32	0.45
3:2:27:ALA:HB2	39:k:61:PRO:HD3	1.99	0.45
6:A:454:A:H5''	6:A:455:G:N2	2.31	0.45
6:A:683:C:OP1	6:A:684:A:O2'	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1212:C:P	19:N:91:ARG:HH12	2.39	0.45
6:A:1433:A:O2'	6:A:1434:A:H5'	2.17	0.45
12:G:177:LEU:HD23	12:G:177:LEU:H	1.80	0.45
30:a:2:C:H2'	30:a:3:A:H8	1.82	0.45
30:a:814:G:H5'	30:a:815:U:H5''	1.99	0.45
30:a:814:G:O2'	30:a:848:G:H4'	2.16	0.45
30:a:1703:G:OP2	30:a:1704:A:O2'	2.32	0.45
30:a:1866:C:H2'	30:a:1867:C:C6	2.51	0.45
30:a:3077:U:H2'	30:a:3078:U:C6	2.51	0.45
34:e:12:VAL:HG12	34:e:14:GLY:N	2.32	0.45
34:e:155:LYS:NZ	34:e:155:LYS:HB3	2.32	0.45
47:s:3:GLU:HG3	47:s:4:LEU:N	2.31	0.45
6:A:220:G:H2'	6:A:221:C:O4'	2.16	0.45
6:A:386:G:H2'	6:A:387:C:H6	1.82	0.45
6:A:1071:U:H3	6:A:1084:G:H22	1.65	0.45
7:B:87:VAL:HG21	7:B:222:ALA:HB3	1.99	0.45
13:H:39:ILE:HG21	13:H:108:ILE:HD12	1.98	0.45
15:J:148:THR:O	15:J:148:THR:OG1	2.34	0.45
16:K:19:LYS:C	16:K:20:LYS:HD3	2.42	0.45
16:K:20:LYS:HD3	16:K:20:LYS:N	2.30	0.45
23:R:55:VAL:O	23:R:59:ILE:HG12	2.17	0.45
30:a:1724:G:H3'	30:a:1725:G:H8	1.82	0.45
30:a:2978:G:H2'	30:a:2979:U:C4	2.52	0.45
41:m:97:VAL:HG22	41:m:113:ILE:HG13	1.97	0.45
6:A:266:U:H2'	6:A:267:G:O4'	2.17	0.45
6:A:1518:A:H2'	6:A:1519:U:C2	2.52	0.45
12:G:128:ALA:HB3	12:G:131:ARG:HG2	1.98	0.45
16:K:25:GLY:HA2	16:K:43:PRO:HD3	1.99	0.45
16:K:41:THR:HA	16:K:47:VAL:HA	1.98	0.45
18:M:54:SER:HB3	18:M:58:TYR:HB2	1.97	0.45
30:a:235:G:H4'	30:a:236:U:C6	2.52	0.45
30:a:361:G:N2	30:a:443:G:N2	2.65	0.45
30:a:1166:G:O2'	30:a:1168:A:N7	2.45	0.45
30:a:1618:U:H2'	30:a:1619:A:H8	1.82	0.45
35:f:144:GLN:HA	35:f:161:MET:HE1	1.98	0.45
6:A:39:G:H2'	6:A:40:C:C6	2.52	0.45
7:B:102:THR:HG22	7:B:176:GLU:OE1	2.17	0.45
7:B:110:ARG:HD2	7:B:110:ARG:HA	1.73	0.45
30:a:630:U:H2'	30:a:631:G:O4'	2.17	0.45
30:a:869:G:H5'	30:a:870:G:OP1	2.17	0.45
30:a:1052:G:H2'	30:a:1053:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1137:A:H61	30:a:1188:U:H3	1.64	0.45
30:a:1417:G:O6	47:s:25:LEU:HD21	2.16	0.45
30:a:2720:C:O2'	30:a:2721:C:OP2	2.35	0.45
41:m:69:THR:HG22	41:m:70:ILE:N	2.32	0.45
42:n:11:LEU:HD23	42:n:12:SER:H	1.80	0.45
6:A:248:A:C2	6:A:284:A:C5	3.05	0.45
6:A:417:C:C2	6:A:418:G:C8	3.05	0.45
6:A:467:G:H4'	6:A:468:U:O5'	2.16	0.45
6:A:999:A:C2	6:A:1205:A:H1'	2.52	0.45
6:A:1244:G:H2'	6:A:1245:C:C6	2.52	0.45
6:A:1304:A:H1'	26:U:37:ARG:NH1	2.32	0.45
11:F:15:GLU:O	11:F:18:GLN:NE2	2.50	0.45
22:Q:28:ILE:HG21	22:Q:60:ALA:HB3	1.99	0.45
29:Y:14:A:H2'	29:Y:14:A:N3	2.31	0.45
30:a:173:A:H2'	30:a:174:G:O4'	2.16	0.45
30:a:201:G:H2'	30:a:202:A:O4'	2.17	0.45
30:a:373:G:H22	30:a:437:G:H1	1.65	0.45
30:a:1862:A:H2'	30:a:1863:A:H8	1.81	0.45
30:a:1908:C:N4	30:a:1909:C:H41	2.14	0.45
30:a:2496:A:H2'	30:a:2497:G:C8	2.52	0.45
6:A:35:G:C8	6:A:308:A:H1'	2.52	0.45
6:A:301:G:H2'	6:A:302:A:C8	2.51	0.45
7:B:6:THR:HA	7:B:9:LEU:HD12	1.97	0.45
7:B:61:VAL:HA	7:B:65:GLY:HA3	1.99	0.45
9:D:82:GLY:HA3	9:D:192:GLU:HG3	1.98	0.45
9:D:150:ILE:O	9:D:154:ARG:HG3	2.17	0.45
30:a:310:C:H2'	30:a:311:A:C8	2.52	0.45
30:a:1416:U:H2'	47:s:62:MET:HE3	1.99	0.45
30:a:2010:U:H5'	30:a:2154:U:H4'	1.98	0.45
30:a:2263:U:H2'	30:a:2264:A:C8	2.52	0.45
30:a:2913:G:H2'	30:a:2914:G:C8	2.52	0.45
47:s:90:GLU:OE1	47:s:90:GLU:HA	2.16	0.45
6:A:1451:G:H2'	6:A:1452:U:H6	1.82	0.44
7:B:189:ASP:OD2	7:B:189:ASP:N	2.35	0.44
17:L:49:LEU:HD12	17:L:49:LEU:HA	1.83	0.44
20:O:7:LYS:HE2	20:O:7:LYS:HB2	1.85	0.44
21:P:111:GLU:OE2	21:P:114:GLU:HB3	2.17	0.44
30:a:306:G:H4'	30:a:307:U:O5'	2.17	0.44
30:a:372:U:C2	30:a:373:G:C8	3.05	0.44
30:a:1465:G:H2'	30:a:1466:U:C6	2.52	0.44
30:a:1901:U:H2'	30:a:1902:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2220:U:H2'	30:a:2221:C:C6	2.52	0.44
30:a:2819:U:H5''	33:d:89:ARG:NH1	2.31	0.44
36:g:142:VAL:O	36:g:145:GLU:HG3	2.17	0.44
41:m:10:LEU:HB2	41:m:17:GLU:HG3	1.98	0.44
42:n:76:ASP:OD2	42:n:76:ASP:C	2.60	0.44
46:r:56:GLN:HE21	54:z:25:THR:H	1.63	0.44
1:0:29:ASN:C	1:0:31:ARG:H	2.25	0.44
6:A:214:G:H2'	6:A:215:U:H6	1.81	0.44
6:A:1152:G:N1	6:A:1155:A:OP2	2.50	0.44
6:A:1230:U:H2'	6:A:1231:G:H8	1.82	0.44
6:A:1302:G:N1	6:A:1305:A:OP2	2.46	0.44
6:A:1411:U:H2'	6:A:1412:A:C8	2.52	0.44
9:D:105:THR:OG1	9:D:106:ARG:N	2.50	0.44
16:K:22:VAL:HG11	16:K:42:ASP:HB2	1.99	0.44
18:M:32:THR:HG22	18:M:82:LYS:HE2	1.99	0.44
30:a:751:C:H2'	30:a:752:U:C6	2.51	0.44
34:e:133:VAL:HG13	34:e:166:ILE:HG22	1.99	0.44
35:f:111:ARG:NE	35:f:149:GLU:OE1	2.49	0.44
6:A:386:G:H2'	6:A:387:C:C6	2.52	0.44
6:A:641:A:H2'	6:A:642:G:C8	2.51	0.44
30:a:20:U:H2'	30:a:21:C:C6	2.53	0.44
30:a:975:G:C2	30:a:976:G:C5	3.05	0.44
30:a:2248:C:H2'	30:a:2249:C:C6	2.52	0.44
30:a:2490:G:H2'	30:a:2490:G:N3	2.32	0.44
31:b:52:U:H1'	31:b:53:C:H5	1.81	0.44
31:b:66:A:H61	31:b:108:A:H2'	1.81	0.44
39:k:97:LEU:HA	39:k:100:VAL:HG22	1.99	0.44
6:A:428:U:H2'	6:A:429:U:C6	2.53	0.44
6:A:1135:C:H2'	6:A:1136:A:C8	2.53	0.44
15:J:63:ILE:HD12	15:J:104:ASP:O	2.17	0.44
30:a:1902:C:H2'	30:a:1903:G:H8	1.81	0.44
30:a:2753:C:O2'	33:d:157:THR:O	2.28	0.44
30:a:2758:G:O2'	30:a:2761:C:OP2	2.29	0.44
38:j:93:PRO:HG3	38:j:114:ILE:HG13	1.98	0.44
1:0:37:MET:HE2	1:0:37:MET:HB3	1.78	0.44
6:A:959:A:H5'	6:A:959:A:H8	1.81	0.44
6:A:1057:G:H2'	6:A:1058:U:C6	2.52	0.44
6:A:1224:A:H2	6:A:1227:G:N3	2.16	0.44
6:A:1500:A:H2'	6:A:1501:C:H6	1.82	0.44
7:B:73:LYS:O	7:B:77:GLN:HG2	2.18	0.44
16:K:112:GLU:OE2	16:K:112:GLU:N	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:76:C:H2'	30:a:77:C:H6	1.83	0.44
30:a:1002:A:H5''	31:b:98:G:O2'	2.17	0.44
30:a:1176:G:H2'	30:a:1177:U:O4'	2.18	0.44
30:a:2428:G:H2'	30:a:2429:A:H8	1.81	0.44
33:d:44:ARG:NE	33:d:87:GLU:OE1	2.47	0.44
34:e:153:LEU:H	34:e:154:ARG:NH2	2.16	0.44
38:j:64:ARG:HB2	38:j:83:ALA:HB3	2.00	0.44
48:t:46:HIS:N	48:t:46:HIS:ND1	2.65	0.44
54:z:35:CYS:SG	54:z:47:SER:HB2	2.57	0.44
6:A:973:G:O6	6:A:1203:C:N4	2.50	0.44
6:A:1053:G:H8	6:A:1053:G:OP2	2.00	0.44
15:J:172:LYS:O	15:J:173:ARG:HG2	2.18	0.44
30:a:188:A:H2'	30:a:189:A:H8	1.83	0.44
30:a:1771:U:H2'	30:a:1772:G:C8	2.53	0.44
30:a:2289:U:OP1	30:a:2289:U:H6	2.01	0.44
33:d:20:LEU:HD12	33:d:30:VAL:HG11	1.98	0.44
6:A:690:C:H2'	6:A:691:A:H8	1.83	0.44
6:A:1103:U:H1'	6:A:1165:A:C5	2.53	0.44
6:A:1274:A:H2'	6:A:1275:A:H8	1.79	0.44
10:E:160:VAL:O	10:E:163:THR:HG22	2.18	0.44
13:H:43:GLU:HA	13:H:43:GLU:OE2	2.18	0.44
15:J:158:LYS:HB2	15:J:161:LEU:HD12	2.00	0.44
21:P:23:MET:HE3	21:P:32:ARG:O	2.17	0.44
30:a:400:G:H2'	30:a:401:U:O4'	2.17	0.44
30:a:580:A:H2'	30:a:581:G:O4'	2.18	0.44
30:a:935:U:H2'	30:a:936:U:C6	2.53	0.44
30:a:993:A:H2'	30:a:996:C:C5	2.53	0.44
30:a:1615:A:H2'	30:a:1616:G:H8	1.83	0.44
36:g:106:GLU:OE2	36:g:116:ILE:HD13	2.17	0.44
47:s:25:LEU:HD22	47:s:30:THR:HG21	1.98	0.44
6:A:12:A:C6	9:D:201:LYS:HB3	2.53	0.44
6:A:45:G:H2'	6:A:46:G:H8	1.83	0.44
6:A:78:G:H2'	6:A:79:C:H6	1.83	0.44
6:A:512:G:C5	29:Y:22:U:H2'	2.52	0.44
6:A:536:U:H2'	6:A:537:C:C6	2.52	0.44
6:A:717:U:H2'	6:A:718:U:C6	2.52	0.44
6:A:984:A:N1	6:A:1025:G:C6	2.85	0.44
16:K:40:ILE:HG22	16:K:85:MET:HE3	2.00	0.44
30:a:437:G:H2'	30:a:438:G:C8	2.53	0.44
30:a:1195:G:H2'	30:a:1196:U:O4'	2.18	0.44
30:a:1232:U:H2'	30:a:1233:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1912:U:OP2	30:a:1913:G:O2'	2.36	0.44
30:a:2047:U:H2'	30:a:2048:G:O4'	2.18	0.44
30:a:2051:U:H2'	30:a:2052:G:O4'	2.17	0.44
6:A:562:C:H2'	6:A:563:G:O4'	2.17	0.44
6:A:618:U:H2'	6:A:619:U:C6	2.53	0.44
6:A:739:U:OP1	6:A:804:G:O2'	2.35	0.44
9:D:182:THR:O	9:D:185:GLN:N	2.50	0.44
10:E:160:VAL:O	10:E:164:VAL:HG23	2.18	0.44
34:e:125:ARG:HH22	34:e:150:LEU:HD13	1.83	0.44
54:z:45:CYS:CB	54:z:48:CYS:SG	3.05	0.44
6:A:934:U:O4	19:N:105:THR:HG21	2.18	0.43
7:B:50:ILE:HD12	7:B:201:ILE:HG12	2.00	0.43
9:D:57:ARG:HG2	9:D:62:VAL:O	2.18	0.43
21:P:120:ILE:HD12	21:P:123:LYS:HB2	1.99	0.43
30:a:671:U:H2'	30:a:672:U:C6	2.52	0.43
30:a:1429:A:H2'	30:a:1430:A:C8	2.52	0.43
30:a:1904:U:OP2	30:a:1921:G:N2	2.51	0.43
30:a:2214:A:N3	30:a:2637:G:O2'	2.50	0.43
35:f:24:ALA:HA	35:f:27:GLU:HG3	2.00	0.43
39:k:144:THR:O	39:k:145:LYS:HB2	2.17	0.43
5:4:12:THR:N	5:4:24:THR:O	2.42	0.43
6:A:865:G:P	17:L:9:ARG:HH22	2.41	0.43
6:A:989:G:H2'	6:A:990:A:C8	2.53	0.43
17:L:16:ILE:HD12	17:L:16:ILE:N	2.33	0.43
23:R:63:ARG:HD3	23:R:70:TYR:HA	2.00	0.43
30:a:51:A:H2'	30:a:52:A:H8	1.83	0.43
30:a:254:G:H4'	30:a:475:G:C6	2.53	0.43
30:a:817:C:H2'	30:a:818:G:O4'	2.19	0.43
30:a:944:G:O2'	30:a:1000:G:O6	2.35	0.43
30:a:2695:G:H2'	30:a:2696:U:C6	2.53	0.43
38:j:64:ARG:O	38:j:82:ASN:HA	2.18	0.43
1:0:25:ILE:HG12	3:2:34:GLU:HG2	1.99	0.43
5:4:18:CYS:SG	5:4:41:CYS:HB2	2.59	0.43
6:A:1284:C:O2'	14:I:114:LYS:NZ	2.51	0.43
10:E:133:SER:O	10:E:137:VAL:HG23	2.18	0.43
11:F:48:LEU:HD11	11:F:86:MET:HE1	1.99	0.43
30:a:283:U:O2'	30:a:315:G:N2	2.50	0.43
30:a:405:G:H4'	30:a:407:A:N7	2.33	0.43
30:a:608:U:H2'	30:a:609:C:C6	2.53	0.43
30:a:672:U:H2'	30:a:673:A:H8	1.82	0.43
30:a:2933:G:H4'	36:g:4:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2992:G:H2'	30:a:2993:U:H6	1.82	0.43
40:l:134:ARG:CZ	49:u:124:ASN:HD21	2.31	0.43
43:o:106:LYS:HA	43:o:109:LYS:HD2	1.99	0.43
6:A:403:C:O2'	6:A:603:A:N3	2.47	0.43
6:A:428:U:OP1	9:D:28:ARG:NH1	2.49	0.43
6:A:1374:G:H2'	6:A:1375:G:H8	1.83	0.43
9:D:15:LEU:HD12	9:D:51:ARG:HG2	2.00	0.43
18:M:21:SER:OG	18:M:96:VAL:HG11	2.18	0.43
18:M:64:HIS:HB3	24:S:59:SER:OG	2.18	0.43
30:a:339:U:H3'	30:a:340:C:C6	2.53	0.43
30:a:728:G:N2	30:a:731:A:H5''	2.33	0.43
30:a:1481:C:H2'	30:a:1482:G:C8	2.52	0.43
30:a:1866:C:H2'	30:a:1867:C:H6	1.83	0.43
30:a:1980:G:O2'	32:c:257:THR:OG1	2.34	0.43
30:a:2274:U:OP2	51:w:61:ARG:NH2	2.43	0.43
30:a:2288:G:HO2'	30:a:2289:U:P	2.41	0.43
30:a:2496:A:H2'	30:a:2497:G:H8	1.84	0.43
34:e:160:LEU:HD13	34:e:163:SER:O	2.19	0.43
35:f:141:LEU:HD22	35:f:146:MET:HE2	2.01	0.43
41:m:70:ILE:HG22	41:m:72:ASP:H	1.84	0.43
42:n:40:VAL:HG13	42:n:49:VAL:HG22	1.99	0.43
45:q:58:VAL:HG22	45:q:100:ILE:HG23	2.00	0.43
6:A:379:G:OP1	21:P:4:LYS:NZ	2.33	0.43
6:A:849:A:H2'	6:A:850:C:C6	2.53	0.43
6:A:1415:A:H2'	6:A:1416:C:H6	1.83	0.43
7:B:163:TRP:CH2	7:B:187:ILE:HD11	2.54	0.43
19:N:33:THR:HA	19:N:59:HIS:CE1	2.53	0.43
30:a:372:U:C2	30:a:373:G:H8	2.36	0.43
30:a:899:C:H1'	30:a:1301:G:N2	2.33	0.43
30:a:1488:U:H2'	30:a:1489:C:C6	2.53	0.43
46:r:68:ILE:O	46:r:72:MET:HG3	2.19	0.43
6:A:21:U:H2'	6:A:22:C:H6	1.81	0.43
6:A:719:C:H2'	6:A:720:U:H6	1.83	0.43
6:A:719:C:H2'	6:A:720:U:C6	2.54	0.43
6:A:793:U:O2'	6:A:885:A:N1	2.51	0.43
6:A:1055:U:H2'	6:A:1056:C:C6	2.53	0.43
8:C:23:C:H2'	8:C:24:U:C6	2.53	0.43
9:D:116:GLY:O	9:D:117:HIS:ND1	2.51	0.43
15:J:138:ARG:N	15:J:139:PRO:HD2	2.34	0.43
26:U:22:GLN:HG2	26:U:31:ILE:HD11	1.99	0.43
30:a:752:U:H2'	30:a:753:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2980:G:O2'	30:a:2981:U:OP1	2.35	0.43
35:f:31:TYR:HD2	35:f:37:ILE:HG13	1.83	0.43
35:f:179:LEU:HD22	35:f:184:PHE:CE1	2.53	0.43
6:A:113:G:H2'	6:A:114:U:C6	2.54	0.43
6:A:677:A:H2'	6:A:678:A:C8	2.54	0.43
6:A:966:U:H4'	6:A:967:A:O4'	2.18	0.43
6:A:1164:G:N2	6:A:1166:A:H3'	2.34	0.43
7:B:134:GLU:O	7:B:137:MET:HG3	2.18	0.43
11:F:15:GLU:N	11:F:18:GLN:OE1	2.36	0.43
13:H:117:THR:OG1	13:H:120:GLN:HG3	2.19	0.43
16:K:89:ASP:HB2	16:K:115:PRO:HD2	2.00	0.43
30:a:172:U:H2'	30:a:173:A:H8	1.83	0.43
30:a:180:U:H2'	30:a:181:G:C8	2.54	0.43
30:a:440:A:H2'	30:a:441:C:C6	2.53	0.43
30:a:852:U:H2'	30:a:853:G:H8	1.84	0.43
30:a:1192:C:H3'	30:a:1193:A:H8	1.83	0.43
30:a:1364:U:H5	30:a:1402:U:O2	2.01	0.43
30:a:1486:U:H2'	30:a:1487:G:C8	2.54	0.43
30:a:1726:U:H4'	30:a:1727:G:H5'	2.01	0.43
30:a:2972:A:C2	30:a:3073:G:H2'	2.53	0.43
42:n:5:LEU:HD23	42:n:5:LEU:HA	1.81	0.43
46:r:56:GLN:NE2	54:z:25:THR:H	2.17	0.43
48:t:8:LYS:HA	48:t:26:VAL:HG23	2.01	0.43
2:1:24:THR:HG23	2:1:27:GLY:H	1.83	0.43
6:A:633:C:H2'	6:A:634:U:C6	2.53	0.43
6:A:717:U:H2'	6:A:718:U:H6	1.82	0.43
6:A:1313:U:H2'	6:A:1314:C:C6	2.53	0.43
6:A:1386:C:O2	6:A:1489:A:N6	2.51	0.43
6:A:1441:U:H2'	6:A:1442:G:H8	1.81	0.43
6:A:1499:U:H2'	6:A:1500:A:C8	2.54	0.43
14:I:21:PRO:O	14:I:25:GLN:HG3	2.19	0.43
30:a:116:G:OP2	30:a:118:A:O2'	2.33	0.43
30:a:145:G:H2'	30:a:146:U:C6	2.53	0.43
30:a:333:U:N3	30:a:334:G:N7	2.67	0.43
30:a:1151:G:H4'	30:a:1153:A:N6	2.34	0.43
30:a:1151:G:H21	30:a:1178:A:H2'	1.83	0.43
30:a:1610:C:H2'	30:a:1611:A:C8	2.54	0.43
30:a:2914:G:H3'	30:a:2915:U:O4'	2.19	0.43
30:a:2922:A:H2'	30:a:2923:A:C8	2.53	0.43
31:b:118:A:H2'	31:b:119:A:O4'	2.19	0.43
32:c:5:LYS:HD2	32:c:17:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:c:134:ARG:HB3	32:c:134:ARG:NH1	2.34	0.43
6:A:149:G:H2'	6:A:150:A:O4'	2.19	0.43
6:A:806:U:H2'	6:A:807:A:H8	1.83	0.43
6:A:1415:A:H2'	6:A:1416:C:C6	2.53	0.43
21:P:46:PRO:O	21:P:47:SER:C	2.60	0.43
30:a:2:C:H2'	30:a:3:A:C8	2.54	0.43
30:a:405:G:H4'	30:a:407:A:C8	2.53	0.43
30:a:1774:C:N4	30:a:1775:G:O6	2.51	0.43
30:a:2289:U:H2'	30:a:2290:U:O4'	2.18	0.43
34:e:119:ASP:CG	39:k:3:ILE:HG12	2.44	0.43
35:f:127:ASN:ND2	35:f:127:ASN:N	2.66	0.43
40:l:127:MET:HE3	40:l:127:MET:HB3	1.80	0.43
48:t:10:ASP:HB3	48:t:77:LEU:HD21	2.01	0.43
6:A:950:2MG:C2	8:C:34:C:H5'	2.54	0.43
6:A:1375:G:H2'	6:A:1376:C:C6	2.53	0.43
10:E:192:MET:HE3	10:E:192:MET:HB2	1.85	0.43
11:F:81:ILE:HD13	11:F:81:ILE:HA	1.84	0.43
12:G:62:ARG:HA	12:G:97:GLN:HG2	2.00	0.43
13:H:73:ARG:HA	13:H:73:ARG:HD2	1.87	0.43
16:K:42:ASP:OD2	16:K:42:ASP:C	2.62	0.43
20:O:1:MET:HA	20:O:5:GLU:OE2	2.19	0.43
20:O:87:ARG:NH2	30:a:799:U:H3'	2.32	0.43
30:a:620:C:H4'	30:a:621:G:C8	2.53	0.43
30:a:2064:G:H2'	30:a:2065:U:O4'	2.19	0.43
30:a:2374:U:H2'	30:a:2375:U:O4'	2.19	0.43
32:c:172:TYR:CD2	32:c:184:MET:HE3	2.54	0.43
35:f:42:LYS:HG3	35:f:166:VAL:HB	2.01	0.43
46:r:90:GLN:HB2	46:r:123:VAL:HB	2.00	0.43
52:x:41:GLU:OE1	52:x:41:GLU:N	2.41	0.43
6:A:192:G:C6	6:A:202:G:C5	3.07	0.42
6:A:482:G:H2'	6:A:483:C:C6	2.54	0.42
6:A:536:U:H2'	6:A:537:C:H6	1.84	0.42
6:A:969:C:H2'	6:A:970:U:C6	2.54	0.42
12:G:176:THR:HG22	12:G:179:ALA:H	1.84	0.42
30:a:147:G:H1'	30:a:1780:C:O2'	2.18	0.42
30:a:1258:G:H2'	30:a:1259:G:C8	2.54	0.42
30:a:1493:G:H1'	30:a:1769:G:N2	2.33	0.42
30:a:1734:U:H2'	30:a:1735:G:O4'	2.19	0.42
30:a:1902:C:H2'	30:a:1903:G:C8	2.54	0.42
30:a:1918:G:H2'	30:a:1919:U:C6	2.53	0.42
30:a:2425:U:H2'	30:a:2426:U:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1453:C:H2'	6:A:1454:G:O4'	2.19	0.42
9:D:15:LEU:HB3	9:D:55:LYS:HZ3	1.83	0.42
9:D:137:ILE:HG12	9:D:176:LEU:HD13	2.01	0.42
10:E:187:ILE:HG13	10:E:188:ALA:N	2.35	0.42
30:a:270:G:H2'	30:a:271:G:O4'	2.19	0.42
30:a:504:A:H2'	30:a:505:C:C6	2.54	0.42
30:a:905:A:H4'	30:a:921:G:N2	2.34	0.42
30:a:1070:C:H2'	30:a:1071:A:O4'	2.19	0.42
30:a:1649:U:H2'	30:a:1704:A:N6	2.34	0.42
30:a:2025:G:H2'	30:a:2026:C:C6	2.54	0.42
30:a:2050:G:H2'	30:a:2051:U:O4'	2.19	0.42
30:a:2106:U:H2'	30:a:2107:C:H6	1.84	0.42
30:a:2432:G:O2'	30:a:2678:C:OP1	2.29	0.42
30:a:2706:G:N1	30:a:2721:C:H5	2.12	0.42
32:c:24:LEU:HD11	32:c:84:TYR:HB2	2.01	0.42
32:c:124:ASP:OD1	32:c:125:ILE:N	2.52	0.42
33:d:59:GLY:O	33:d:83:ARG:N	2.47	0.42
39:k:123:LEU:HB2	39:k:143:VAL:HG12	2.01	0.42
41:m:82:GLU:O	41:m:86:ARG:HB2	2.20	0.42
6:A:828:A:H2'	6:A:829:C:C6	2.54	0.42
6:A:829:C:H4'	23:R:14:LYS:NZ	2.35	0.42
6:A:990:A:H4'	6:A:1023:C:H4'	2.00	0.42
7:B:58:LYS:HA	7:B:58:LYS:HD3	1.72	0.42
17:L:72:HIS:HE2	17:L:74:LEU:HD12	1.84	0.42
19:N:37:THR:HG23	19:N:39:ILE:HG13	2.01	0.42
30:a:305:U:H2'	30:a:306:G:N2	2.34	0.42
30:a:532:A:C2	34:e:48:ARG:HG3	2.54	0.42
30:a:947:G:H2'	30:a:948:A:O4'	2.18	0.42
30:a:1084:A:H2'	30:a:1085:G:O4'	2.19	0.42
30:a:1881:G:OP2	30:a:1882:A:O2'	2.33	0.42
30:a:2234:A:OP2	30:a:2234:A:H8	2.02	0.42
30:a:2248:C:H2'	30:a:2249:C:H6	1.84	0.42
30:a:2546:C:H2'	30:a:2547:G:O4'	2.19	0.42
34:e:63:GLY:HA3	34:e:82:ARG:HG2	2.00	0.42
34:e:157:LEU:HD12	34:e:182:ALA:HA	2.01	0.42
34:e:210:ARG:CZ	34:e:210:ARG:HB3	2.49	0.42
44:p:109:LEU:HD23	44:p:109:LEU:HA	1.82	0.42
47:s:26:LEU:HD21	47:s:31:TYR:CE2	2.55	0.42
6:A:187:C:O2'	25:T:84:ASN:OD1	2.31	0.42
6:A:474:G:H2'	6:A:475:U:C6	2.53	0.42
6:A:576:C:H2'	6:A:577:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1240:A:OP1	18:M:47:ASN:ND2	2.49	0.42
6:A:1511:C:H2'	6:A:1512:G:C8	2.55	0.42
7:B:107:ILE:O	7:B:111:ILE:HG12	2.18	0.42
7:B:155:MET:HE2	7:B:155:MET:HB3	1.86	0.42
13:H:3:MET:HE2	13:H:3:MET:HA	2.01	0.42
30:a:568:A:N3	30:a:570:G:H5''	2.34	0.42
30:a:718:A:H2'	30:a:719:A:C8	2.55	0.42
30:a:948:A:H2'	30:a:949:G:C8	2.54	0.42
30:a:1199:U:H2'	30:a:1200:U:H6	1.83	0.42
30:a:1251:C:H2'	30:a:1252:C:C6	2.54	0.42
30:a:1260:U:H2'	30:a:1261:U:O4'	2.20	0.42
30:a:1631:G:H2'	30:a:1632:U:C6	2.54	0.42
30:a:2694:C:H2'	30:a:2695:G:O4'	2.19	0.42
34:e:157:LEU:HD13	34:e:157:LEU:HA	1.95	0.42
37:i:104:ALA:O	37:i:108:MET:HG3	2.20	0.42
49:u:29:VAL:HG21	49:u:50:THR:HG21	2.01	0.42
6:A:449:G:O6	6:A:467:G:O2'	2.34	0.42
6:A:575:U:H2'	6:A:576:C:C6	2.55	0.42
6:A:652:A:H2'	6:A:653:A:C8	2.54	0.42
6:A:1040:A:O2'	12:G:155:ARG:NH1	2.51	0.42
6:A:1267:U:O4	18:M:9:ARG:NH2	2.52	0.42
7:B:187:ILE:HD12	7:B:214:LEU:HD13	2.01	0.42
10:E:104:ILE:O	10:E:121:PRO:HB3	2.20	0.42
13:H:22:HIS:O	13:H:69:TYR:OH	2.30	0.42
19:N:91:ARG:HB2	19:N:98:VAL:HG12	2.01	0.42
30:a:172:U:H2'	30:a:173:A:C8	2.54	0.42
30:a:587:U:H2'	30:a:588:G:O4'	2.19	0.42
30:a:948:A:H2'	30:a:949:G:H8	1.85	0.42
30:a:1160:A:N6	30:a:1171:A:N1	2.67	0.42
