



Full wwPDB EM Validation Report ⓘ

Dec 11, 2025 – 05:11 PM EST

PDB ID : 9YQ0 / pdb_00009yq0
EMDB ID : EMD-73316
Title : Vacant ribosome with P-site tRNA, substate 2, Structure Ib
Authors : Susorov, D.; Korostelev, A.A.
Deposited on : 2025-10-14
Resolution : 2.90 Å(reported)
Based on initial model : 5LZS

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:

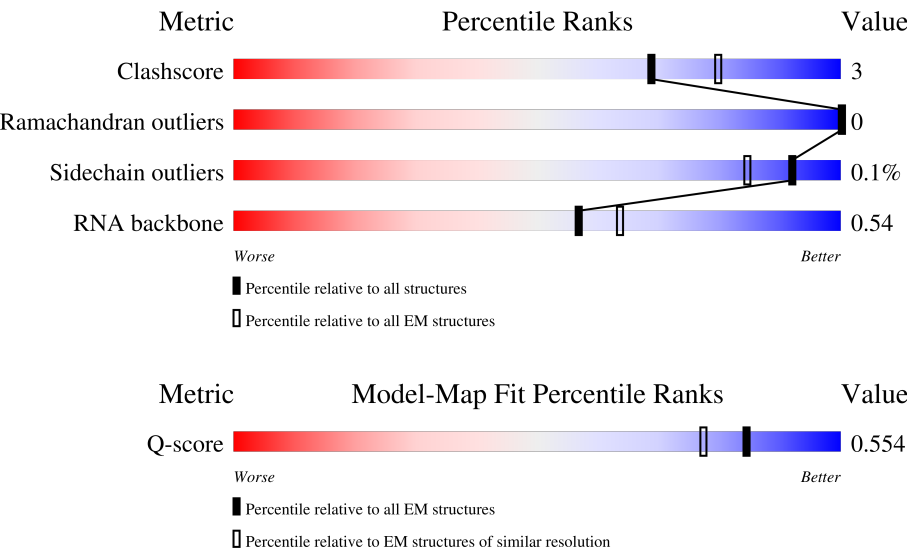
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.47

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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.




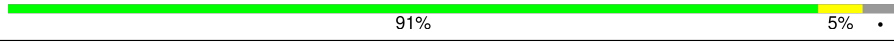
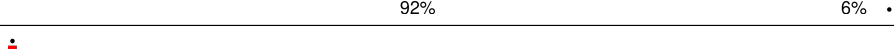
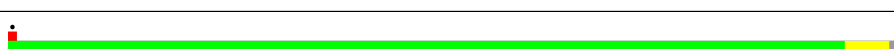


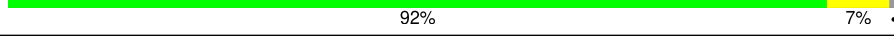
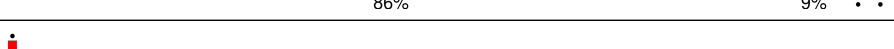

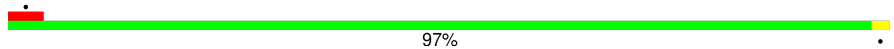

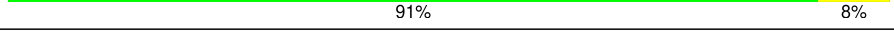
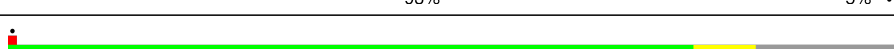



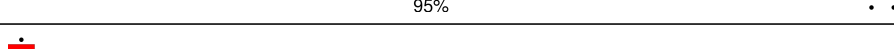







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	5	3601	<div><div></div><div>69%27%5%</div></div>
2	7	120	<div><div></div><div>85%13%. .</div></div>
3	8	156	<div><div></div><div>74%19%. .</div></div>

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Mol	Chain	Length	Quality of chain
4	9	1869	
5	A	257	
6	B	403	
7	C	425	
8	D	297	
9	E	291	
10	G	319	
11	H	192	
12	I	214	
13	J	178	
14	K	247	
15	L	211	
16	M	218	
17	N	204	
18	O	203	
19	P	184	
20	Q	188	
21	R	196	
22	S	176	
23	T	160	
24	U	128	
25	V	140	
26	W	157	
27	X	156	
28	Y	145	