30:a:2287:G:H1'	30:a:2288:G:H5'	2.01	0.42
30:a:2934:C:H2'	30:a:2935:A:O4'	2.20	0.42
31:b:28:C:H2'	31:b:29:A:O4'	2.19	0.42
33:d:57:GLY:O	33:d:58:TYR:HB3	2.19	0.42
34:e:160:LEU:C	34:e:162:ARG:N	2.75	0.42
41:m:38:VAL:HG22	41:m:111:ALA:HB2	2.01	0.42
6:A:270:U:H2'	6:A:271:U:C6	2.54	0.42
6:A:1268:C:H2'	6:A:1269:U:C6	2.54	0.42
6:A:1505:MA6:H8	6:A:1505:MA6:O5'	2.19	0.42
7:B:81:VAL:O	7:B:85:THR:OG1	2.28	0.42
11:F:43:TRP:HB2	11:F:60:TYR:HB2	2.01	0.42
14:I:79:ARG:HE	14:I:79:ARG:HB3	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:135:G:OP1	30:a:1767:G:H5''	2.20	0.42
30:a:979:U:H2'	30:a:981:C:H41	1.84	0.42
30:a:1014:G:H3'	30:a:1015:U:C6	2.55	0.42
30:a:2919:G:H2'	30:a:2920:A:C8	2.55	0.42
32:c:5:LYS:HE2	32:c:5:LYS:HB3	1.86	0.42
35:f:86:PHE:HB2	35:f:88:LEU:HD22	2.02	0.42
35:f:146:MET:HB3	35:f:146:MET:HE3	1.77	0.42
36:g:20:ASP:OD1	36:g:20:ASP:N	2.52	0.42
52:x:48:GLU:OE1	52:x:48:GLU:HA	2.19	0.42
6:A:214:G:H2'	6:A:215:U:C6	2.55	0.42
6:A:561:U:H2'	6:A:562:C:H6	1.83	0.42
6:A:1167:G:H1'	6:A:1168:G:C5	2.55	0.42
21:P:95:GLN:HB2	21:P:98:ARG:NH1	2.28	0.42
30:a:658:A:OP2	30:a:2681:C:O2'	2.38	0.42
30:a:764:G:H2'	30:a:765:G:H8	1.85	0.42
47:s:20:GLU:OE1	47:s:20:GLU:N	2.41	0.42
5:4:60:ARG:HA	5:4:63:ARG:CZ	2.50	0.42
6:A:449:G:N1	6:A:468:U:OP2	2.51	0.42
6:A:584:A:H2'	6:A:585:A:H8	1.84	0.42
6:A:1301:U:H2'	6:A:1302:G:O4'	2.20	0.42
7:B:166:ASP:OD2	7:B:169:LYS:HB2	2.20	0.42
15:J:156:ARG:O	15:J:158:LYS:HE3	2.20	0.42
17:L:72:HIS:NE2	17:L:74:LEU:HD12	2.35	0.42
30:a:629:C:H2'	30:a:630:U:O4'	2.20	0.42
30:a:1183:C:H2'	30:a:1184:U:O4'	2.19	0.42
30:a:2001:U:H2'	32:c:157:ARG:HB2	2.02	0.42
31:b:66:A:N6	31:b:108:A:H2'	2.35	0.42
54:z:48:CYS:SG	54:z:57:ARG:NH2	2.93	0.42
6:A:161:A:H2'	6:A:162:A:O4'	2.20	0.42
6:A:478:A:O2'	6:A:479:G:C8	2.73	0.42
6:A:1497:C:H2'	6:A:1498:G:H8	1.85	0.42
9:D:165:TRP:CD1	9:D:181:PRO:HB3	2.55	0.42
11:F:56:SER:OG	11:F:56:SER:O	2.32	0.42
30:a:406:G:OP2	34:e:138:PRO:HA	2.20	0.42
35:f:31:TYR:CD2	35:f:37:ILE:HG13	2.54	0.42
43:o:14:ARG:H	43:o:77:HIS:CD2	2.38	0.42
46:r:62:GLU:O	46:r:66:LYS:HG3	2.20	0.42
48:t:116:LEU:HD23	48:t:116:LEU:H	1.84	0.42
6:A:229:G:H2'	6:A:230:A:C8	2.55	0.42
6:A:1033:G:H5''	24:S:3:LYS:HG2	2.01	0.42
14:I:69:ILE:HD11	14:I:127:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:I:93:PRO:O	14:I:96:GLN:HG2	2.20	0.42
21:P:9:ARG:C	21:P:10:LEU:HD12	2.44	0.42
30:a:26:G:H22	30:a:600:G:H1'	1.85	0.42
30:a:238:U:H2'	30:a:239:G:O4'	2.20	0.42
30:a:271:G:O2'	30:a:272:A:OP1	2.36	0.42
30:a:2066:G:C2	30:a:2067:A:H1'	2.55	0.42
30:a:2180:C:H5'	33:d:128:MET:CE	2.49	0.42
30:a:2560:A:C5	30:a:2561:G:H1'	2.55	0.42
36:g:47:ASP:O	36:g:47:ASP:CG	2.62	0.42
4:3:26:ILE:HD12	4:3:26:ILE:C	2.45	0.41
5:4:8:ASP:OD2	5:4:8:ASP:C	2.62	0.41
6:A:90:U:H1'	6:A:91:G:O5'	2.20	0.41
6:A:177:C:H2'	6:A:178:G:H5''	2.02	0.41
6:A:520:U:H2'	6:A:521:A:H8	1.85	0.41
7:B:137:MET:HA	7:B:140:ARG:HG2	2.01	0.41
9:D:197:GLU:HA	9:D:197:GLU:OE2	2.20	0.41
10:E:104:ILE:HD12	10:E:170:LEU:HD11	2.01	0.41
12:G:133:MET:HE3	12:G:150:ILE:HG22	2.02	0.41
15:J:61:VAL:HG21	15:J:125:ILE:HD12	2.02	0.41
15:J:93:PRO:HA	15:J:96:THR:HG22	2.02	0.41
18:M:26:VAL:HG22	18:M:36:VAL:HG21	2.01	0.41
19:N:87:TYR:O	19:N:91:ARG:HG2	2.20	0.41
19:N:91:ARG:HA	19:N:91:ARG:HD2	1.92	0.41
20:O:87:ARG:N	20:O:87:ARG:HD3	2.35	0.41
30:a:18:G:H2'	30:a:19:A:C8	2.55	0.41
30:a:145:G:H2'	30:a:146:U:H6	1.85	0.41
30:a:422:U:H2'	30:a:423:G:O4'	2.20	0.41
30:a:1607:A:H4'	30:a:1608:C:O4'	2.20	0.41
31:b:5:C:OP1	31:b:62:U:H5'	2.19	0.41
38:j:34:TYR:N	38:j:37:ASP:OD2	2.42	0.41
46:r:128:GLU:CD	46:r:128:GLU:H	2.28	0.41
6:A:97:C:H2'	6:A:98:U:H5'	2.02	0.41
6:A:352:G:H2'	6:A:353:G:C8	2.55	0.41
6:A:373:A:H2'	6:A:374:C:O4'	2.19	0.41
6:A:934:U:OP2	19:N:102:ARG:HD2	2.20	0.41
6:A:970:U:H2'	6:A:971:G:O4'	2.20	0.41
6:A:1236:A:H2'	6:A:1237:G:C8	2.55	0.41
6:A:1299:U:P	26:U:5:LEU:HB2	2.60	0.41
11:F:91:MET:HE2	11:F:91:MET:HB3	1.84	0.41
15:J:54:ARG:NH1	15:J:150:ASP:OD1	2.53	0.41
30:a:3:A:N6	30:a:3079:C:H42	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:975:G:H2'	30:a:976:G:C8	2.55	0.41
30:a:1984:G:C6	30:a:2385:U:H5''	2.55	0.41
30:a:2014:U:H2'	30:a:2015:C:C6	2.56	0.41
30:a:2113:G:O2'	30:a:2151:G:O6	2.34	0.41
30:a:2871:U:H5''	30:a:2872:G:C8	2.54	0.41
30:a:2961:U:P	30:a:2961:U:H3'	2.60	0.41
34:e:160:LEU:CB	34:e:164:ASP:HB2	2.48	0.41
41:m:65:PHE:O	41:m:68:ARG:HB2	2.21	0.41
6:A:45:G:H2'	6:A:46:G:C8	2.55	0.41
11:F:75:LEU:O	11:F:79:LEU:HG	2.20	0.41
23:R:33:ILE:HD12	23:R:68:LEU:HD22	2.02	0.41
30:a:2468:A:H4'	30:a:2469:A:O4'	2.21	0.41
43:o:10:LYS:HE2	43:o:10:LYS:HB2	1.90	0.41
45:q:27:ASP:OD2	45:q:27:ASP:N	2.52	0.41
6:A:1314:C:H5''	19:N:28:THR:HG21	2.03	0.41
6:A:1497:C:H2'	6:A:1498:G:C8	2.55	0.41
8:C:9:G:O2'	8:C:10:G:N7	2.45	0.41
15:J:133:ASP:OD2	15:J:136:ALA:HB3	2.20	0.41
21:P:45:ASP:CB	21:P:46:PRO:HD3	2.49	0.41
30:a:670:G:H22	39:k:34:ARG:NH1	2.18	0.41
30:a:936:U:H2'	30:a:937:G:H8	1.85	0.41
30:a:1156:A:O2'	30:a:2656:U:O3'	2.35	0.41
30:a:1982:G:N7	32:c:179:SER:OG	2.47	0.41
30:a:2194:U:H2'	30:a:2195:G:O4'	2.21	0.41
33:d:20:LEU:O	33:d:27:LEU:HD12	2.20	0.41
33:d:21:TRP:CE2	33:d:27:LEU:HD13	2.56	0.41
45:q:56:VAL:HA	45:q:102:GLY:HA2	2.02	0.41
48:t:26:VAL:HG12	48:t:38:VAL:HG22	2.01	0.41
6:A:26:G:H2'	6:A:27:C:C6	2.55	0.41
6:A:36:A:OP2	6:A:400:C:O2'	2.33	0.41
6:A:401:G:H2'	6:A:402:C:C6	2.56	0.41
6:A:624:A:C5	13:H:112:SER:HA	2.56	0.41
6:A:852:C:H2'	6:A:853:U:O4'	2.20	0.41
9:D:118:PHE:O	9:D:119:LEU:HD23	2.20	0.41
10:E:201:GLU:OE1	10:E:201:GLU:HA	2.19	0.41
14:I:13:MET:HE3	14:I:14:VAL:H	1.84	0.41
30:a:279:A:H62	30:a:319:G:N2	2.18	0.41
30:a:742:U:H2'	30:a:743:C:C6	2.55	0.41
30:a:1010:A:H2'	30:a:1011:A:C8	2.55	0.41
30:a:1912:U:H5''	30:a:1914:C:H5'	2.02	0.41
31:b:90:A:C2	31:b:91:U:H1'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:38:ARG:HA	36:g:38:ARG:HD3	1.81	0.41
38:j:112:MET:HE2	38:j:112:MET:HA	2.02	0.41
6:A:23:C:H2'	6:A:24:U:C6	2.56	0.41
6:A:201:U:H4'	22:Q:4:ASN:HD22	1.85	0.41
6:A:831:G:H5'	6:A:832:G:OP2	2.21	0.41
6:A:938:G:H2'	6:A:939:A:H8	1.85	0.41
6:A:989:G:H3'	6:A:1009:G:N2	2.36	0.41
6:A:1312:C:H2'	6:A:1313:U:C6	2.55	0.41
7:B:16:PHE:O	7:B:204:ASN:ND2	2.53	0.41
9:D:52:GLU:CD	9:D:191:ASN:HB2	2.45	0.41
30:a:141:A:H2'	30:a:142:G:C8	2.56	0.41
30:a:432:A:H2'	30:a:433:G:O4'	2.21	0.41
30:a:672:U:H2'	30:a:673:A:C8	2.55	0.41
30:a:824:A:H1'	30:a:825:C:H5	1.86	0.41
30:a:1402:U:O2'	30:a:2193:G:O2'	2.38	0.41
30:a:2098:3TD:H2'	30:a:2099:A:O4'	2.21	0.41
30:a:2288:G:H1'	30:a:2289:U:OP2	2.21	0.41
30:a:2584:G:H1'	30:a:2585:G:N7	2.36	0.41
30:a:2649:C:H2'	30:a:2650:G:O4'	2.20	0.41
30:a:2956:C:H2'	30:a:2957:A:O4'	2.21	0.41
30:a:3026:G:H2'	30:a:3027:U:C6	2.56	0.41
35:f:105:MET:HE2	35:f:105:MET:HB3	1.94	0.41
36:g:72:LEU:HD12	36:g:72:LEU:HA	1.87	0.41
6:A:886:G:H2'	6:A:887:G:H8	1.85	0.41
6:A:1002:U:H2'	6:A:1003:G:O4'	2.21	0.41
6:A:1164:G:N7	15:J:142:LYS:NZ	2.38	0.41
6:A:1217:A:H2'	6:A:1218:U:C6	2.55	0.41
6:A:1266:A:H5'	18:M:42:LEU:HD12	2.03	0.41
7:B:54:TYR:CE1	7:B:58:LYS:HE2	2.56	0.41
12:G:17:ASP:N	12:G:17:ASP:OD2	2.54	0.41
14:I:26:LEU:HG	14:I:101:MET:HE2	2.02	0.41
30:a:353:A:H2'	30:a:354:U:H5	1.86	0.41
30:a:445:U:H2'	30:a:446:G:H8	1.84	0.41
30:a:459:G:OP2	30:a:512:A:N6	2.54	0.41
30:a:488:U:H2'	30:a:489:G:O4'	2.21	0.41
30:a:1661:C:H2'	30:a:1662:U:C6	2.56	0.41
30:a:2831:U:H2'	30:a:2832:C:C6	2.56	0.41
34:e:15:LYS:HE2	34:e:15:LYS:N	2.36	0.41
36:g:53:VAL:HG11	36:g:69:THR:HG23	2.03	0.41
52:x:34:GLN:HB3	52:x:40:LEU:HB2	2.02	0.41
1:0:18:GLU:OE1	1:0:18:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:48:LYS:HB3	5:4:48:LYS:HE3	1.95	0.41
6:A:569:G:N1	6:A:736:C:OP2	2.54	0.41
6:A:1159:C:H2'	6:A:1160:G:H8	1.86	0.41
6:A:1184:G:H2'	6:A:1185:U:C6	2.56	0.41
6:A:1333:G:H5''	15:J:152:ARG:HB2	2.02	0.41
7:B:45:GLN:H	7:B:45:GLN:HG2	1.66	0.41
12:G:7:PRO:HA	12:G:11:ARG:HH21	1.85	0.41
12:G:165:GLU:OE2	12:G:166:GLY:N	2.54	0.41
20:O:27:VAL:HG12	20:O:83:LEU:HD13	2.03	0.41
28:X:21:LEU:O	28:X:28:ARG:NH2	2.53	0.41
30:a:31:C:N4	30:a:536:A:OP2	2.54	0.41
30:a:331:C:O2'	30:a:332:U:O5'	2.36	0.41
30:a:622:U:O2'	44:p:49:ASP:OD1	2.32	0.41
30:a:1836:U:C4	41:m:8:PRO:HG2	2.55	0.41
30:a:2036:A:N1	30:a:2269:G:H1'	2.36	0.41
30:a:2704:U:O2'	30:a:2829:U:OP1	2.24	0.41
30:a:2871:U:H5''	30:a:2872:G:H8	1.85	0.41
30:a:3071:A:H2'	30:a:3072:G:O4'	2.20	0.41
34:e:153:LEU:C	34:e:154:ARG:HE	2.29	0.41
49:u:81:ASP:N	49:u:81:ASP:OD1	2.51	0.41
5:4:65:TYR:CE2	26:U:5:LEU:HD12	2.55	0.41
6:A:79:C:H2'	6:A:80:C:H6	1.85	0.41
6:A:300:A:H2'	6:A:301:G:C8	2.56	0.41
6:A:409:C:OP1	9:D:107:ARG:NH1	2.54	0.41
6:A:678:A:H2'	6:A:679:U:C6	2.55	0.41
6:A:1357:G:C2	6:A:1358:G:C8	3.09	0.41
6:A:1388:G:H2'	6:A:1389:4OC:O4'	2.20	0.41
11:F:87:ARG:HG2	11:F:88:THR:H	1.86	0.41
12:G:115:VAL:O	12:G:119:ILE:HG13	2.20	0.41
15:J:41:ARG:HA	15:J:42:PRO:HD3	1.88	0.41
15:J:149:ARG:NH1	15:J:150:ASP:O	2.54	0.41
21:P:52:ASP:O	21:P:56:VAL:HG12	2.20	0.41
21:P:100:ASN:OD1	21:P:103:ASP:HB2	2.21	0.41
30:a:330:C:N4	30:a:331:C:H41	2.19	0.41
30:a:377:G:O6	30:a:432:A:N6	2.54	0.41
30:a:649:U:H2'	30:a:650:U:O4'	2.21	0.41
30:a:838:U:H2'	30:a:839:G:C8	2.51	0.41
30:a:911:U:O2'	39:k:52:GLY:HA3	2.21	0.41
30:a:913:U:H4'	30:a:916:G:N1	2.36	0.41
30:a:1138:G:N2	30:a:1168:A:H1'	2.30	0.41
30:a:1142:G:N2	30:a:1163:C:C2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1486:U:H2'	30:a:1487:G:H8	1.86	0.41
30:a:1664:U:H2'	30:a:1665:C:C6	2.55	0.41
30:a:1709:G:N2	30:a:1729:G:O6	2.54	0.41
30:a:2025:G:H2'	30:a:2026:C:H6	1.86	0.41
30:a:2500:G:H5''	30:a:2501:G:OP2	2.21	0.41
30:a:2555:A:H2'	30:a:2556:C:C6	2.56	0.41
30:a:2929:G:O6	30:a:2937:C:H5''	2.21	0.41
30:a:2978:G:H21	30:a:2981:U:C5'	2.33	0.41
32:c:267:LEU:HD13	32:c:267:LEU:HA	1.80	0.41
33:d:20:LEU:HD11	33:d:194:LEU:HD13	2.02	0.41
35:f:59:MET:O	35:f:63:ILE:HG23	2.21	0.41
39:k:96:ASP:O	39:k:100:VAL:HG13	2.20	0.41
42:n:98:THR:O	42:n:98:THR:OG1	2.38	0.41
48:t:45:LYS:HG3	48:t:63:ILE:O	2.21	0.41
49:u:159:LEU:H	49:u:159:LEU:HD12	1.85	0.41
6:A:26:G:H2'	6:A:27:C:H6	1.85	0.41
6:A:638:G:O2'	20:O:26:GLN:OE1	2.38	0.41
6:A:1109:G:N2	6:A:1110:U:O4	2.54	0.41
16:K:54:GLY:HA2	16:K:58:PHE:O	2.21	0.41
18:M:19:ASP:OD1	18:M:23:ARG:NH1	2.54	0.41
19:N:14:ARG:HE	19:N:42:ASP:HA	1.85	0.41
20:O:74:GLU:H	20:O:74:GLU:CD	2.18	0.41
30:a:442:U:H3'	30:a:443:G:C8	2.55	0.41
30:a:1358:U:H2'	30:a:1359:G:O4'	2.21	0.41
30:a:1462:C:H2'	30:a:1463:C:C6	2.55	0.41
30:a:1919:U:H2'	30:a:1920:G:O4'	2.21	0.41
35:f:102:GLY:N	35:f:105:MET:HE2	2.36	0.41
47:s:10:ARG:HG2	52:x:29:PHE:CD2	2.56	0.41
50:v:38:VAL:CG1	50:v:59:LEU:HB2	2.50	0.41
53:y:11:LYS:HB2	53:y:54:LEU:HD22	2.03	0.41
6:A:745:G:H2'	6:A:746:C:C6	2.55	0.40
6:A:1010:C:H2'	6:A:1011:C:O4'	2.21	0.40
6:A:1134:U:O4'	15:J:60:ARG:HD3	2.21	0.40
6:A:1400:A:H2	6:A:1474:G:H22	1.69	0.40
8:C:58:A:O2'	8:C:60:U:OP2	2.31	0.40
12:G:11:ARG:NH1	12:G:177:LEU:HA	2.36	0.40
12:G:72:PRO:HA	12:G:75:VAL:HG12	2.03	0.40
12:G:195:ILE:O	12:G:195:ILE:HG13	2.18	0.40
13:H:40:LEU:HB3	13:H:46:ILE:HG12	2.03	0.40
16:K:132:ARG:CZ	16:K:132:ARG:HB3	2.51	0.40
19:N:12:ASP:OD2	19:N:12:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:16:HIS:CD2	20:O:19:ASP:HB2	2.56	0.40
30:a:54:G:H2'	30:a:55:A:C8	2.55	0.40
30:a:1142:G:C8	30:a:1143:U:H2'	2.56	0.40
30:a:1189:G:H2'	30:a:1190:G:C8	2.55	0.40
30:a:1685:G:H2'	30:a:1686:C:O4'	2.21	0.40
30:a:2008:A:H2'	30:a:2009:C:C6	2.56	0.40
30:a:2176:U:H4'	33:d:139:THR:OG1	2.21	0.40
30:a:2247:C:H2'	30:a:2248:C:H6	1.85	0.40
30:a:2832:C:H2'	30:a:2833:U:H6	1.86	0.40
36:g:105:LEU:HD12	36:g:105:LEU:HA	1.82	0.40
37:i:36:LEU:O	37:i:51:GLY:HA3	2.21	0.40
47:s:14:LEU:O	52:x:32:ARG:NH1	2.54	0.40
6:A:408:G:H5'	9:D:5:THR:OG1	2.21	0.40
6:A:439:U:H2'	6:A:440:U:C6	2.56	0.40
6:A:499:G:H1	6:A:515:A:P	2.44	0.40
6:A:933:A:H2'	6:A:934:U:C6	2.56	0.40
6:A:968:C:H2'	6:A:969:C:H6	1.86	0.40
6:A:1020:G:C2	6:A:1021:G:H1'	2.57	0.40
6:A:1027:U:H2'	6:A:1028:C:O4'	2.21	0.40
6:A:1056:C:H2'	6:A:1057:G:C8	2.54	0.40
6:A:1202:U:OP1	24:S:3:LYS:HE3	2.21	0.40
6:A:1396:A:H5''	30:a:2098:3TD:H10	2.03	0.40
13:H:50:LYS:HD3	13:H:51:VAL:H	1.86	0.40
14:I:57:ASP:O	14:I:61:THR:HG22	2.21	0.40
14:I:78:ARG:HH11	14:I:78:ARG:HG2	1.86	0.40
16:K:73:ALA:HB1	16:K:106:LEU:HD13	2.02	0.40
16:K:125:ASN:HB3	16:K:126:GLY:H	1.70	0.40
26:U:3:ARG:HH12	26:U:10:PHE:HD1	1.70	0.40
30:a:659:U:H2'	30:a:660:G:C8	2.56	0.40
30:a:898:U:H2'	30:a:899:C:H6	1.86	0.40
30:a:2927:C:H2'	30:a:2928:U:C6	2.56	0.40
32:c:134:ARG:HA	32:c:168:ARG:HD3	2.03	0.40
49:u:107:LEU:HD23	49:u:139:ILE:HG23	2.02	0.40
6:A:1088:C:H4'	7:B:97:LEU:HD13	2.04	0.40
6:A:1092:C:C4	6:A:1093:G:C8	3.10	0.40
6:A:1277:C:H2'	6:A:1278:C:C6	2.57	0.40
7:B:112:ALA:HA	7:B:115:LYS:HG2	2.03	0.40
7:B:172:LEU:O	7:B:176:GLU:HG3	2.22	0.40
9:D:3:ARG:HG3	9:D:110:ARG:HH21	1.86	0.40
20:O:42:LYS:HE2	20:O:42:LYS:HB3	1.68	0.40
22:Q:45:MET:HE3	22:Q:45:MET:HB3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1709:G:O6	30:a:1726:U:O2'	2.34	0.40
34:e:13:LYS:HD2	34:e:13:LYS:HA	1.72	0.40
34:e:29:VAL:HG12	34:e:30:ASN:H	1.87	0.40
35:f:11:PRO:HB3	35:f:107:GLU:OE1	2.21	0.40
39:k:99:SER:HA	39:k:103:VAL:HG12	2.03	0.40
53:y:37:ILE:N	53:y:37:ILE:HD12	2.37	0.40
6:A:37:A:H2'	6:A:38:C:C6	2.56	0.40
6:A:392:U:H2'	6:A:393:G:H8	1.86	0.40
6:A:614:U:H5'	6:A:615:G:C8	2.57	0.40
6:A:892:A:H2'	6:A:893:A:C8	2.56	0.40
6:A:976:U:H4'	6:A:977:G:H5''	2.03	0.40
10:E:170:LEU:HD23	10:E:170:LEU:HA	1.90	0.40
14:I:42:ILE:HG21	14:I:116:MET:HB3	2.04	0.40
15:J:173:ARG:HG2	15:J:173:ARG:NH1	2.37	0.40
16:K:70:GLN:O	16:K:74:GLU:HG2	2.21	0.40
21:P:40:TYR:CZ	21:P:42:PRO:HB3	2.56	0.40
30:a:381:G:H2'	30:a:382:U:C6	2.57	0.40
30:a:2141:C:H2'	30:a:2142:G:H8	1.87	0.40
30:a:2398:G:H2'	30:a:2399:G:H8	1.86	0.40
30:a:2749:G:H2'	30:a:2750:C:C6	2.56	0.40
30:a:3027:U:H2'	30:a:3028:G:O4'	2.21	0.40
41:m:77:HIS:O	41:m:78:ILE:C	2.65	0.40
6:A:1161:G:H2'	6:A:1162:A:H8	1.86	0.40
6:A:1236:A:H2	6:A:1357:G:H1'	1.86	0.40
14:I:60:GLN:OE1	14:I:60:GLN:C	2.64	0.40
16:K:89:ASP:OD2	16:K:89:ASP:C	2.64	0.40
30:a:384:A:N1	30:a:407:A:O2'	2.51	0.40
30:a:1315:G:H2'	30:a:1316:U:O4'	2.21	0.40
30:a:1754:A:H2'	30:a:1755:A:H8	1.85	0.40
30:a:1984:G:N1	30:a:2384:G:OP1	2.44	0.40
30:a:2185:U:H2'	30:a:2186:G:C8	2.56	0.40
30:a:2245:A:O2'	30:a:2246:C:H5'	2.20	0.40
30:a:2817:C:H5''	33:d:85:LEU:O	2.21	0.40
35:f:17:TYR:HA	35:f:21:ILE:HG12	2.04	0.40
36:g:35:PHE:HB2	36:g:76:MET:HE3	2.04	0.40
39:k:134:GLU:HA	39:k:137:GLU:OE2	2.21	0.40
42:n:44:SER:O	42:n:77:LYS:NZ	2.48	0.40
46:r:82:ARG:HB3	46:r:82:ARG:NH1	2.36	0.40
47:s:27:ASP:OD1	47:s:27:ASP:C	2.64	0.40
47:s:27:ASP:OD1	47:s:28:GLN:HG2	2.20	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	
1	0	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	65/68 (96%)	65 (100%)	0	0	100	100
4	3	35/37 (95%)	35 (100%)	0	0	100	100
5	4	64/69 (93%)	57 (89%)	7 (11%)	0	100	100
7	B	231/283 (82%)	214 (93%)	15 (6%)	2 (1%)	14	27
9	D	198/201 (98%)	184 (93%)	14 (7%)	0	100	100
10	E	177/215 (82%)	174 (98%)	3 (2%)	0	100	100
11	F	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
12	G	204/269 (76%)	198 (97%)	6 (3%)	0	100	100
13	H	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
14	I	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
15	J	132/173 (76%)	120 (91%)	11 (8%)	1 (1%)	16	31
16	K	115/135 (85%)	105 (91%)	9 (8%)	1 (1%)	14	27
17	L	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
18	M	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	24
19	N	120/123 (98%)	110 (92%)	10 (8%)	0	100	100
20	O	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
21	P	126/147 (86%)	112 (89%)	13 (10%)	1 (1%)	16	31
22	Q	88/90 (98%)	78 (89%)	9 (10%)	1 (1%)	11	22
23	R	65/79 (82%)	60 (92%)	4 (6%)	1 (2%)	8	16
24	S	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7	13
25	T	85/88 (97%)	85 (100%)	0	0	100	100
26	U	82/93 (88%)	75 (92%)	6 (7%)	1 (1%)	10	20
27	V	21/24 (88%)	20 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	X	30/33 (91%)	29 (97%)	0	1 (3%)	3	4
32	c	272/278 (98%)	260 (96%)	11 (4%)	1 (0%)	30	49
33	d	212/223 (95%)	204 (96%)	8 (4%)	0	100	100
34	e	208/301 (69%)	178 (86%)	26 (12%)	4 (2%)	6	11
35	f	182/210 (87%)	169 (93%)	13 (7%)	0	100	100
36	g	175/180 (97%)	168 (96%)	7 (4%)	0	100	100
37	i	144/147 (98%)	141 (98%)	3 (2%)	0	100	100
38	j	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
39	k	142/146 (97%)	124 (87%)	17 (12%)	1 (1%)	18	34
40	l	134/139 (96%)	125 (93%)	9 (7%)	0	100	100
41	m	118/187 (63%)	110 (93%)	7 (6%)	1 (1%)	16	31
42	n	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
43	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
44	p	117/123 (95%)	116 (99%)	1 (1%)	0	100	100
45	q	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
46	r	130/153 (85%)	125 (96%)	5 (4%)	0	100	100
47	s	93/102 (91%)	85 (91%)	7 (8%)	1 (1%)	11	22
48	t	103/122 (84%)	94 (91%)	8 (8%)	1 (1%)	12	24
49	u	177/205 (86%)	168 (95%)	9 (5%)	0	100	100
50	v	76/89 (85%)	74 (97%)	1 (1%)	1 (1%)	9	18
51	w	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	13
52	x	67/77 (87%)	62 (92%)	5 (8%)	0	100	100
53	y	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
54	z	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
All	All	5646/6322 (89%)	5320 (94%)	304 (5%)	22 (0%)	31	49

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	B	100	MET
22	Q	9	THR
24	S	27	CYS
26	U	84	VAL
28	X	4	VAL

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Mol	Chain	Res	Type
34	e	133	VAL
34	e	151	ALA
47	s	93	ARG
16	K	23	VAL
18	M	6	ILE
34	e	159	VAL
21	P	112	ALA
32	c	262	LYS
15	J	43	ALA
23	R	73	THR
34	e	186	ASN
41	m	37	THR
48	t	64	ILE
51	w	41	ASN
50	v	73	ARG
7	B	4	VAL
39	k	124	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/51 (92%)	47 (100%)	0	100	100
2	1	36/36 (100%)	35 (97%)	1 (3%)	38	66
3	2	54/55 (98%)	53 (98%)	1 (2%)	50	76
4	3	35/35 (100%)	35 (100%)	0	100	100
5	4	56/59 (95%)	52 (93%)	4 (7%)	13	29
7	B	197/234 (84%)	189 (96%)	8 (4%)	27	53
9	D	175/176 (99%)	169 (97%)	6 (3%)	32	60
10	E	130/155 (84%)	125 (96%)	5 (4%)	29	56
11	F	89/89 (100%)	87 (98%)	2 (2%)	45	73
12	G	160/200 (80%)	155 (97%)	5 (3%)	35	62
13	H	108/109 (99%)	104 (96%)	4 (4%)	30	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	I	132/133 (99%)	125 (95%)	7 (5%)	20	42
15	J	97/131 (74%)	94 (97%)	3 (3%)	35	62
16	K	88/101 (87%)	83 (94%)	5 (6%)	18	39
17	L	103/104 (99%)	99 (96%)	4 (4%)	28	55
18	M	89/93 (96%)	87 (98%)	2 (2%)	45	73
19	N	99/100 (99%)	97 (98%)	2 (2%)	48	75
20	O	74/74 (100%)	73 (99%)	1 (1%)	59	81
21	P	103/115 (90%)	99 (96%)	4 (4%)	28	55
22	Q	81/81 (100%)	78 (96%)	3 (4%)	30	57
23	R	55/65 (85%)	53 (96%)	2 (4%)	31	58
24	S	48/49 (98%)	47 (98%)	1 (2%)	47	74
25	T	68/69 (99%)	64 (94%)	4 (6%)	18	37
26	U	72/80 (90%)	69 (96%)	3 (4%)	26	52
27	V	16/17 (94%)	16 (100%)	0	100	100
28	X	28/29 (97%)	27 (96%)	1 (4%)	31	58
32	c	216/220 (98%)	209 (97%)	7 (3%)	34	62
33	d	166/172 (96%)	165 (99%)	1 (1%)	78	91
34	e	165/237 (70%)	157 (95%)	8 (5%)	23	46
35	f	154/175 (88%)	146 (95%)	8 (5%)	21	42
36	g	150/152 (99%)	144 (96%)	6 (4%)	28	54
37	i	118/120 (98%)	114 (97%)	4 (3%)	32	60
38	j	101/101 (100%)	98 (97%)	3 (3%)	36	64
39	k	111/113 (98%)	107 (96%)	4 (4%)	31	58
40	l	108/110 (98%)	105 (97%)	3 (3%)	38	66
41	m	100/142 (70%)	96 (96%)	4 (4%)	28	54
42	n	95/96 (99%)	92 (97%)	3 (3%)	34	62
43	o	97/99 (98%)	96 (99%)	1 (1%)	68	86
44	p	98/99 (99%)	96 (98%)	2 (2%)	48	75
45	q	84/84 (100%)	74 (88%)	10 (12%)	5	11
46	r	105/118 (89%)	100 (95%)	5 (5%)	23	46
47	s	84/89 (94%)	83 (99%)	1 (1%)	63	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	t	91/103 (88%)	87 (96%)	4 (4%)	25	50
49	u	149/168 (89%)	143 (96%)	6 (4%)	28	54
50	v	60/67 (90%)	57 (95%)	3 (5%)	22	44
51	w	52/53 (98%)	50 (96%)	2 (4%)	29	56
52	x	61/68 (90%)	59 (97%)	2 (3%)	33	61
53	y	53/55 (96%)	51 (96%)	2 (4%)	29	56
54	z	51/52 (98%)	49 (96%)	2 (4%)	28	55
All	All	4709/5133 (92%)	4540 (96%)	169 (4%)	32	58