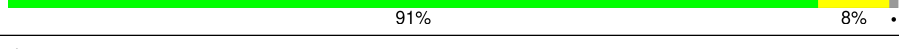
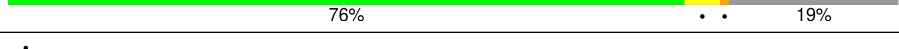
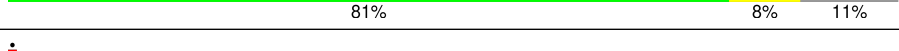
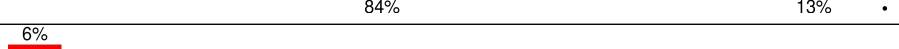
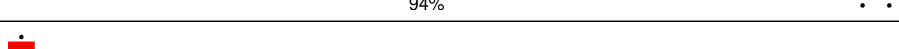
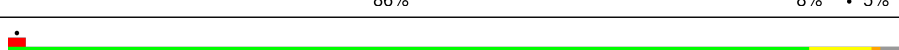

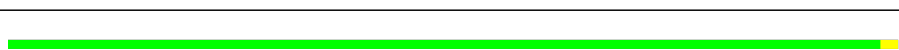

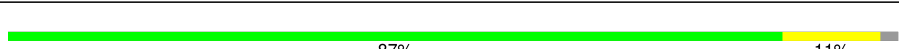





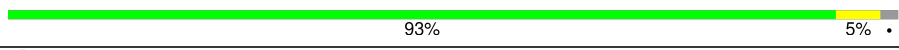




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Mol	Chain	Length	Quality of chain
29	Z	136	
30	a	148	
31	b	245	
32	c	115	
33	d	125	
34	e	135	
35	f	110	
36	g	116	
37	h	123	
38	i	105	
39	k	70	
40	l	51	
41	m	102	
42	n	25	
43	o	106	
44	p	92	
45	r	137	
46	AA	295	
47	BB	264	
48	CC	293	
49	DD	243	
50	EE	263	
51	FF	204	
52	GG	249	
53	HH	194	

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Mol	Chain	Length	Quality of chain
54	II	208	
55	JJ	194	
56	KK	165	
57	LL	158	
58	MM	132	
59	NN	151	
60	OO	168	
61	PP	145	
62	QQ	146	
63	RR	135	
64	SS	152	
65	TT	145	
66	UU	119	
67	VV	83	
68	WW	130	
69	XX	143	
70	YY	130	
71	ZZ	125	
72	aa	115	
73	bb	84	
74	cc	69	
75	dd	56	
76	ee	133	
77	ff	156	
78	gg	317	

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Mol	Chain	Length	Quality of chain
79	10	185	 94%
80	11	75	 15% 39%55%5%
80	13	75	 56%32%11%
81	j	97	 77%11%11%

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 213916 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3601	Total	C	N	O	P	0	0
			77221	34390	14143	25087	3601		

There are 59 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1	C	N	conflict	GB 5LZS_5
5	3948	C	-	insertion	GB 5LZS_5
5	3949	A	-	insertion	GB 5LZS_5
5	3950	U	-	insertion	GB 5LZS_5
5	3951	G	-	insertion	GB 5LZS_5
5	3952	A	-	insertion	GB 5LZS_5
5	3953	G	-	insertion	GB 5LZS_5
5	3954	A	-	insertion	GB 5LZS_5
5	3955	G	-	insertion	GB 5LZS_5
5	3956	G	-	insertion	GB 5LZS_5
5	3957	U	-	insertion	GB 5LZS_5
5	3958	G	-	insertion	GB 5LZS_5
5	3959	U	-	insertion	GB 5LZS_5
5	3960	A	-	insertion	GB 5LZS_5
5	3961	G	-	insertion	GB 5LZS_5
5	3962	A	-	insertion	GB 5LZS_5
5	3963	A	-	insertion	GB 5LZS_5
5	3964	U	-	insertion	GB 5LZS_5
5	3965	A	-	insertion	GB 5LZS_5
5	3966	A	-	insertion	GB 5LZS_5
5	3967	G	-	insertion	GB 5LZS_5
5	3968	U	-	insertion	GB 5LZS_5
5	3969	G	-	insertion	GB 5LZS_5
5	3970	G	-	insertion	GB 5LZS_5
5	3971	G	-	insertion	GB 5LZS_5
5	3972	A	-	insertion	GB 5LZS_5
5	3973	G	-	insertion	GB 5LZS_5
5	3974	G	-	insertion	GB 5LZS_5