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	24	THR
3	2	38	SER
5	4	10	ARG
5	4	23	THR
5	4	28	SER
5	4	62	GLU
7	B	1	MET
7	B	20	THR
7	B	155	MET
7	B	164	VAL
7	B	182	ILE
7	B	189	ASP
7	B	193	ASP
7	B	208	ILE
9	D	41	THR
9	D	47	SER
9	D	112	MET
9	D	134	THR
9	D	146	ASP
9	D	190	VAL
10	E	108	VAL
10	E	111	GLU
10	E	146	VAL
10	E	151	LEU
10	E	192	MET
11	F	19	VAL
11	F	88	THR
12	G	93	LEU

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Mol	Chain	Res	Type
12	G	97	GLN
12	G	103	LEU
12	G	161	MET
12	G	197	VAL
13	H	10	MET
13	H	40	LEU
13	H	76	SER
13	H	123	GLU
14	I	12	VAL
14	I	31	LEU
14	I	33	ASP
14	I	40	GLN
14	I	55	ASN
14	I	68	ASN
14	I	146	GLU
15	J	86	HIS
15	J	105	VAL
15	J	148	THR
16	K	22	VAL
16	K	47	VAL
16	K	83	HIS
16	K	111	LEU
16	K	125	ASN
17	L	41	THR
17	L	73	ASN
17	L	101	SER
17	L	104	THR
18	M	76	ILE
18	M	99	GLU
19	N	4	LEU
19	N	103	THR
20	O	9	ILE
21	P	3	THR
21	P	53	SER
21	P	62	VAL
21	P	124	SER
22	Q	24	MET
22	Q	34	ASP
22	Q	62	MET
23	R	44	VAL
23	R	67	LEU
24	S	44	LEU

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Mol	Chain	Res	Type
25	T	17	SER
25	T	22	LYS
25	T	33	ARG
25	T	37	ARG
26	U	62	VAL
26	U	71	LEU
26	U	79	THR
28	X	30	ARG
32	c	23	GLU
32	c	34	LEU
32	c	44	ASN
32	c	95	LEU
32	c	119	SER
32	c	169	GLU
32	c	267	LEU
33	d	94	SER
34	e	7	ILE
34	e	71	LYS
34	e	134	ASP
34	e	150	LEU
34	e	158	VAL
34	e	179	VAL
34	e	185	LEU
34	e	210	ARG
35	f	41	GLU
35	f	73	LYS
35	f	77	THR
35	f	81	LYS
35	f	121	ARG
35	f	127	ASN
35	f	141	LEU
35	f	146	MET
36	g	60	ARG
36	g	72	LEU
36	g	81	THR
36	g	118	ASP
36	g	124	THR
36	g	135	VAL
37	i	30	THR
37	i	91	GLU
37	i	98	ARG
37	i	102	GLU

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Mol	Chain	Res	Type
38	j	28	SER
38	j	65	THR
38	j	73	ASP
39	k	103	VAL
39	k	114	THR
39	k	117	LEU
39	k	143	VAL
40	l	18	THR
40	l	52	ILE
40	l	94	ILE
41	m	23	ASN
41	m	57	THR
41	m	113	ILE
41	m	114	GLU
42	n	11	LEU
42	n	47	VAL
42	n	72	GLU
43	o	30	VAL
44	p	93	LYS
44	p	108	SER
45	q	6	ARG
45	q	14	VAL
45	q	21	GLU
45	q	23	ASP
45	q	36	THR
45	q	49	ASP
45	q	51	ASP
45	q	59	THR
45	q	83	LYS
45	q	95	VAL
46	r	1	MET
46	r	3	LYS
46	r	5	GLU
46	r	41	VAL
46	r	102	ILE
47	s	6	ILE
48	t	33	ARG
48	t	37	VAL
48	t	42	ASN
48	t	46	HIS
49	u	8	LYS
49	u	61	LEU

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Mol	Chain	Res	Type
49	u	81	ASP
49	u	102	ASP
49	u	124	ASN
49	u	150	THR
50	v	49	ASP
50	v	75	ARG
50	v	83	VAL
51	w	25	THR
51	w	47	MET
52	x	8	GLU
52	x	39	GLN
53	y	22	GLU
53	y	58	GLU
54	z	11	SER
54	z	56	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	32	HIS
5	4	34	ASN
7	B	15	HIS
7	B	160	GLN
7	B	204	ASN
9	D	54	GLN
10	E	155	ASN
12	G	6	ASN
12	G	45	ASN
12	G	113	GLN
13	H	18	ASN
13	H	22	HIS
15	J	88	GLN
19	N	52	GLN
25	T	7	GLN
32	c	44	ASN
32	c	96	HIS
32	c	135	ASN
33	d	143	HIS
34	e	93	HIS
34	e	102	GLN
35	f	75	GLN
35	f	127	ASN

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Mol	Chain	Res	Type
35	f	130	GLN
37	i	130	HIS
39	k	106	ASN
39	k	133	GLN
41	m	31	HIS
41	m	62	ASN
49	u	134	ASN
51	w	48	ASN
54	z	12	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	Y	9/22 (40%)	4 (44%)	0
30	a	2891/3086 (93%)	518 (17%)	0
31	b	117/120 (97%)	11 (9%)	0
6	A	1503/1537 (97%)	253 (16%)	17 (1%)
8	C	75/77 (97%)	13 (17%)	1 (1%)
All	All	4595/4842 (94%)	799 (17%)	18 (0%)

All (799) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	7	A
6	A	9	U
6	A	10	G
6	A	13	G
6	A	36	A
6	A	43	G
6	A	51	C
6	A	52	U
6	A	55	A
6	A	58	C
6	A	74	A
6	A	82	U
6	A	91	G
6	A	92	G
6	A	93	G
6	A	96	G
6	A	98	U
6	A	119	A

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Mol	Chain	Res	Type
6	A	120	A
6	A	121	C
6	A	130	A
6	A	143	C
6	A	164	C
6	A	173	A
6	A	174	U
6	A	178	G
6	A	183	G
6	A	184	G
6	A	185	A
6	A	192	G
6	A	204	G
6	A	205	G
6	A	213	A
6	A	214	G
6	A	218	C
6	A	222	G
6	A	226	G
6	A	233	G
6	A	242	C
6	A	247	C
6	A	249	G
6	A	253	G
6	A	268	G
6	A	269	C
6	A	291	G
6	A	308	A
6	A	323	A
6	A	331	A
6	A	332	C
6	A	349	G
6	A	354	C
6	A	356	G
6	A	358	A
6	A	369	U
6	A	374	C
6	A	390	G
6	A	399	A
6	A	408	G
6	A	414	U
6	A	415	G

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Mol	Chain	Res	Type
6	A	416	A
6	A	417	C
6	A	420	C
6	A	423	U
6	A	424	C
6	A	425	G
6	A	426	G
6	A	431	U
6	A	441	U
6	A	453	A
6	A	455	G
6	A	461	G
6	A	463	G
6	A	466	G
6	A	467	G
6	A	468	U
6	A	474	G
6	A	476	A
6	A	477	A
6	A	478	A
6	A	491	A
6	A	492	A
6	A	493	C
6	A	499	G
6	A	500	C
6	A	503	G
6	A	509	G7M
6	A	513	U
6	A	514	G
6	A	515	A
6	A	529	A
6	A	546	U
6	A	554	A
6	A	555	A
6	A	558	G
6	A	559	G
6	A	578	C
6	A	600	C
6	A	614	U
6	A	615	G
6	A	635	U
6	A	647	G

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Mol	Chain	Res	Type
6	A	703	A
6	A	704	G
6	A	716	G
6	A	729	U
6	A	730	U
6	A	737	G
6	A	759	A
6	A	774	A
6	A	775	U
6	A	776	A
6	A	791	G
6	A	797	A
6	A	799	C
6	A	803	G
6	A	825	U
6	A	826	C
6	A	827	C
6	A	828	A
6	A	831	G
6	A	832	G
6	A	837	G
6	A	874	G
6	A	898	A
6	A	900	G
6	A	910	G
6	A	911	G
6	A	918	C
6	A	919	A
6	A	944	U
6	A	945	U
6	A	950	2MG
6	A	952	A
6	A	953	A
6	A	955	G
6	A	956	C
6	A	959	A
6	A	960	G
6	A	961	A
6	A	975	U
6	A	976	U
6	A	977	G
6	A	978	A

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Mol	Chain	Res	Type
6	A	984	A
6	A	987	G
6	A	988	G
6	A	989	G
6	A	990	A
6	A	992	U
6	A	993	G
6	A	994	C
6	A	1003	G
6	A	1004	G
6	A	1009	G
6	A	1010	C
6	A	1012	U
6	A	1015	U
6	A	1021	G
6	A	1025	G
6	A	1026	U
6	A	1027	U
6	A	1029	A
6	A	1030	C
6	A	1031	A
6	A	1038	G
6	A	1040	A
6	A	1041	U
6	A	1050	U
6	A	1051	C
6	A	1053	G
6	A	1055	U
6	A	1066	G
6	A	1070	U
6	A	1079	G
6	A	1080	U
6	A	1086	A
6	A	1088	C
6	A	1110	U
6	A	1111	U
6	A	1121	U
6	A	1122	U
6	A	1125	G
6	A	1126	G
6	A	1131	G
6	A	1132	A

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Mol	Chain	Res	Type
6	A	1138	U
6	A	1140	G
6	A	1145	C
6	A	1146	G
6	A	1153	U
6	A	1162	A
6	A	1168	G
6	A	1170	G
6	A	1182	A
6	A	1183	A
6	A	1188	U
6	A	1192	G
6	A	1198	U
6	A	1199	A
6	A	1200	U
6	A	1210	U
6	A	1213	A
6	A	1224	A
6	A	1227	G
6	A	1237	G
6	A	1242	U
6	A	1244	G
6	A	1246	G
6	A	1256	G
6	A	1261	A
6	A	1266	A
6	A	1272	G
6	A	1273	A
6	A	1274	A
6	A	1278	C
6	A	1285	A
6	A	1286	G
6	A	1291	G
6	A	1298	G
6	A	1303	C
6	A	1306	C
6	A	1326	G
6	A	1332	A
6	A	1333	G
6	A	1339	G
6	A	1351	C
6	A	1368	U

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Mol	Chain	Res	Type
6	A	1382	C
6	A	1385	A
6	A	1401	U
6	A	1406	G
6	A	1415	A
6	A	1429	G
6	A	1433	A
6	A	1437	G
6	A	1438	U
6	A	1439	U
6	A	1440	G
6	A	1474	G
6	A	1479	A
6	A	1480	A
6	A	1481	G
6	A	1484	G
6	A	1493	U
6	A	1504	G
6	A	1506	MA6
6	A	1516	G
6	A	1517	G
6	A	1518	A
6	A	1519	U
6	A	1520	C
6	A	1521	A
8	C	6	G
8	C	9	G
8	C	16	C
8	C	17	C
8	C	17(A)	U
8	C	18	G
8	C	19	G
8	C	20	U
8	C	21	A
8	C	47	U
8	C	48	C
8	C	69	C
8	C	76	A
29	Y	19	U
29	Y	20	U
29	Y	21	U
29	Y	22	U

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Mol	Chain	Res	Type
30	a	11	G
30	a	12	U
30	a	32	U
30	a	34	G
30	a	42	G
30	a	44	G
30	a	50	G
30	a	62	G
30	a	70	A
30	a	73	A
30	a	74	G
30	a	82	G
30	a	91	A
30	a	92	G
30	a	93	C
30	a	99	G
30	a	101	G
30	a	117	A
30	a	118	A
30	a	119	U
30	a	132	A
30	a	133	A
30	a	135	G
30	a	136	U
30	a	147	G
30	a	166	A
30	a	169	G
30	a	171	A
30	a	180	U
30	a	185	G
30	a	188	A
30	a	203	A
30	a	206	A
30	a	222	G
30	a	223	A
30	a	229	A
30	a	230	A
30	a	235	G
30	a	236	U
30	a	237	G
30	a	240	A
30	a	255	G

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Mol	Chain	Res	Type
30	a	272	A
30	a	273	G
30	a	275	C
30	a	276	U
30	a	279	A
30	a	283	U
30	a	284	G
30	a	285	U
30	a	286	G
30	a	287	U
30	a	288	G
30	a	290	G
30	a	307	U
30	a	308	U
30	a	309	G
30	a	310	C
30	a	312	U
30	a	313	G
30	a	314	U
30	a	318	G
30	a	322	U
30	a	324	U
30	a	325	G
30	a	332	U
30	a	337	G
30	a	338	U
30	a	339	U
30	a	345	G
30	a	346	C
30	a	347	C
30	a	348	G
30	a	353	A
30	a	354	U
30	a	356	G
30	a	357	G
30	a	358	C
30	a	359	C
30	a	360	A
30	a	362	U
30	a	366	A
30	a	367	A
30	a	369	U

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Mol	Chain	Res	Type
30	a	370	G
30	a	373	G
30	a	375	G
30	a	377	G
30	a	378	A
30	a	379	A
30	a	380	G
30	a	387	C
30	a	389	U
30	a	393	G
30	a	396	A
30	a	402	A
30	a	408	G
30	a	415	A
30	a	419	U
30	a	423	G
30	a	431	A
30	a	433	G
30	a	434	C
30	a	435	G
30	a	445	U
30	a	447	U
30	a	451	G
30	a	454	G
30	a	455	C
30	a	460	A
30	a	475	G
30	a	476	U
30	a	477	G
30	a	478	G
30	a	480	A
30	a	494	U
30	a	500	G
30	a	501	A
30	a	516	U
30	a	532	A
30	a	533	C
30	a	535	G
30	a	536	A
30	a	537	U
30	a	540	U
30	a	544	U

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Mol	Chain	Res	Type
30	a	545	G
30	a	546	A
30	a	569	A
30	a	570	G
30	a	589	A
30	a	592	G
30	a	593	A
30	a	596	U
30	a	618	G
30	a	619	C
30	a	620	C
30	a	621	G
30	a	631	G
30	a	632	U
30	a	633	G
30	a	634	U
30	a	635	G
30	a	646	G
30	a	656	G
30	a	657	A
30	a	658	A
30	a	674	G
30	a	675	U
30	a	676	G
30	a	687	A
30	a	698	U
30	a	699	G
30	a	700	G
30	a	701	U
30	a	704	G
30	a	713	A
30	a	720	G
30	a	723	A
30	a	731	A
30	a	734	G
30	a	739	G
30	a	740	A
30	a	741	G
30	a	770	A
30	a	771	U
30	a	794	G
30	a	797	G

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Mol	Chain	Res	Type
30	a	802	G
30	a	815	U
30	a	832	U
30	a	849	A
30	a	860	G
30	a	861	G
30	a	867	A
30	a	869	G
30	a	870	G
30	a	875	U
30	a	877	A
30	a	890	G
30	a	897	C
30	a	912	U
30	a	930	G
30	a	931	G
30	a	944	G
30	a	951	A
30	a	966	G
30	a	968	G
30	a	969	C
30	a	970	U
30	a	971	U
30	a	973	U
30	a	974	C
30	a	979	U
30	a	981	C
30	a	994	A
30	a	1014	G
30	a	1015	U
30	a	1028	A
30	a	1029	G
30	a	1042	A
30	a	1044	G
30	a	1057	G
30	a	1063	A
30	a	1066	A
30	a	1079	A
30	a	1096	G
30	a	1105	G
30	a	1109	G
30	a	1116	U

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Mol	Chain	Res	Type
30	a	1120	G
30	a	1124	U
30	a	1128	U
30	a	1129	A
30	a	1130	G
30	a	1135	C
30	a	1137	A
30	a	1140	A
30	a	1141	G
30	a	1144	U
30	a	1145	G
30	a	1149	U
30	a	1150	G
30	a	1153	A
30	a	1154	G
30	a	1156	A
30	a	1157	G
30	a	1159	C
30	a	1161	U
30	a	1162	C
30	a	1163	C
30	a	1164	U
30	a	1165	U
30	a	1171	A
30	a	1178	A
30	a	1179	A
30	a	1181	A
30	a	1183	C
30	a	1188	U
30	a	1191	U
30	a	1194	A
30	a	1195	G
30	a	1196	U
30	a	1211	A
30	a	1215	U
30	a	1216	A
30	a	1218	C
30	a	1225	U
30	a	1227	A
30	a	1254	G
30	a	1255	U
30	a	1256	G

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Mol	Chain	Res	Type
30	a	1257	U
30	a	1283	G
30	a	1297	G
30	a	1306	U
30	a	1307	G
30	a	1327	G
30	a	1333	G
30	a	1348	G
30	a	1351	U
30	a	1376	A
30	a	1377	U
30	a	1388	U
30	a	1397	C
30	a	1405	U
30	a	1417	G
30	a	1420	U
30	a	1426	C
30	a	1428	U
30	a	1441	A
30	a	1455	U
30	a	1460	A
30	a	1471	A
30	a	1472	U
30	a	1493	G
30	a	1601	G
30	a	1607	A
30	a	1608	C
30	a	1625	U
30	a	1626	C
30	a	1630	G
30	a	1633	G
30	a	1639	U
30	a	1641	U
30	a	1642	C
30	a	1663	G
30	a	1667	G
30	a	1673	U
30	a	1674	A
30	a	1685	G
30	a	1688	U
30	a	1690	A
30	a	1691	A

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Mol	Chain	Res	Type
30	a	1692	G
30	a	1695	U
30	a	1697	A
30	a	1706	G
30	a	1710	A
30	a	1713	C
30	a	1714	C
30	a	1717	G
30	a	1718	G
30	a	1719	U
30	a	1720	U
30	a	1721	G
30	a	1724	G
30	a	1725	G
30	a	1726	U
30	a	1727	G
30	a	1737	U
30	a	1743	A
30	a	1749	G
30	a	1752	A
30	a	1761	G
30	a	1763	G
30	a	1769	G
30	a	1791	U
30	a	1792	A
30	a	1794	A
30	a	1818	U
30	a	1830	A
30	a	1832	C
30	a	1837	G
30	a	1838	A
30	a	1858	G
30	a	1897	G
30	a	1904	U
30	a	1905	G
30	a	1906	C
30	a	1908	C
30	a	1911	G
30	a	1912	U
30	a	1913	G
30	a	1914	C
30	a	1915	G

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Mol	Chain	Res	Type
30	a	1916	G
30	a	1919	U
30	a	1929	G
30	a	1939	G
30	a	1947	G
30	a	1956	A
30	a	1965	C
30	a	1974	A
30	a	1983	C
30	a	1984	G
30	a	1985	A
30	a	1999	U
30	a	2012	A
30	a	2031	A
30	a	2041	G
30	a	2042	A
30	a	2052	G
30	a	2053	U
30	a	2054	A
30	a	2055	U
30	a	2066	G
30	a	2067	A
30	a	2068	A
30	a	2069	C
30	a	2089	G
30	a	2096	A
30	a	2097	C
30	a	2098	3TD
30	a	2101	A
30	a	2103	C
30	a	2112	G
30	a	2113	G
30	a	2120	A
30	a	2121	A
30	a	2124	C
30	a	2138	U
30	a	2150	C
30	a	2153	A
30	a	2154	U
30	a	2155	G
30	a	2174	U
30	a	2176	U

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Mol	Chain	Res	Type
30	a	2203	A
30	a	2204	U
30	a	2206	A
30	a	2210	G
30	a	2214	A
30	a	2215	G
30	a	2216	A
30	a	2222	G
30	a	2226	C
30	a	2233	C
30	a	2235	G
30	a	2238	C
30	a	2239	G
30	a	2243	A
30	a	2245	A
30	a	2246	C
30	a	2275	G
30	a	2278	G
30	a	2280	U
30	a	2282	G
30	a	2283	G
30	a	2284	G
30	a	2287	G
30	a	2288	G
30	a	2289	U
30	a	2291	U
30	a	2361	C
30	a	2364	A
30	a	2366	U
30	a	2367	G
30	a	2369	U
30	a	2381	A
30	a	2384	G
30	a	2385	U
30	a	2386	G
30	a	2393	G
30	a	2394	A
30	a	2395	U
30	a	2407	A
30	a	2420	G
30	a	2421	G
30	a	2460	A

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Mol	Chain	Res	Type
30	a	2461	G
30	a	2464	G
30	a	2465	C
30	a	2469	A
30	a	2470	A
30	a	2487	U
30	a	2489	G
30	a	2490	G
30	a	2493	A
30	a	2501	G
30	a	2502	U
30	a	2503	G
30	a	2509	A
30	a	2517	A
30	a	2518	A
30	a	2529	C
30	a	2532	U
30	a	2536	A
30	a	2543	G
30	a	2565	G
30	a	2567	A
30	a	2585	G
30	a	2588	U
30	a	2607	A
30	a	2608	A
30	a	2611	G
30	a	2612	A
30	a	2617	A
30	a	2623	C
30	a	2627	2MG
30	a	2630	A
30	a	2655	C
30	a	2657	C
30	a	2658	A
30	a	2673	U
30	a	2676	G
30	a	2680	OMC
30	a	2684	G
30	a	2687	G
30	a	2688	U
30	a	2700	A
30	a	2702	C

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Mol	Chain	Res	Type
30	a	2712	G
30	a	2717	G
30	a	2721	C
30	a	2722	C
30	a	2748	A
30	a	2749	G
30	a	2763	G
30	a	2764	G
30	a	2767	U
30	a	2784	A
30	a	2791	U
30	a	2792	C
30	a	2795	U
30	a	2796	A
30	a	2811	A
30	a	2828	C
30	a	2836	A
30	a	2845	G
30	a	2852	G
30	a	2870	G
30	a	2872	G
30	a	2873	C
30	a	2896	G
30	a	2908	C
30	a	2914	G
30	a	2915	U
30	a	2926	G
30	a	2930	A
30	a	2939	A
30	a	2948	G
30	a	2960	A
30	a	2962	A
30	a	2963	A
30	a	2971	C
30	a	2972	A
30	a	2973	C
30	a	2978	G
30	a	2979	U
30	a	2981	U
30	a	2982	U
30	a	2983	C
30	a	2988	U

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Mol	Chain	Res	Type
30	a	3013	U
30	a	3014	G
30	a	3015	A
30	a	3041	G
30	a	3047	G
30	a	3052	G
30	a	3053	A
30	a	3063	A
30	a	3064	U
30	a	3066	G
30	a	3071	A
30	a	3073	G
30	a	3074	A
30	a	3075	C
31	b	34	G
31	b	35	U
31	b	45	A
31	b	52	U
31	b	56	U
31	b	84	C
31	b	91	U
31	b	100	A
31	b	109	C
31	b	110	G
31	b	119	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	9	U
6	A	90	U
6	A	418	G
6	A	467	G
6	A	869	G
6	A	1009	G
6	A	1050	U
6	A	1052	A
6	A	1130	G
6	A	1131	G
6	A	1187	A
6	A	1271	G
6	A	1350	A

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Mol	Chain	Res	Type
6	A	1384	C
6	A	1479	A
6	A	1480	A
6	A	1520	C
8	C	17(A)	U

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

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
6	UR3	A	1485	6	19,22,23	2.70	8 (42%)	26,32,35	1.63	2 (7%)
6	5MC	A	1394	6	19,22,23	4.37	8 (42%)	26,32,35	1.03	2 (7%)
30	PSU	a	1038	30	18,21,22	0.91	1 (5%)	21,30,33	0.88	0
30	PSU	a	2762	30	18,21,22	0.95	1 (5%)	21,30,33	0.90	1 (4%)
6	5MC	A	1387	6	19,22,23	4.48	8 (42%)	26,32,35	1.07	1 (3%)
30	3TD	a	2098	30	19,22,23	4.13	7 (36%)	23,32,35	1.86	5 (21%)
30	OMG	a	2433	30,8	23,26,27	2.53	9 (39%)	32,38,41	2.41	11 (34%)
6	5MC	A	1391	6	19,22,23	4.40	8 (42%)	26,32,35	0.96	2 (7%)
6	2MG	A	950	6	23,26,27	3.12	8 (34%)	33,38,41	2.51	12 (36%)
30	H2U	a	2631	30	18,21,22	3.06	5 (27%)	19,30,33	1.49	4 (21%)
6	PSU	A	498	6,56	18,21,22	0.93	1 (5%)	21,30,33	0.69	0
30	2MG	a	2018	30	23,26,27	3.04	8 (34%)	33,38,41	2.62	12 (36%)
30	PSU	a	2786	30	18,21,22	0.91	1 (5%)	21,30,33	0.77	0
6	2MG	A	1503	6	23,26,27	3.05	8 (34%)	33,38,41	2.62	12 (36%)
6	MA6	A	1505	6	23,26,27	1.38	4 (17%)	33,38,41	3.02	12 (36%)
6	4OC	A	1389	6	20,23,24	3.10	8 (40%)	25,32,35	0.92	1 (4%)
6	G7M	A	509	6	23,26,27	2.61	9 (39%)	34,39,42	1.72	7 (20%)
8	5MC	C	32	8	19,22,23	4.42	8 (42%)	26,32,35	1.01	1 (3%)
30	2MG	a	2627	30	23,26,27	3.03	8 (34%)	33,38,41	2.46	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	a	2094	30	18,21,22	0.92	1 (5%)	21,30,33	0.67	0
30	PSU	a	2639	30	18,21,22	0.92	1 (5%)	21,30,33	0.74	0
30	5MC	a	2145	30	19,22,23	4.36	8 (42%)	26,32,35	1.08	2 (7%)
30	OMC	a	2680	30,56	19,22,23	3.16	8 (42%)	25,31,34	0.89	0
30	OMU	a	2734	30	19,22,23	2.90	6 (31%)	25,31,34	1.89	5 (20%)
30	5MU	a	2122	30	19,22,23	0.30	0	27,32,35	0.41	0
6	5MC	A	951	6	19,22,23	4.50	8 (42%)	26,32,35	0.99	1 (3%)
30	PSU	a	2787	30	18,21,22	0.94	1 (5%)	21,30,33	0.77	0
8	PSU	C	55	8	18,21,22	0.93	1 (5%)	21,30,33	0.71	0
8	4SU	C	8	8	18,21,22	3.75	7 (38%)	25,30,33	2.31	4 (16%)
6	MA6	A	1506	6	23,26,27	1.41	4 (17%)	33,38,41	3.15	13 (39%)
30	2MA	a	2685	30,56	22,25,26	0.85	1 (4%)	32,37,40	1.20	5 (15%)
30	PSU	a	2100	30	18,21,22	0.90	1 (5%)	21,30,33	0.66	0
8	5MU	C	54	8	19,22,23	0.25	0	27,32,35	0.42	0
30	PSU	a	2686	30	18,21,22	0.92	1 (5%)	21,30,33	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	UR3	A	1485	6	-	0/7/25/26	0/2/2/2
6	5MC	A	1394	6	-	0/7/25/26	0/2/2/2
30	PSU	a	1038	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2762	30	-	0/7/25/26	0/2/2/2
6	5MC	A	1387	6	-	2/7/25/26	0/2/2/2
30	3TD	a	2098	30	-	2/7/25/26	0/2/2/2
30	OMG	a	2433	30,8	-	1/9/27/28	0/3/3/3
6	5MC	A	1391	6	-	0/7/25/26	0/2/2/2
6	2MG	A	950	6	-	0/9/27/28	0/3/3/3
30	H2U	a	2631	30	-	0/7/38/39	0/2/2/2
6	PSU	A	498	6,56	-	0/7/25/26	0/2/2/2
30	2MG	a	2018	30	-	2/9/27/28	0/3/3/3
30	PSU	a	2786	30	-	0/7/25/26	0/2/2/2
6	2MG	A	1503	6	-	0/9/27/28	0/3/3/3
6	MA6	A	1505	6	-	0/11/29/30	0/3/3/3
6	4OC	A	1389	6	-	1/9/29/30	0/2/2/2
6	G7M	A	509	6	-	3/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	5MC	C	32	8	-	0/7/25/26	0/2/2/2
30	2MG	a	2627	30	-	2/9/27/28	0/3/3/3
30	PSU	a	2094	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2639	30	-	0/7/25/26	0/2/2/2
30	5MC	a	2145	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2680	30,56	-	0/9/27/28	0/2/2/2
30	OMU	a	2734	30	-	0/9/27/28	0/2/2/2
30	5MU	a	2122	30	-	0/7/25/26	0/2/2/2
6	5MC	A	951	6	-	0/7/25/26	0/2/2/2
30	PSU	a	2787	30	-	0/7/25/26	0/2/2/2
8	PSU	C	55	8	-	0/7/25/26	0/2/2/2
8	4SU	C	8	8	-	0/7/25/26	0/2/2/2
6	MA6	A	1506	6	-	2/11/29/30	0/3/3/3
30	2MA	a	2685	30,56	-	1/7/25/26	0/3/3/3
30	PSU	a	2100	30	-	0/7/25/26	0/2/2/2
8	5MU	C	54	8	-	0/7/25/26	0/2/2/2
30	PSU	a	2686	30	-	1/7/25/26	0/2/2/2

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2098	3TD	C6-C5	12.83	1.49	1.35
6	A	951	5MC	C6-C5	9.70	1.50	1.34
6	A	1387	5MC	C6-C5	9.61	1.50	1.34
6	A	1394	5MC	C6-C5	9.53	1.50	1.34
8	C	32	5MC	C6-C5	9.53	1.50	1.34
6	A	951	5MC	C5-C4	9.43	1.51	1.44
6	A	1391	5MC	C6-C5	9.39	1.49	1.34
30	a	2631	H2U	C2-N1	9.37	1.48	1.35
30	a	2145	5MC	C6-C5	9.36	1.49	1.34
6	A	1387	5MC	C5-C4	9.26	1.51	1.44
30	a	2098	3TD	C2-N1	9.09	1.48	1.37
6	A	1391	5MC	C5-C4	9.01	1.50	1.44
8	C	32	5MC	C5-C4	8.96	1.50	1.44
30	a	2145	5MC	C5-C4	8.96	1.50	1.44
6	A	1394	5MC	C5-C4	8.80	1.50	1.44
6	A	950	2MG	C2-N3	8.12	1.47	1.32
30	a	2627	2MG	C2-N3	7.89	1.47	1.32
6	A	1503	2MG	C2-N3	7.86	1.47	1.32
30	a	2018	2MG	C2-N3	7.82	1.46	1.32
6	A	951	5MC	C4-N3	7.61	1.46	1.34
6	A	1387	5MC	C4-N3	7.54	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	32	5MC	C4-N3	7.54	1.46	1.34
30	a	2145	5MC	C4-N3	7.43	1.46	1.34
6	A	1391	5MC	C4-N3	7.41	1.46	1.34
6	A	1394	5MC	C4-N3	7.35	1.45	1.34
8	C	8	4SU	C2-N3	7.26	1.50	1.38
8	C	8	4SU	C2-N1	7.23	1.49	1.38
6	A	950	2MG	C4-N3	7.12	1.50	1.34
8	C	32	5MC	C2-N3	7.11	1.50	1.36
30	a	2018	2MG	C4-N3	7.08	1.50	1.34
6	A	1389	4OC	C4-N3	7.07	1.44	1.32
6	A	1485	UR3	C2-N1	7.05	1.48	1.38
6	A	1387	5MC	C2-N3	7.02	1.50	1.36
6	A	951	5MC	C2-N3	7.01	1.50	1.36
6	A	1391	5MC	C2-N3	7.00	1.50	1.36
30	a	2145	5MC	C2-N3	6.95	1.50	1.36
30	a	2627	2MG	C4-N3	6.95	1.50	1.34
30	a	2734	OMU	C2-N1	6.91	1.49	1.38
6	A	1503	2MG	C4-N3	6.90	1.50	1.34
6	A	1394	5MC	C2-N3	6.89	1.50	1.36
30	a	2680	OMC	C2-N3	6.81	1.49	1.36
6	A	950	2MG	C2-N2	6.79	1.47	1.33
8	C	8	4SU	C4-N3	6.78	1.44	1.37
30	a	2433	OMG	C4-N3	6.62	1.49	1.34
30	a	2018	2MG	C2-N2	6.59	1.47	1.33
30	a	2734	OMU	C2-N3	6.57	1.49	1.38
6	A	1503	2MG	C2-N2	6.51	1.47	1.33
6	A	509	G7M	C4-N3	6.48	1.49	1.34
30	a	2631	H2U	C2-N3	6.38	1.49	1.38
30	a	2627	2MG	C2-N2	6.37	1.46	1.33
6	A	1389	4OC	C6-C5	6.15	1.49	1.35
6	A	1389	4OC	C2-N3	6.04	1.48	1.36
6	A	1485	UR3	C6-C5	6.02	1.49	1.35
8	C	8	4SU	C5-C4	6.01	1.49	1.42
30	a	2680	OMC	C6-C5	5.82	1.48	1.35
30	a	2098	3TD	C6-N1	5.80	1.45	1.36
6	A	951	5MC	C4-N4	5.79	1.48	1.34
6	A	1387	5MC	C4-N4	5.78	1.48	1.34
6	A	951	5MC	C6-N1	5.76	1.47	1.38
6	A	1387	5MC	C6-N1	5.76	1.47	1.38
8	C	32	5MC	C4-N4	5.76	1.48	1.34
6	A	1394	5MC	C4-N4	5.75	1.48	1.34
6	A	1391	5MC	C6-N1	5.74	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1391	5MC	C4-N4	5.72	1.48	1.34
30	a	2145	5MC	C4-N4	5.71	1.48	1.34
30	a	2734	OMU	C6-C5	5.67	1.48	1.35
6	A	1394	5MC	C6-N1	5.62	1.47	1.38
8	C	32	5MC	C6-N1	5.59	1.47	1.38
8	C	8	4SU	C6-C5	5.56	1.48	1.35
30	a	2433	OMG	C2-N3	5.52	1.46	1.33
30	a	2145	5MC	C6-N1	5.43	1.47	1.38
6	A	509	G7M	C2-N3	5.33	1.46	1.33
30	a	2433	OMG	C2-N2	5.32	1.46	1.34
30	a	2680	OMC	C4-N3	5.27	1.44	1.34
6	A	950	2MG	C2-N1	5.21	1.45	1.36
6	A	1503	2MG	C2-N1	5.16	1.44	1.36
30	a	2018	2MG	C2-N1	4.98	1.44	1.36
8	C	8	4SU	C4-S4	-4.86	1.60	1.68
30	a	2627	2MG	C2-N1	4.85	1.44	1.36
30	a	2680	OMC	C4-N4	4.84	1.45	1.33
6	A	509	G7M	C2-N2	4.75	1.45	1.34
6	A	1387	5MC	C2-N1	4.73	1.50	1.40
30	a	2631	H2U	C4-N3	4.69	1.45	1.37
6	A	1485	UR3	C2-N3	4.69	1.48	1.39
6	A	509	G7M	C5-N7	-4.64	1.33	1.39
30	a	2098	3TD	C2-N3	4.64	1.48	1.38
6	A	1394	5MC	C2-N1	4.60	1.49	1.40
6	A	1391	5MC	C2-N1	4.52	1.49	1.40
6	A	951	5MC	C2-N1	4.51	1.49	1.40
8	C	32	5MC	C2-N1	4.49	1.49	1.40
30	a	2145	5MC	C2-N1	4.45	1.49	1.40
30	a	2680	OMC	C2-N1	4.40	1.49	1.40
30	a	2680	OMC	O2-C2	-4.34	1.15	1.23
6	A	1389	4OC	C4-N4	4.34	1.45	1.36
6	A	1389	4OC	C2-N1	4.04	1.48	1.40
6	A	509	G7M	C5-C6	3.74	1.53	1.43
6	A	1389	4OC	C5-C4	3.65	1.49	1.41
8	C	55	PSU	C6-C5	3.59	1.39	1.35
30	a	2094	PSU	C6-C5	3.57	1.39	1.35
30	a	2686	PSU	C6-C5	3.57	1.39	1.35
30	a	2787	PSU	C6-C5	3.55	1.39	1.35
6	A	1506	MA6	C6-N6	3.55	1.46	1.36
30	a	2762	PSU	C6-C5	3.53	1.39	1.35
30	a	1038	PSU	C6-C5	3.53	1.39	1.35
30	a	2639	PSU	C6-C5	3.51	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	498	PSU	C6-C5	3.51	1.39	1.35
30	a	2680	OMC	C6-N1	3.49	1.46	1.38
30	a	2786	PSU	C6-C5	3.49	1.39	1.35
6	A	1505	MA6	C6-N6	3.48	1.46	1.36
30	a	2100	PSU	C6-C5	3.46	1.39	1.35
30	a	2734	OMU	C4-N3	3.41	1.44	1.38
6	A	1506	MA6	C5-C4	-3.16	1.33	1.39
6	A	1389	4OC	C6-N1	3.12	1.45	1.38
30	a	2627	2MG	C5-N7	-3.08	1.32	1.39
6	A	1505	MA6	C5-C4	-3.01	1.33	1.39
30	a	2734	OMU	O2-C2	-2.99	1.17	1.23
30	a	2433	OMG	O6-C6	-2.97	1.17	1.23
6	A	1389	4OC	O2-C2	-2.95	1.18	1.23
6	A	1485	UR3	C6-N1	2.88	1.45	1.38
30	a	2018	2MG	C5-N7	-2.88	1.33	1.39
6	A	1503	2MG	C5-C6	2.82	1.54	1.44
6	A	950	2MG	C5-C6	2.79	1.54	1.44
30	a	2734	OMU	O4-C4	-2.79	1.19	1.24
30	a	2433	OMG	C2-N1	2.78	1.44	1.37
30	a	2018	2MG	C5-C6	2.77	1.54	1.44
6	A	1503	2MG	C5-N7	-2.73	1.33	1.39
6	A	950	2MG	C5-N7	-2.73	1.33	1.39
6	A	1506	MA6	C5-N7	-2.71	1.34	1.39
6	A	509	G7M	C2-N1	2.70	1.44	1.37
30	a	2627	2MG	C5-C6	2.69	1.54	1.44
8	C	8	4SU	C6-N1	2.68	1.44	1.38
30	a	2433	OMG	C5-C6	2.67	1.54	1.44
6	A	509	G7M	O6-C6	-2.64	1.18	1.23
30	a	2631	H2U	O2-C2	-2.63	1.18	1.23
30	a	2627	2MG	O6-C6	-2.63	1.18	1.23
6	A	1505	MA6	C5-N7	-2.60	1.34	1.39
30	a	2098	3TD	C4-N3	2.59	1.45	1.40
6	A	1391	5MC	O2-C2	-2.55	1.19	1.23
6	A	950	2MG	C6-N1	2.55	1.43	1.38
6	A	1394	5MC	O2-C2	-2.51	1.19	1.23
30	a	2018	2MG	O6-C6	-2.51	1.18	1.23
8	C	32	5MC	O2-C2	-2.49	1.19	1.23
30	a	2145	5MC	O2-C2	-2.49	1.19	1.23
6	A	1503	2MG	O6-C6	-2.48	1.18	1.23
6	A	1387	5MC	O2-C2	-2.46	1.19	1.23
6	A	1503	2MG	C6-N1	2.46	1.43	1.38
30	a	2018	2MG	C6-N1	2.45	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2680	OMC	C5-C4	2.45	1.48	1.42
6	A	951	5MC	O2-C2	-2.43	1.19	1.23
30	a	2685	2MA	C6-N6	-2.42	1.28	1.34
30	a	2433	OMG	C5-N7	-2.41	1.34	1.39
6	A	950	2MG	O6-C6	-2.41	1.19	1.23
30	a	2433	OMG	C6-N1	2.37	1.43	1.38
6	A	1485	UR3	O4-C4	-2.34	1.18	1.23
30	a	2631	H2U	O4-C4	-2.33	1.18	1.23
6	A	509	G7M	C6-N1	2.29	1.43	1.38
6	A	1485	UR3	C4-N3	2.28	1.45	1.40
6	A	1505	MA6	C8-N9	-2.27	1.33	1.37
6	A	1485	UR3	O2-C2	-2.25	1.18	1.22
6	A	1506	MA6	C8-N9	-2.24	1.33	1.37
6	A	1485	UR3	C5-C4	2.19	1.49	1.43
30	a	2098	3TD	O4-C4	-2.18	1.18	1.23
6	A	509	G7M	C4-N9	-2.17	1.32	1.38
30	a	2627	2MG	C6-N1	2.15	1.42	1.38
30	a	2098	3TD	O2-C2	-2.06	1.19	1.23
30	a	2433	OMG	C4-N9	-2.03	1.32	1.38