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Chain	Residue	Modelled	Actual	Comment	Reference
5	3975	C	-	insertion	GB 5LZS_5
5	3976	C	-	insertion	GB 5LZS_5
5	4035	G	-	insertion	GB 5LZS_5
5	4036	G	-	insertion	GB 5LZS_5
5	4037	C	-	insertion	GB 5LZS_5
5	4038	C	-	insertion	GB 5LZS_5
5	4039	G	-	insertion	GB 5LZS_5
5	4040	C	-	insertion	GB 5LZS_5
5	4041	C	-	insertion	GB 5LZS_5
5	4042	G	-	insertion	GB 5LZS_5
5	4043	G	-	insertion	GB 5LZS_5
5	4044	U	-	insertion	GB 5LZS_5
5	4045	G	-	insertion	GB 5LZS_5
5	4046	A	-	insertion	GB 5LZS_5
5	4047	A	-	insertion	GB 5LZS_5
5	4048	A	-	insertion	GB 5LZS_5
5	4049	U	-	insertion	GB 5LZS_5
5	4050	A	-	insertion	GB 5LZS_5
5	4051	C	-	insertion	GB 5LZS_5
5	4052	C	-	insertion	GB 5LZS_5
5	4053	A	-	insertion	GB 5LZS_5
5	4054	C	-	insertion	GB 5LZS_5
5	4055	U	-	insertion	GB 5LZS_5
5	4056	A	-	insertion	GB 5LZS_5
5	4057	C	-	insertion	GB 5LZS_5
5	4058	U	-	insertion	GB 5LZS_5
5	4059	C	-	insertion	GB 5LZS_5
5	4060	U	-	insertion	GB 5LZS_5
5	4061	G	-	insertion	GB 5LZS_5
5	4062	A	-	insertion	GB 5LZS_5
5	4063	U	-	insertion	GB 5LZS_5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	2	U	N	conflict	GB X06789.1

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Chain	Residue	Modelled	Actual	Comment	Reference
7	36	C	N	conflict	GB X06789.1
7	102	U	N	conflict	GB X06789.1
7	112	U	N	conflict	GB X06789.1
7	114	U	N	conflict	GB X06789.1
7	119	U	C	conflict	GB X06789.1
7	120	U	N	conflict	GB X06789.1

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 4 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	9	1697	Total	C	N	O	P	0	0
			36229	16171	6507	11855	1696		

- Molecule 5 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 6 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 7 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	378	LYS	-	insertion	UNP G1SVW5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	379	VAL	-	insertion	UNP G1SVW5
C	380	LYS	-	insertion	UNP G1SVW5
C	381	LYS	-	insertion	UNP G1SVW5
C	382	PRO	-	insertion	UNP G1SVW5
C	383	ARG	-	insertion	UNP G1SVW5
C	384	ALA	-	insertion	UNP G1SVW5
C	385	VAL	-	insertion	UNP G1SVW5
C	386	GLY	-	insertion	UNP G1SVW5
C	387	ILE	-	insertion	UNP G1SVW5
C	388	LYS	-	insertion	UNP G1SVW5
C	389	GLN	-	insertion	UNP G1SVW5

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 13 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 14 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	61	ARG	GLY	conflict	UNP G1TUB1
K	93	ARG	GLY	conflict	UNP G1TUB1
K	131	MET	VAL	conflict	UNP G1TUB1
K	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 15 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ILE	-	insertion	UNP G1TPV0
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 17 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 18 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 19 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 20 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	4	ASP	ASN	conflict	UNP G1TFE0
Q	14	ARG	TRP	conflict	UNP G1TFE0
Q	53	MET	LEU	conflict	UNP G1TFE0
Q	58	ARG	TRP	conflict	UNP G1TFE0
Q	75	ARG	GLN	conflict	UNP G1TFE0
Q	80	ALA	PRO	conflict	UNP G1TFE0
Q	86	VAL	ILE	conflict	UNP G1TFE0
Q	104	ARG	HIS	conflict	UNP G1TFE0
Q	110	ARG	CYS	conflict	UNP G1TFE0
Q	137	VAL	GLY	conflict	UNP G1TFE0
Q	157	GLY	ARG	conflict	UNP G1TFE0