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1506	MA6	N1-C6-N6	-11.15	103.27	116.86
6	A	1505	MA6	N1-C6-N6	-10.56	103.99	116.86
8	C	8	4SU	C4-N3-C2	-7.90	119.74	127.31
30	a	2018	2MG	C2-N3-C4	7.36	121.21	112.00
6	A	1506	MA6	C5-C6-N6	7.19	136.72	125.33
30	a	2433	OMG	C1'-N9-C8	-6.79	107.45	126.73
6	A	1505	MA6	C5-C6-N6	6.61	135.79	125.33
6	A	1503	2MG	C2-N3-C4	6.44	120.06	112.00
6	A	950	2MG	C2-N3-C4	6.29	119.87	112.00
30	a	2627	2MG	C2-N3-C4	6.21	119.77	112.00
30	a	2018	2MG	C5-C4-N3	-6.19	118.53	128.39
30	a	2734	OMU	C4-N3-C2	-5.91	119.28	126.61
30	a	2098	3TD	N1-C2-N3	5.85	120.39	116.13
6	A	1485	UR3	C4-N3-C2	-5.83	119.89	124.58
6	A	1505	MA6	N1-C2-N3	-5.79	119.82	128.58
6	A	950	2MG	C1'-N9-C4	-5.79	109.39	126.49
6	A	1506	MA6	N1-C2-N3	-5.68	119.98	128.58
6	A	1503	2MG	C1'-N9-C4	-5.67	109.73	126.49
30	a	2627	2MG	C5-C4-N3	-5.56	119.54	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1503	2MG	C1'-N9-C8	5.52	142.41	126.73
6	A	950	2MG	C1'-N9-C8	5.50	142.36	126.73
30	a	2433	OMG	C1'-N9-C4	5.47	142.64	126.49
8	C	8	4SU	C5-C4-N3	5.39	119.77	114.75
6	A	1503	2MG	C5-C4-N3	-5.27	120.00	128.39
6	A	950	2MG	C5-C4-N3	-5.11	120.27	128.39
30	a	2627	2MG	C1'-N9-C4	-5.00	111.72	126.49
6	A	1506	MA6	C5-C4-N3	-4.92	119.95	126.72
6	A	1505	MA6	C5-C4-N3	-4.91	119.96	126.72
30	a	2018	2MG	C2-N1-C6	-4.87	118.66	124.55
30	a	2627	2MG	C1'-N9-C8	4.85	140.51	126.73
30	a	2627	2MG	C2-N1-C6	-4.67	118.90	124.55
6	A	1503	2MG	C2-N1-C6	-4.64	118.94	124.55
30	a	2433	OMG	C5-C4-N3	-4.59	121.09	128.39
6	A	509	G7M	C2-N3-C4	4.37	119.83	112.30
30	a	2433	OMG	C2-N3-C4	4.28	119.67	112.30
6	A	1506	MA6	N9-C8-N7	-4.26	107.90	113.94
30	a	2018	2MG	C1'-N9-C4	-4.23	114.00	126.49
30	a	2018	2MG	C1'-N9-C8	4.21	138.69	126.73
6	A	950	2MG	C2-N1-C6	-4.15	119.53	124.55
30	a	2734	OMU	N3-C2-N1	4.06	120.18	114.89
6	A	1505	MA6	N9-C8-N7	-4.02	108.23	113.94
30	a	2018	2MG	N1-C2-N2	4.00	120.64	116.56
6	A	509	G7M	C5-C6-N1	3.98	120.08	111.84
6	A	1503	2MG	N1-C2-N2	3.96	120.61	116.56
8	C	8	4SU	C5-C4-S4	-3.93	119.81	124.31
30	a	2098	3TD	C4-N3-C2	-3.93	120.45	124.61
30	a	2018	2MG	N9-C4-N3	3.91	133.78	125.95
6	A	1506	MA6	C4-C5-C6	3.90	119.94	115.91
8	C	8	4SU	N3-C2-N1	3.88	119.94	114.89
6	A	509	G7M	C5-C4-N3	-3.85	120.88	128.15
6	A	1505	MA6	C4-C5-C6	3.75	119.79	115.91
6	A	1485	UR3	C5-C4-N3	3.75	119.97	115.04
30	a	2734	OMU	C5-C4-N3	3.69	119.97	114.80
30	a	2433	OMG	N9-C8-N7	-3.69	106.55	113.40
30	a	2631	H2U	N3-C2-N1	3.61	120.28	116.65
6	A	1387	5MC	C5-C6-N1	-3.56	119.45	123.31
30	a	2145	5MC	C5-C6-N1	-3.53	119.48	123.31
30	a	2627	2MG	N9-C4-N3	3.42	132.78	125.95
6	A	1505	MA6	C2-N3-C4	3.42	120.17	111.83
6	A	1506	MA6	C2-N3-C4	3.40	120.12	111.83
6	A	1505	MA6	C2-N1-C6	3.36	120.05	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	951	5MC	C5-C6-N1	-3.35	119.67	123.31
6	A	1506	MA6	C2-N1-C6	3.34	120.00	111.83
6	A	509	G7M	O6-C6-C5	-3.32	120.60	128.01
30	a	2685	2MA	C5-C4-N3	-3.32	123.68	127.18
6	A	509	G7M	N9-C4-N3	3.23	132.42	125.95
8	C	32	5MC	C5-C6-N1	-3.17	119.87	123.31
30	a	2734	OMU	O4-C4-C5	-3.11	119.80	125.16
30	a	2433	OMG	C2-N1-C6	-3.10	119.49	125.11
6	A	1394	5MC	C5-C6-N1	-3.07	119.98	123.31
30	a	2098	3TD	C1'-C5-C4	3.07	122.26	117.61
6	A	950	2MG	N1-C2-N2	3.05	119.67	116.56
6	A	1505	MA6	N3-C4-N9	3.05	132.35	127.17
6	A	950	2MG	N9-C4-N3	3.02	132.00	125.95
6	A	1506	MA6	C5-N7-C8	3.02	108.19	103.45
6	A	950	2MG	N9-C8-N7	-2.94	107.95	113.40
30	a	2433	OMG	N9-C4-N3	2.93	131.81	125.95
30	a	2631	H2U	C5-C6-N1	2.93	120.38	111.52
6	A	1503	2MG	N9-C4-N3	2.91	131.78	125.95
30	a	2018	2MG	C5-C6-N1	2.91	120.67	113.25
6	A	509	G7M	C2-N1-C6	-2.91	119.83	125.11
6	A	1503	2MG	N9-C8-N7	-2.89	108.03	113.40
30	a	2631	H2U	C5-C4-N3	2.81	119.68	116.69
6	A	1506	MA6	N3-C4-N9	2.80	131.93	127.17
6	A	1503	2MG	C5-C6-N1	2.78	120.32	113.25
6	A	1391	5MC	C5-C6-N1	-2.77	120.30	123.31
6	A	1503	2MG	CM2-N2-C2	-2.77	117.70	123.65
30	a	2433	OMG	C5-C6-N1	2.75	120.26	113.25
6	A	1505	MA6	C5-N7-C8	2.72	107.73	103.45
30	a	2627	2MG	N9-C8-N7	-2.71	108.37	113.40
30	a	2627	2MG	C5-C6-N1	2.71	120.15	113.25
6	A	950	2MG	C5-C6-N1	2.71	120.14	113.25
30	a	2018	2MG	O6-C6-C5	-2.69	119.42	126.53
30	a	2631	H2U	O2-C2-N1	-2.66	119.91	123.10
30	a	2685	2MA	N3-C2-N1	-2.59	121.19	125.77
30	a	2433	OMG	O6-C6-C5	-2.58	119.72	126.53
6	A	509	G7M	N9-C8-N7	-2.55	106.29	112.48
30	a	2627	2MG	N1-C2-N2	2.55	119.16	116.56
6	A	950	2MG	O6-C6-C5	-2.52	119.89	126.53
30	a	2627	2MG	O6-C6-C5	-2.47	120.01	126.53
6	A	1503	2MG	O6-C6-C5	-2.47	120.02	126.53
30	a	2685	2MA	CM2-C2-N1	2.45	120.80	117.13
30	a	2627	2MG	CM2-N2-C2	-2.43	118.42	123.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2018	2MG	N9-C8-N7	-2.42	108.90	113.40
6	A	1506	MA6	C4-C5-N7	-2.39	107.84	110.58
30	a	2018	2MG	CM2-N2-C2	-2.37	118.55	123.65
30	a	2762	PSU	C3'-C2'-C1'	2.37	104.48	101.69
30	a	2098	3TD	C6-C5-C4	2.35	119.77	118.19
30	a	2145	5MC	CM5-C5-C6	-2.35	119.67	122.85
30	a	2433	OMG	C8-N7-C5	2.29	108.35	104.26
30	a	2685	2MA	C2-N1-C6	2.29	121.61	118.10
30	a	2734	OMU	O2-C2-N1	-2.25	119.86	122.80
6	A	1389	4OC	C6-C5-C4	2.25	119.71	117.00
6	A	1505	MA6	C4-N9-C8	2.23	108.08	105.74
6	A	1503	2MG	C8-N7-C5	2.12	108.04	104.26
6	A	1506	MA6	C5-C4-N9	2.12	108.12	105.81
6	A	1506	MA6	C4-N9-C8	2.10	107.94	105.74
6	A	950	2MG	N1-C2-N3	-2.10	120.14	123.68
30	a	2098	3TD	O4'-C1'-C2'	2.09	108.04	105.15
30	a	2433	OMG	C8-N9-C4	2.07	109.90	106.03
6	A	950	2MG	C8-N7-C5	2.06	107.93	104.26
30	a	2018	2MG	N1-C2-N3	-2.06	120.21	123.68
6	A	1394	5MC	C5-C4-N3	-2.06	119.65	121.75
30	a	2685	2MA	N3-C4-N9	2.03	129.57	126.99
6	A	1391	5MC	CM5-C5-C6	-2.02	120.11	122.85
6	A	1505	MA6	C4-C5-N7	-2.02	108.27	110.58
30	a	2627	2MG	C8-N7-C5	2.00	107.83	104.26

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1506	MA6	O4'-C4'-C5'-O5'
30	a	2098	3TD	O4'-C4'-C5'-O5'
6	A	509	G7M	C3'-C4'-C5'-O5'
30	a	2098	3TD	C3'-C4'-C5'-O5'
30	a	2627	2MG	C3'-C4'-C5'-O5'
6	A	1387	5MC	O4'-C4'-C5'-O5'
30	a	2627	2MG	O4'-C4'-C5'-O5'
6	A	509	G7M	O4'-C4'-C5'-O5'
6	A	1506	MA6	C3'-C4'-C5'-O5'
30	a	2018	2MG	O4'-C4'-C5'-O5'
30	a	2018	2MG	C3'-C4'-C5'-O5'
6	A	1387	5MC	C3'-C4'-C5'-O5'
30	a	2433	OMG	C1'-C2'-O2'-CM2

Continued on next page...

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Mol	Chain	Res	Type	Atoms
6	A	509	G7M	C4'-C5'-O5'-P
6	A	1389	4OC	O4'-C4'-C5'-O5'
30	a	2686	PSU	O4'-C4'-C5'-O5'
30	a	2685	2MA	C4'-C5'-O5'-P

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	a	2098	3TD	2	0
6	A	950	2MG	1	0
30	a	2631	H2U	1	0
6	A	1503	2MG	2	0
6	A	1505	MA6	1	0
6	A	1389	4OC	1	0
6	A	1506	MA6	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 309 ligands modelled in this entry, 307 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	$\# Z > 2$
57	V7A	A	1602	56	37,38,38	1.11	2 (5%)	43,60,60	1.02	3 (6%)
57	V7A	a	3145	56	37,38,38	1.09	2 (5%)	43,60,60	0.92	1 (2%)

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
57	V7A	A	1602	56	-	5/13/72/72	0/4/4/4
57	V7A	a	3145	56	-	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)
57	A	1602	V7A	CBC-NBD	5.10	1.48	1.33
57	a	3145	V7A	CBC-NBD	5.01	1.47	1.33
57	a	3145	V7A	OAY-CAH	2.23	1.27	1.23
57	A	1602	V7A	OAY-CAH	2.12	1.27	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A	1602	V7A	CAH-CAI-CAL	2.93	121.12	118.80
57	A	1602	V7A	OBA-CAM-CAL	-2.41	106.29	110.14
57	a	3145	V7A	CAM-CAP-CAQ	2.39	119.55	115.75
57	A	1602	V7A	OAZ-CAL-CAM	2.28	116.67	113.37

There are no chirality outliers.

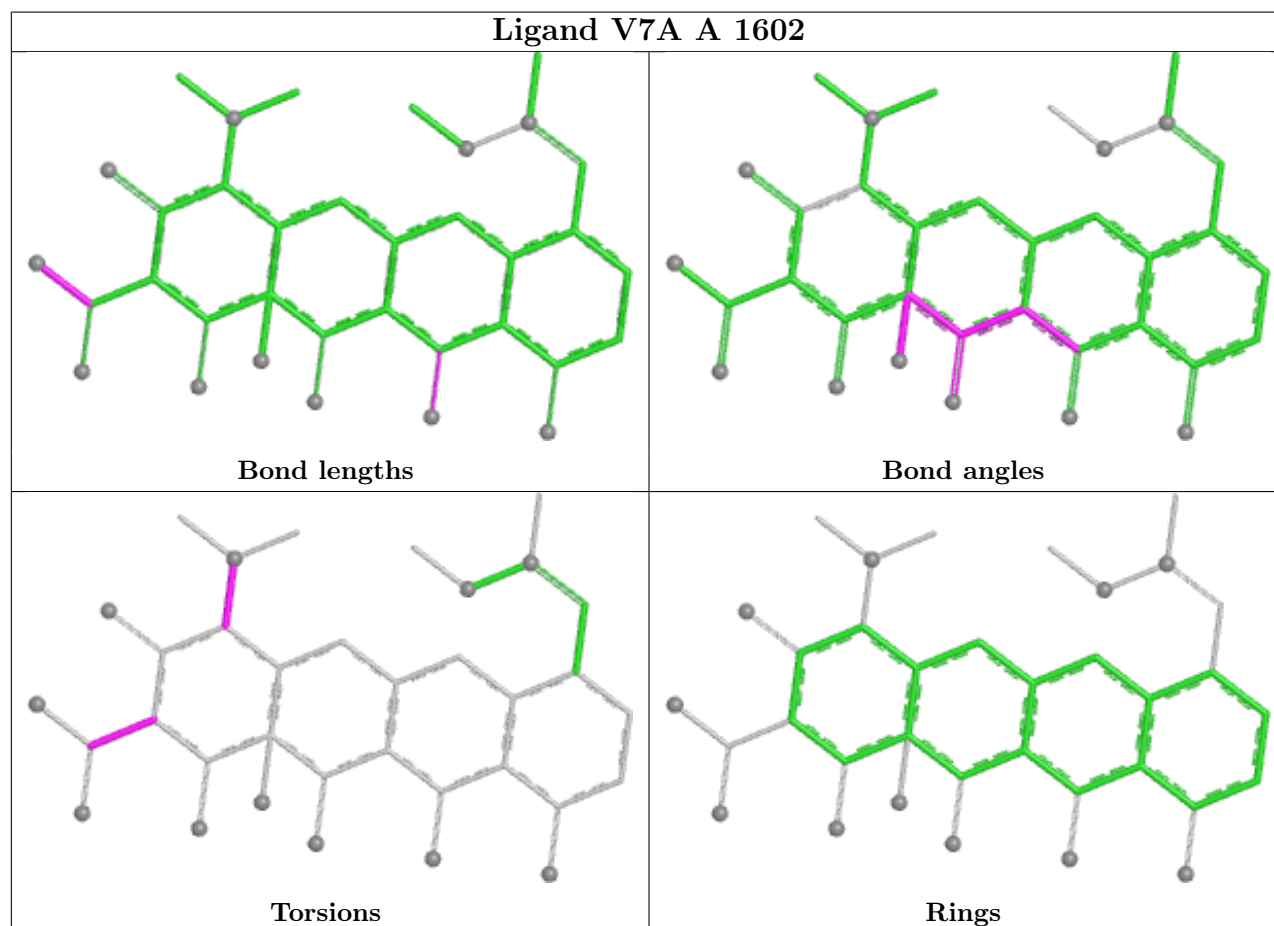
All (13) torsion outliers are listed below:

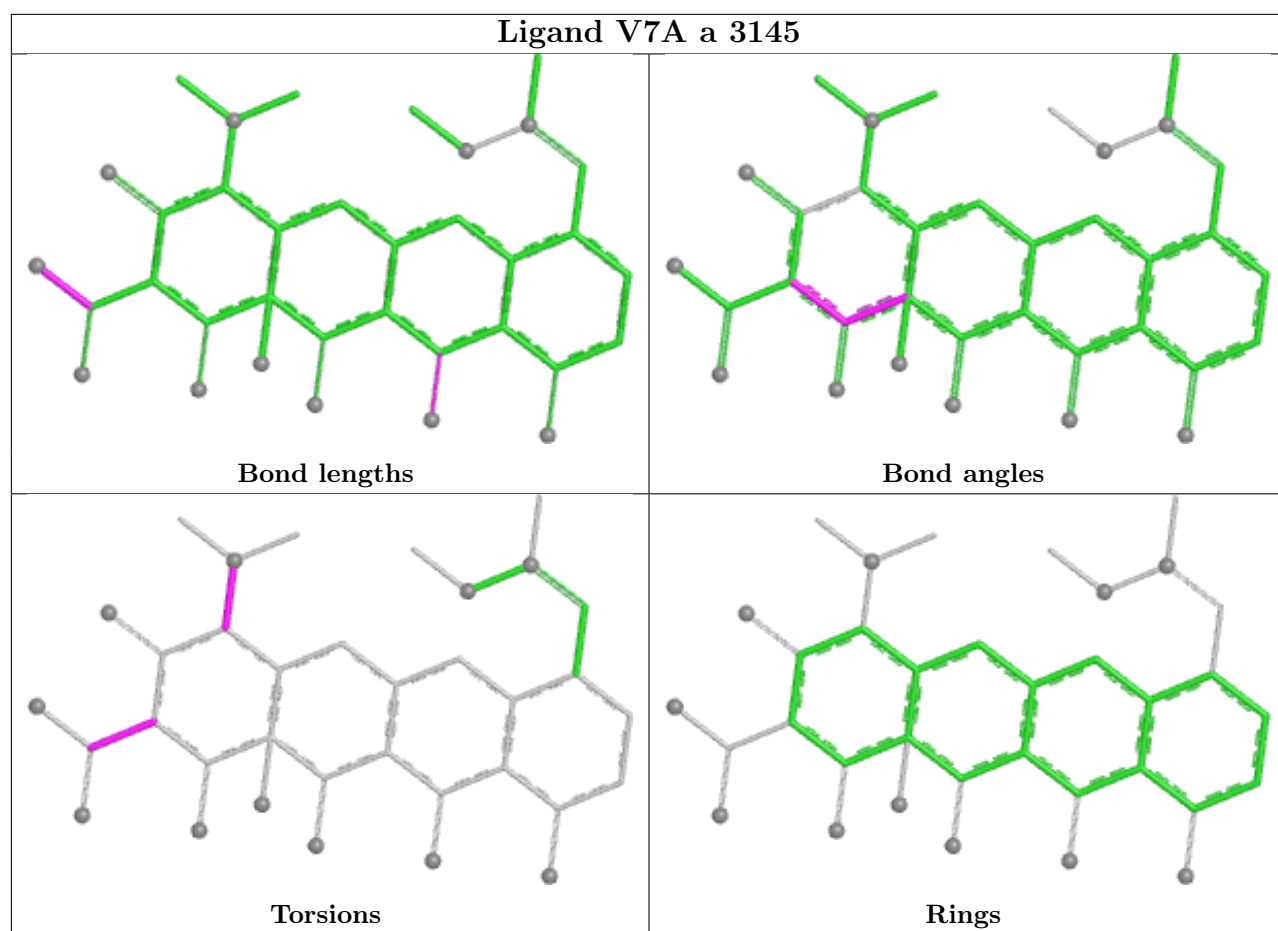
Mol	Chain	Res	Type	Atoms
57	A	1602	V7A	CAN-CAO-NBF-CBG
57	A	1602	V7A	CAP-CAQ-CBC-NBD
57	A	1602	V7A	CAP-CAQ-CBC-OBE
57	a	3145	V7A	CAR-CAO-NBF-CBG
57	a	3145	V7A	CAR-CAO-NBF-CBH
57	a	3145	V7A	CAP-CAQ-CBC-OBE
57	a	3145	V7A	CAR-CAQ-CBC-NBD
57	a	3145	V7A	CAR-CAQ-CBC-OBE
57	A	1602	V7A	CAR-CAQ-CBC-NBD
57	A	1602	V7A	CAR-CAQ-CBC-OBE
57	a	3145	V7A	CAP-CAQ-CBC-NBD
57	a	3145	V7A	CAN-CAO-NBF-CBG
57	a	3145	V7A	CAN-CAO-NBF-CBH

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

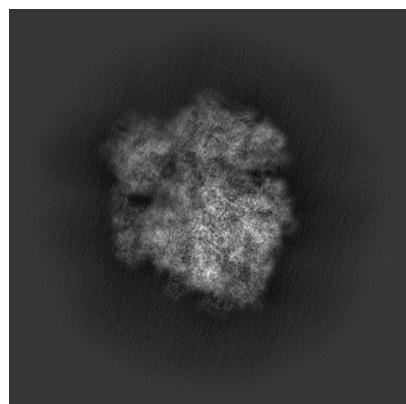
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71683. These allow visual inspection of the internal detail of the map and identification of artifacts.

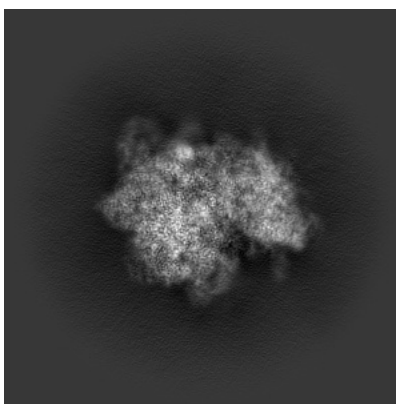
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

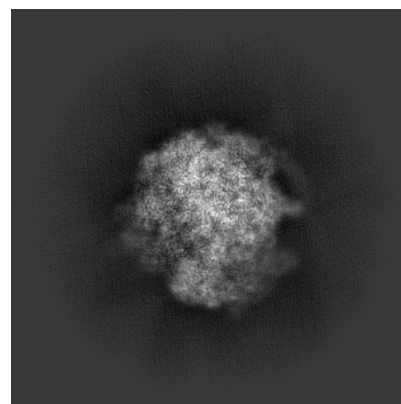
6.1.1 Primary map



X

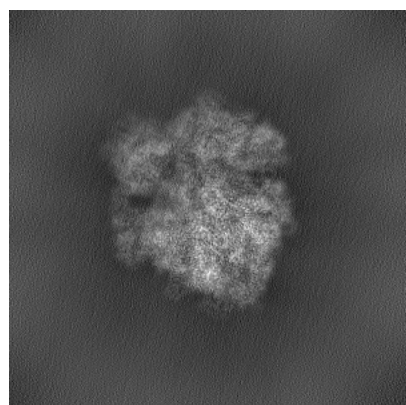


Y

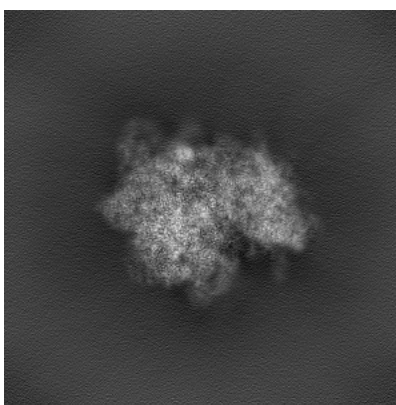


Z

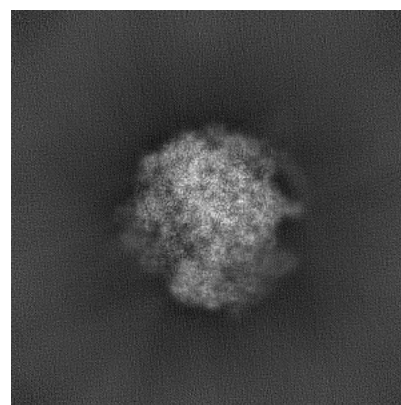
6.1.2 Raw map



X



Y

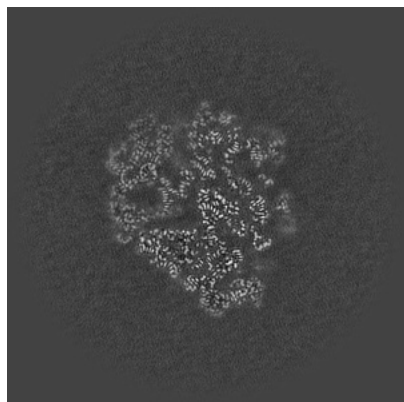


Z

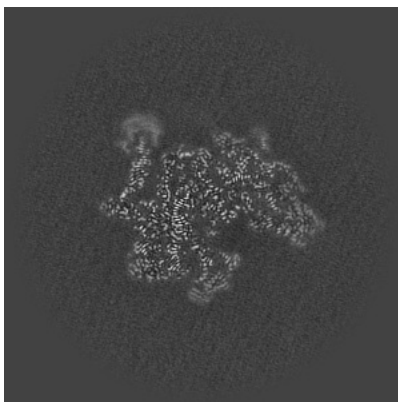
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

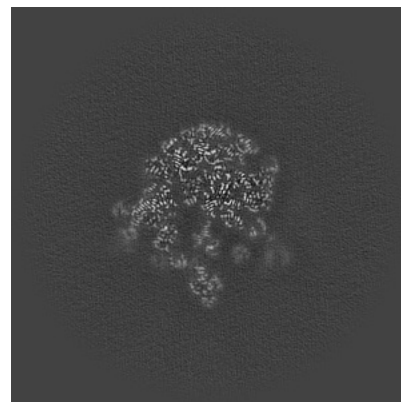
6.2.1 Primary map



X Index: 220

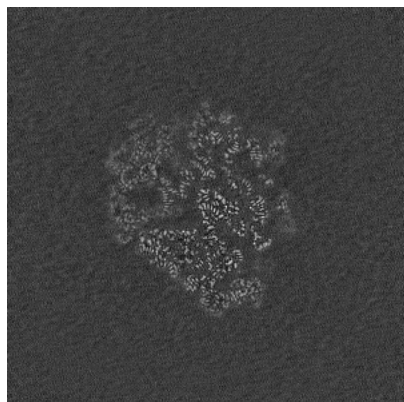


Y Index: 220

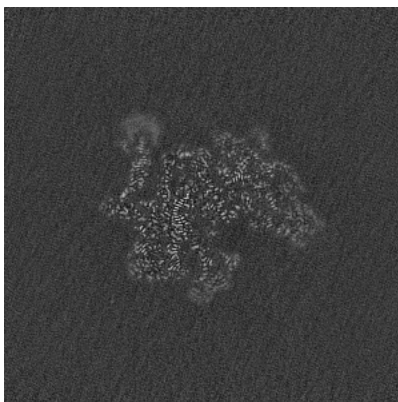


Z Index: 220

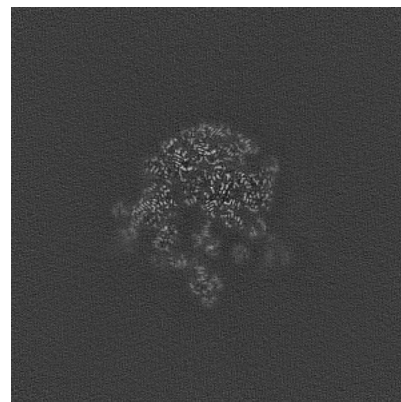
6.2.2 Raw map



X Index: 220



Y Index: 220

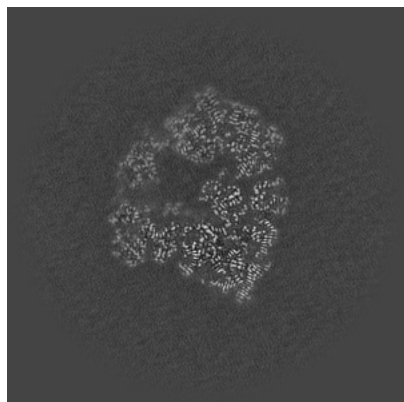


Z Index: 220

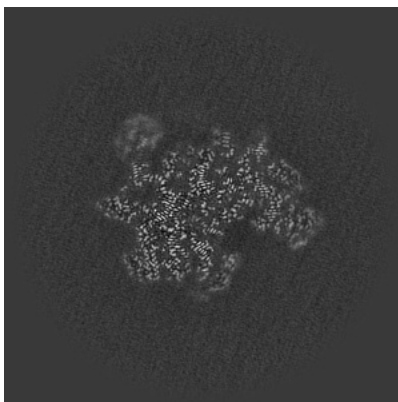
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

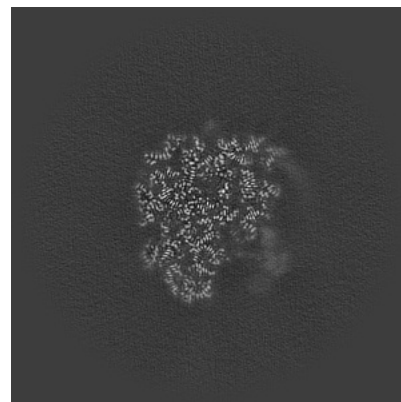
6.3.1 Primary map



X Index: 203

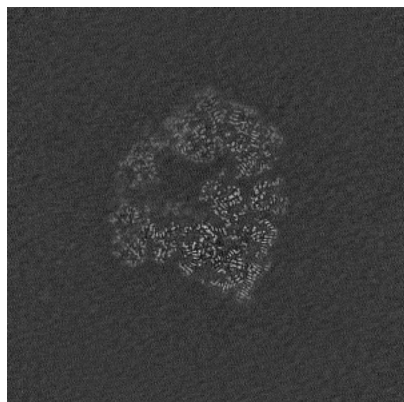


Y Index: 225

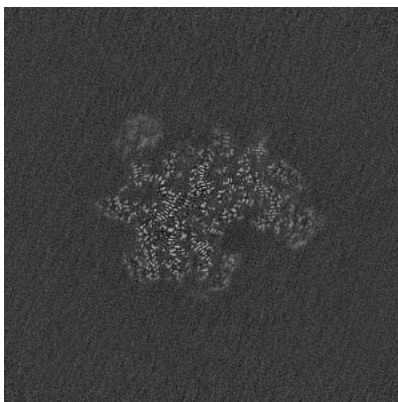


Z Index: 190

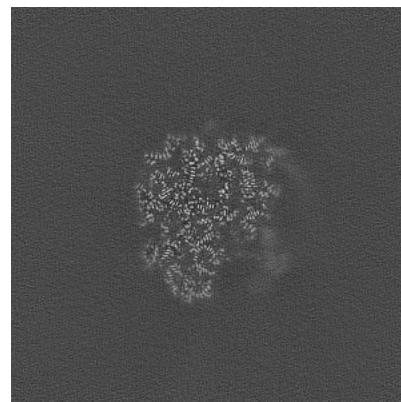
6.3.2 Raw map



X Index: 203



Y Index: 225

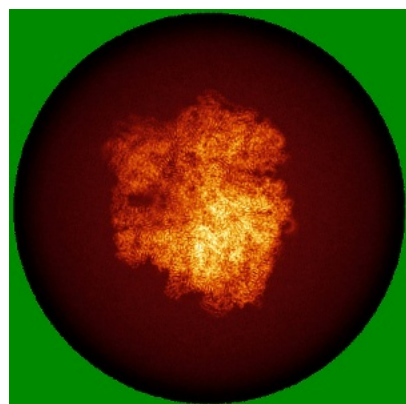


Z Index: 190

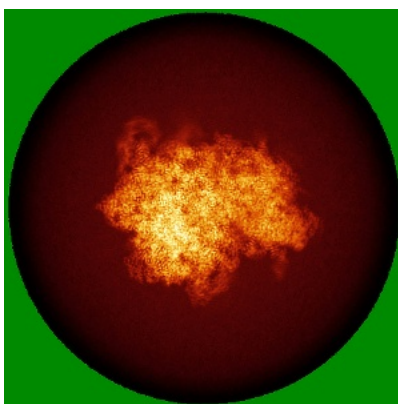
The images above show the largest variance slices of the map in three orthogonal directions.

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

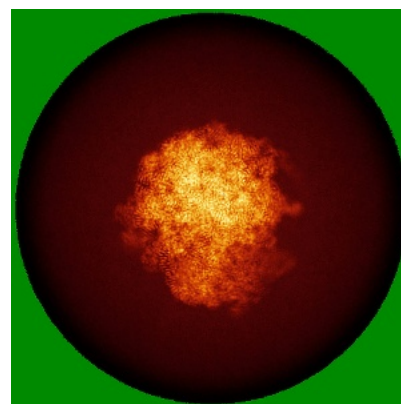
6.4.1 Primary map



X

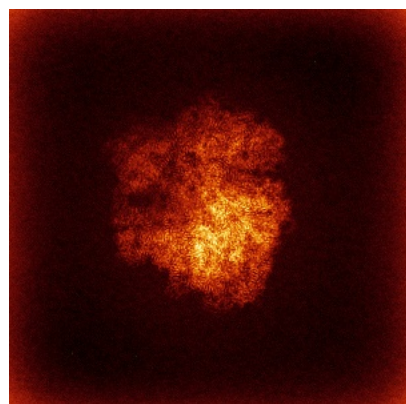


Y

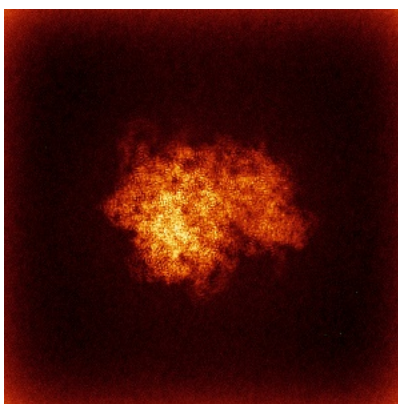


Z

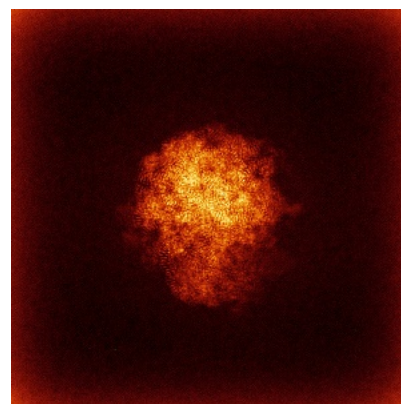
6.4.2 Raw map



X



Y

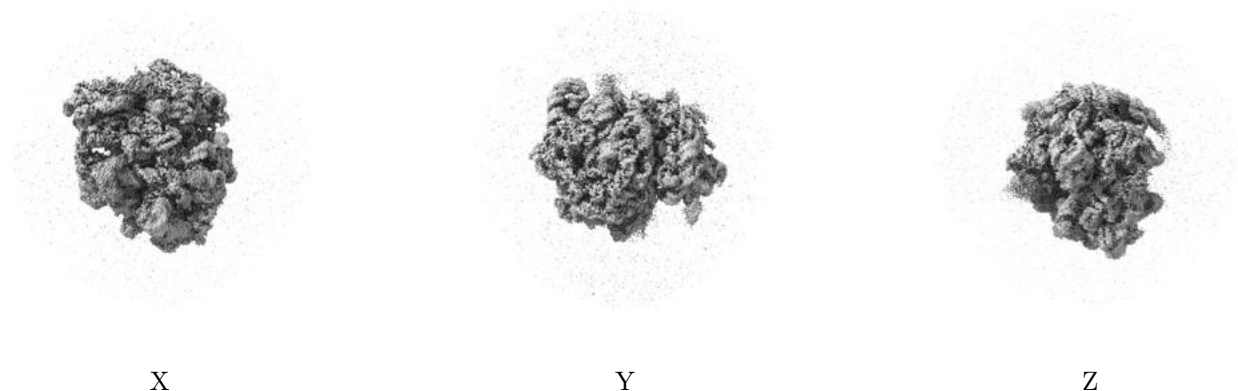


Z

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

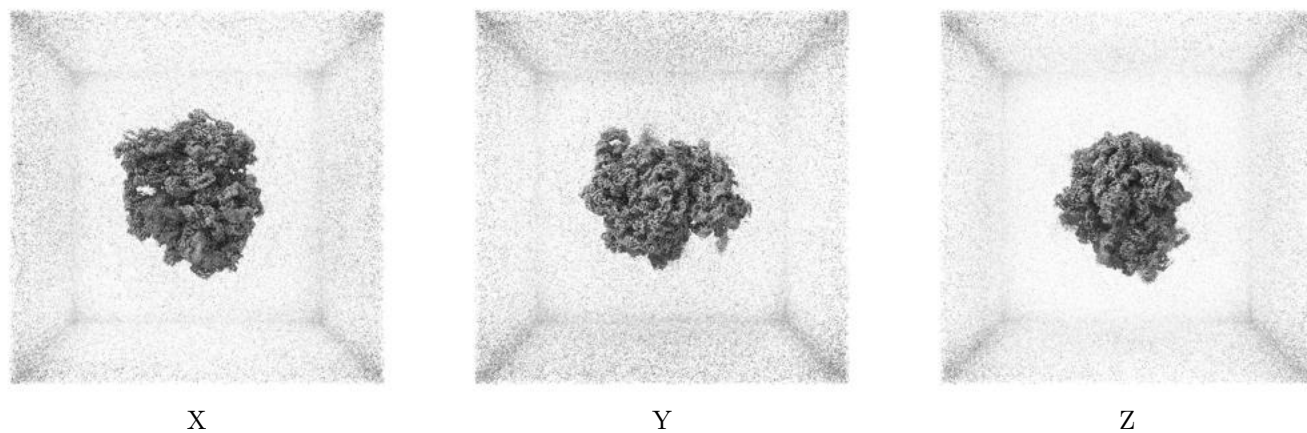
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

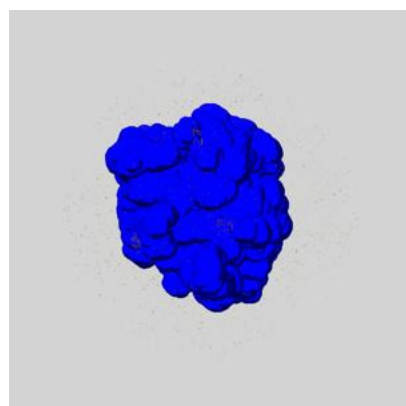
6.6 Mask visualisation [i](#)

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

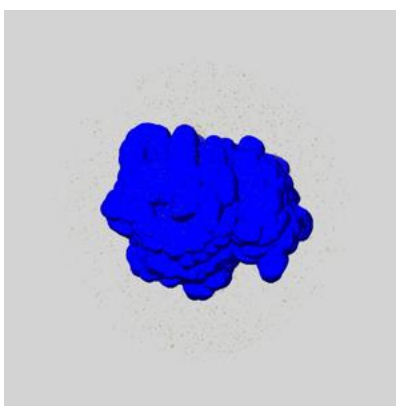
A mask typically either:

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

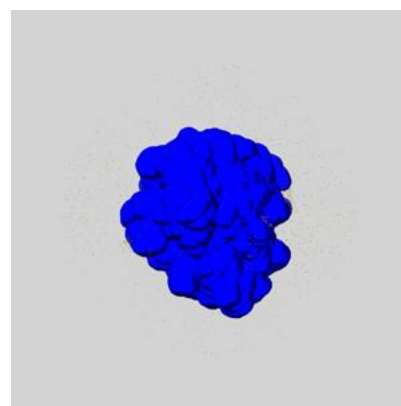
6.6.1 emd_71683_msk_1.map [i](#)



X



Y

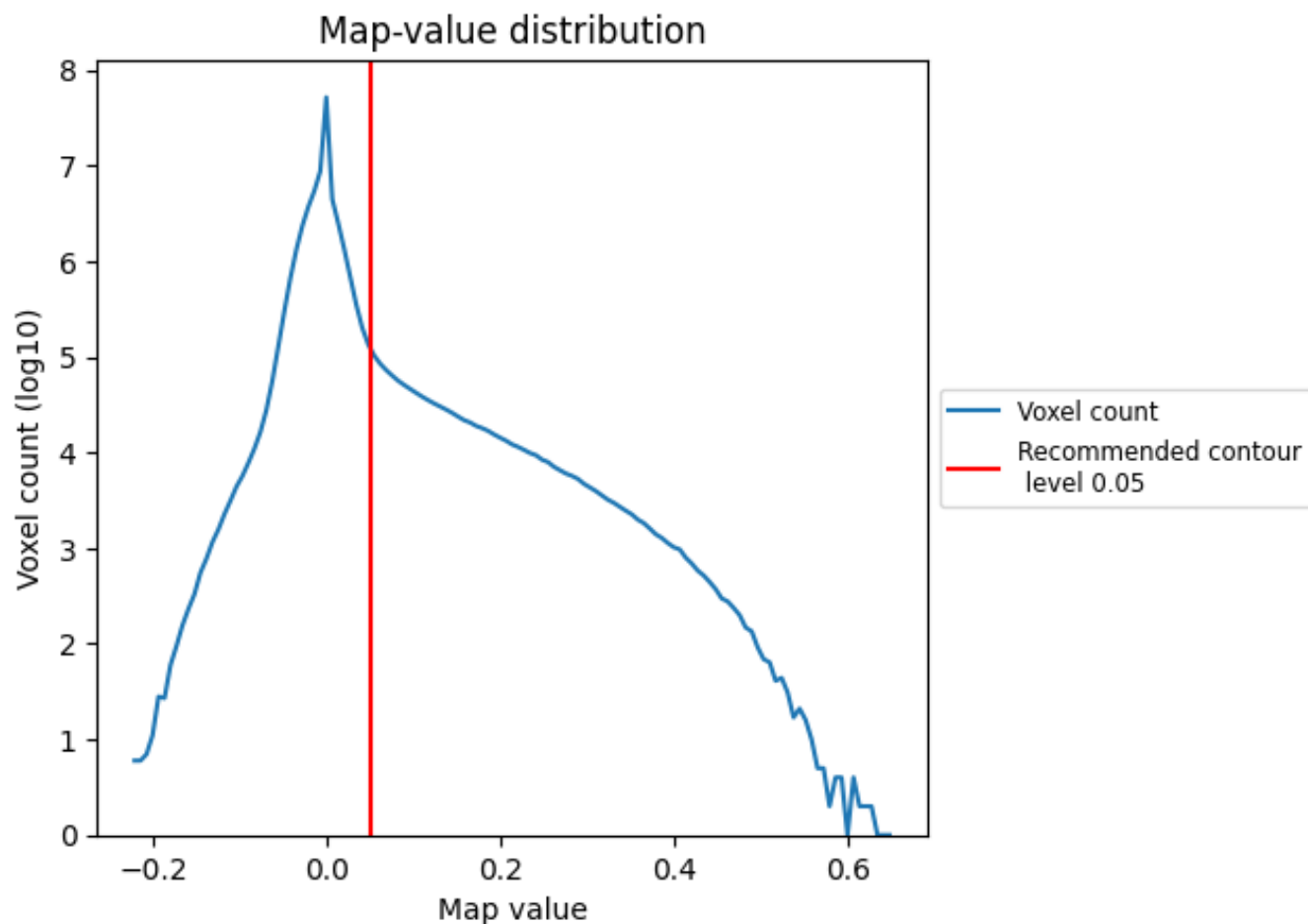


Z

7 Map analysis [i](#)

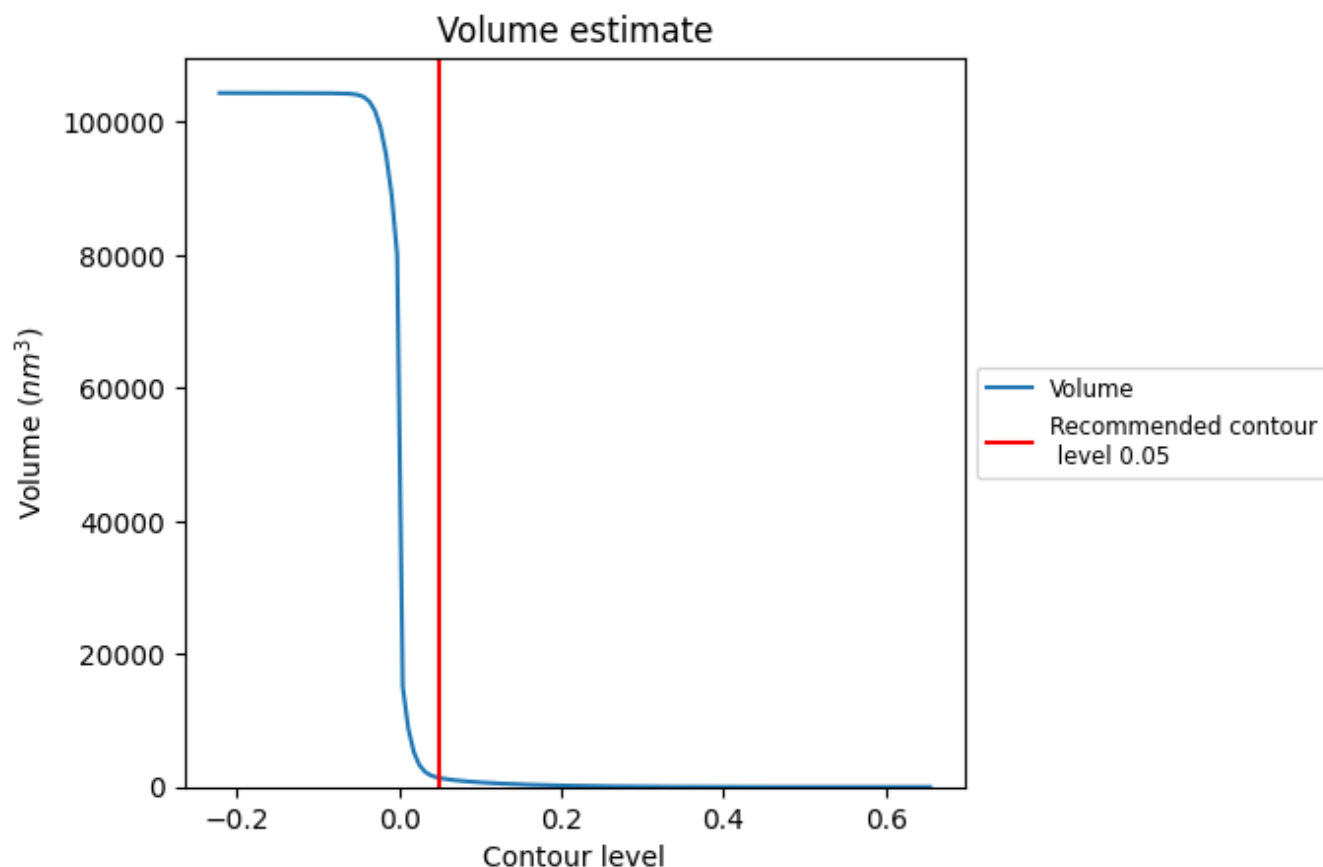
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

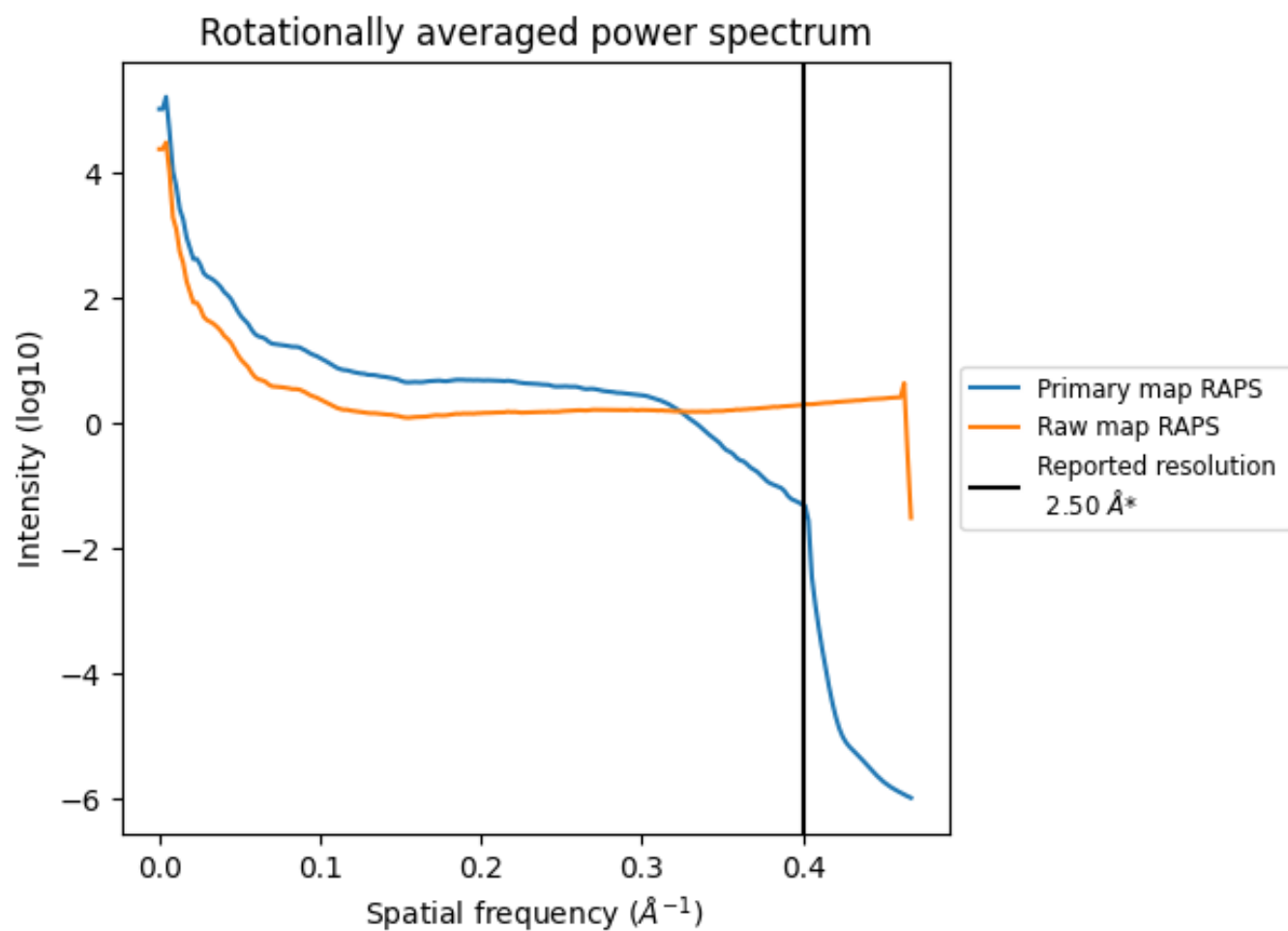
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1360 nm^3 ; this corresponds to an approximate mass of 1229 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 ⓘ

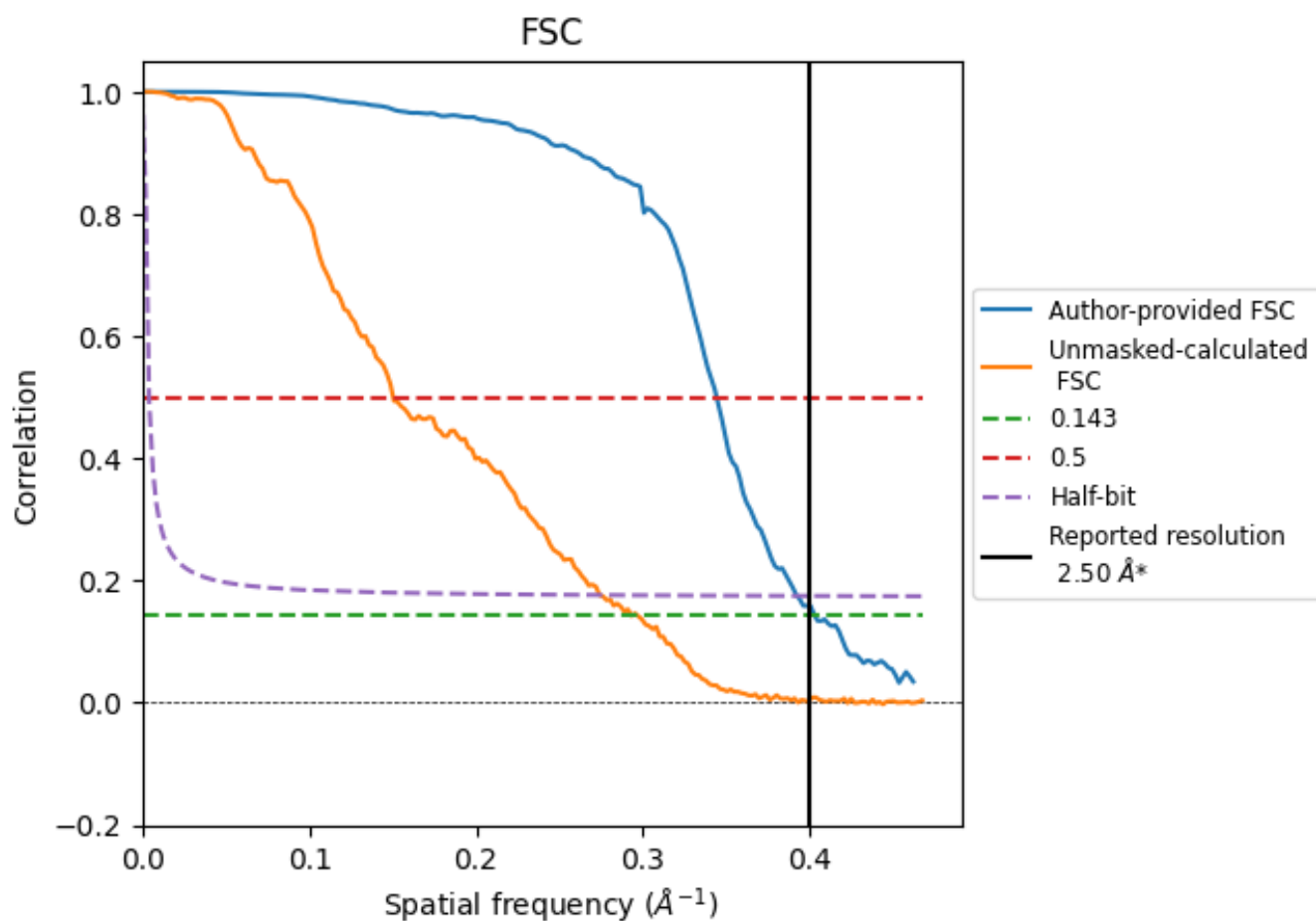


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

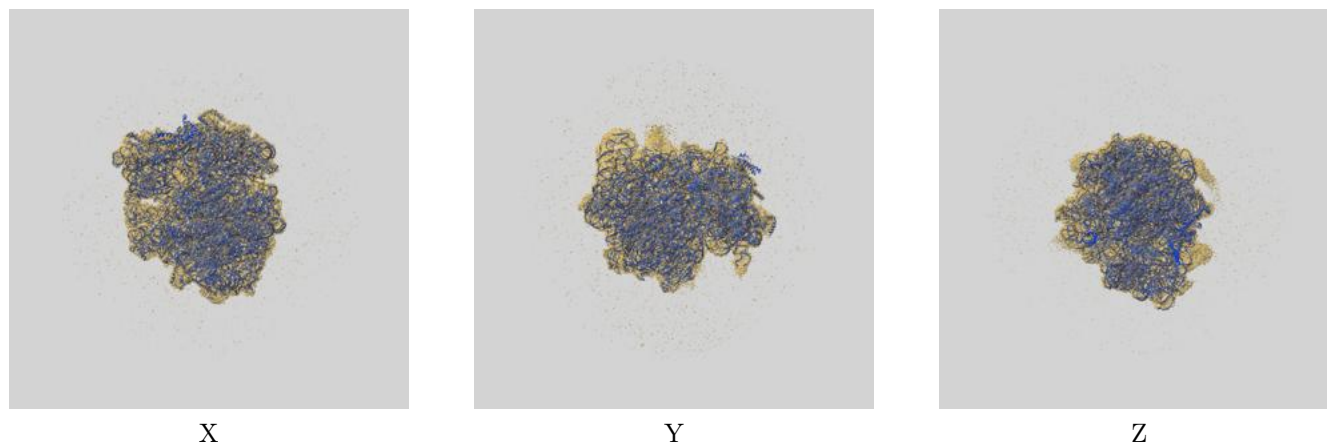
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.48	2.91	2.55
Unmasked-calculated*	3.41	6.65	3.65

*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 3.41 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

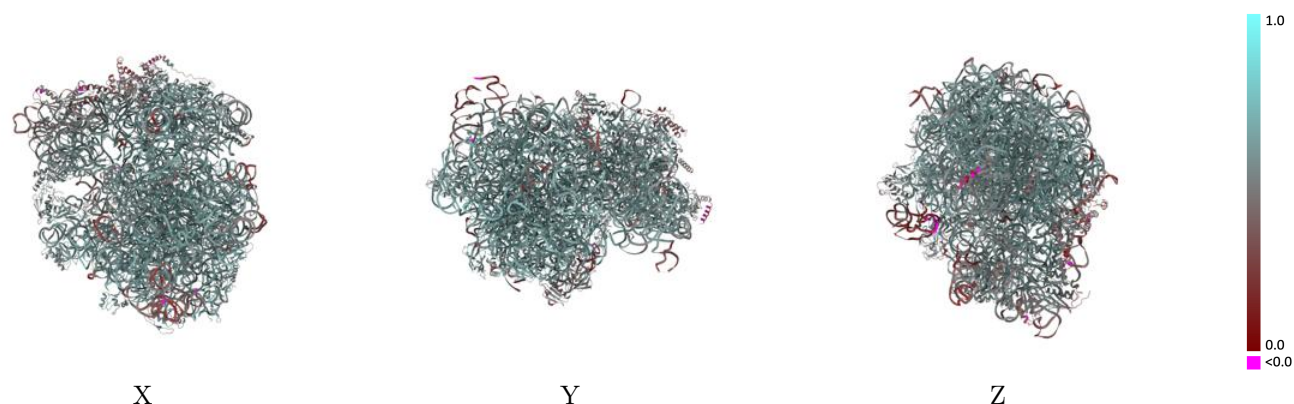
This section contains information regarding the fit between EMDB map EMD-71683 and PDB model 9PJ8. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



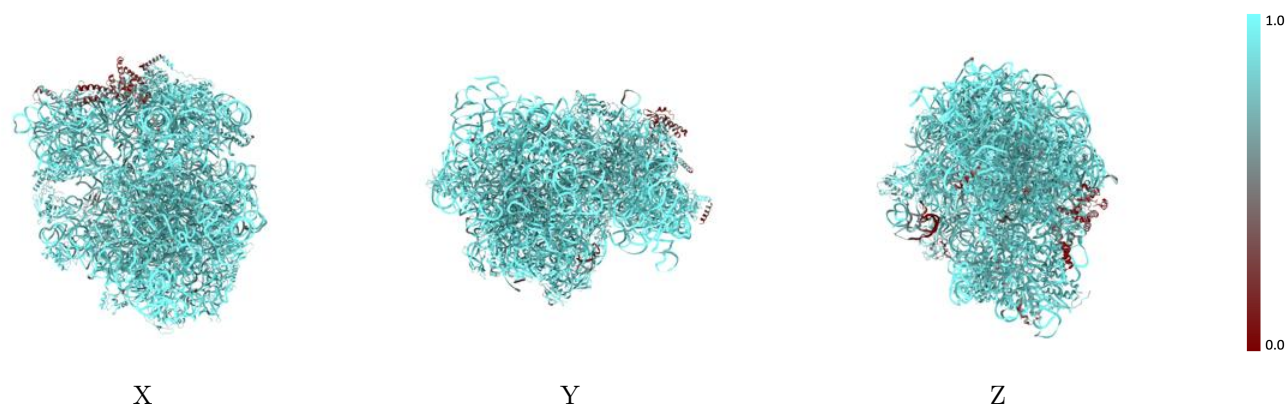
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



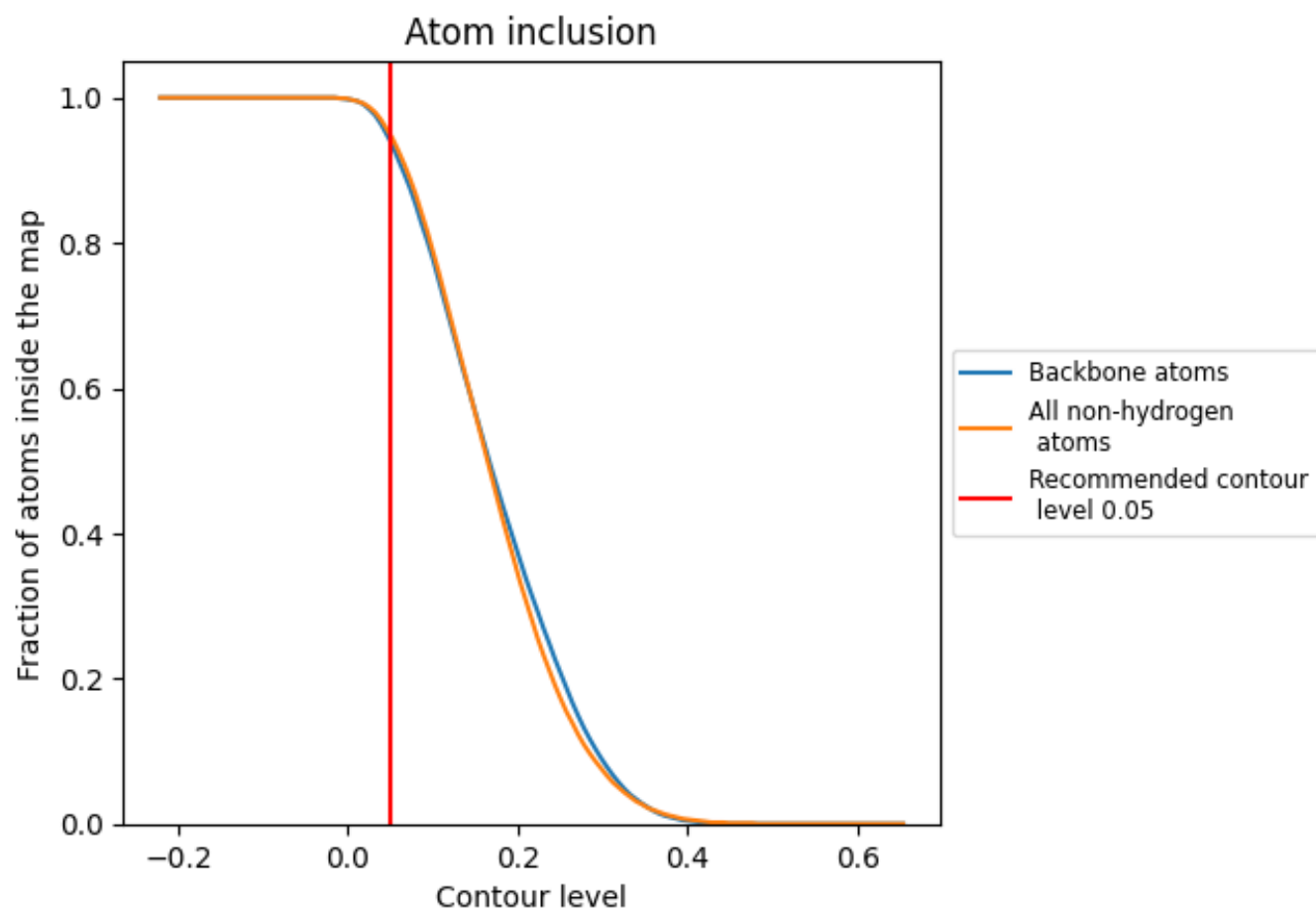
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary









































The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.5680
0	 0.9580	 0.6020
1	 0.9940	 0.6400
2	 0.9680	 0.6250
3	 0.9490	 0.6080
4	 0.8960	 0.5030
A	 0.9830	 0.5610
B	 0.2570	 0.3670
C	 0.9610	 0.5600
D	 0.9060	 0.5040
E	 0.8750	 0.5530
F	 0.8960	 0.5240
G	 0.7980	 0.5000
H	 0.9390	 0.5740
I	 0.9020	 0.5240
J	 0.8970	 0.4760
K	 0.9510	 0.5540
L	 0.9390	 0.5870
M	 0.7200	 0.4460
N	 0.8750	 0.5200
O	 0.9460	 0.5570
P	 0.8710	 0.4960
Q	 0.8920	 0.5490
R	 0.8510	 0.5230
S	 0.8900	 0.5480
T	 0.9310	 0.5590
U	 0.9260	 0.5000
V	 0.9770	 0.6370
X	 0.9110	 0.5860
Y	 0.7390	 0.4520
a	 0.9710	 0.5830
b	 0.9960	 0.5910
c	 0.9670	 0.6220
d	 0.9750	 0.6070
e	 0.9510	 0.5800



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.9440	 0.5440
g	 0.9040	 0.4950
i	 0.9730	 0.6160
j	 0.9390	 0.5990
k	 0.9490	 0.5950
l	 0.9640	 0.6060
m	 0.9690	 0.6070
n	 0.9590	 0.5610
o	 0.9460	 0.6060
p	 0.9620	 0.6130
q	 0.9530	 0.5900
r	 0.9460	 0.6060
s	 0.9590	 0.5900
t	 0.9420	 0.5670
u	 0.7270	 0.4660
v	 0.9630	 0.6220
w	 0.9800	 0.6260
x	 0.9360	 0.5610
y	 0.9510	 0.6100
z	 0.9610	 0.6170