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	181	ARG	TRP	conflict	UNP G1TFE0

- Molecule 21 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	CYS	conflict	UNP G1TJR3
R	64	ARG	GLN	conflict	UNP G1TJR3
R	94	THR	LYS	conflict	UNP G1TJR3

- Molecule 22 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1	MET	THR	conflict	UNP G1TTY7
S	18	PRO	-	insertion	UNP G1TTY7
S	19	THR	-	insertion	UNP G1TTY7
S	20	PRO	SER	conflict	UNP G1TTY7
S	22	CYS	SER	conflict	UNP G1TTY7
S	23	ARG	PRO	conflict	UNP G1TTY7
S	24	THR	ALA	conflict	UNP G1TTY7
S	49	SER	LEU	conflict	UNP G1TTY7
S	50	GLN	GLU	conflict	UNP G1TTY7
S	95	ARG	HIS	conflict	UNP G1TTY7
S	101	THR	ILE	conflict	UNP G1TTY7
S	102	THR	MET	conflict	UNP G1TTY7
S	104	GLY	SER	conflict	UNP G1TTY7
S	126	ILE	VAL	conflict	UNP G1TTY7
S	132	ILE	MET	conflict	UNP G1TTY7
S	135	SER	ALA	conflict	UNP G1TTY7
S	136	LYS	ARG	conflict	UNP G1TTY7
S	138	ARG	PRO	conflict	UNP G1TTY7

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Chain	Residue	Modelled	Actual	Comment	Reference
S	149	LYS	ARG	conflict	UNP G1TTY7
S	151	LYS	ARG	conflict	UNP G1TTY7
S	168	THR	TYR	conflict	UNP G1TTY7
S	169	THR	ALA	conflict	UNP G1TTY7
S	176	PHE	-	insertion	UNP G1TTY7

- Molecule 23 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 24 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	18	LEU	VAL	conflict	UNP G1TSG1
U	32	GLY	ARG	conflict	UNP G1TSG1
U	36	ALA	GLU	conflict	UNP G1TSG1
U	39	PHE	SER	conflict	UNP G1TSG1
U	54	GLY	ARG	conflict	UNP G1TSG1
U	60	VAL	ALA	conflict	UNP G1TSG1
U	62	SER	THR	conflict	UNP G1TSG1
U	63	LEU	ILE	conflict	UNP G1TSG1
U	97	ARG	HIS	conflict	UNP G1TSG1
U	106	THR	SER	conflict	UNP G1TSG1
U	126	GLU	ASP	conflict	UNP G1TSG1

- Molecule 25 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 26 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 27 is a protein called eL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 28 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 29 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 30 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 31 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	98	Total	C	N	O	S	0	0
			806	498	182	123	3		

- Molecule 32 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 33 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 34 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 35 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 36 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 37 is a protein called eL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 39 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	3	ARG	GLN	conflict	UNP G1U3J0
k	38	CYS	TYR	conflict	UNP G1U3J0
k	48	THR	MET	conflict	UNP G1U3J0
k	66	VAL	MET	conflict	UNP G1U3J0

- Molecule 40 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 41 is a protein called Ubiquitin A-52 residue ribosomal protein fusion product 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	1	MET	-	initiating methionine	UNP A0A2K5PSA0
m	2	GLY	-	expression tag	UNP A0A2K5PSA0
m	3	ASP	-	expression tag	UNP A0A2K5PSA0
m	4	PRO	-	expression tag	UNP A0A2K5PSA0
m	5	GLU	-	expression tag	UNP A0A2K5PSA0
m	6	SER	-	expression tag	UNP A0A2K5PSA0
m	7	GLY	-	expression tag	UNP A0A2K5PSA0
m	8	GLY	-	expression tag	UNP A0A2K5PSA0
m	9	CYS	-	expression tag	UNP A0A2K5PSA0

- Molecule 42 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 43 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 44 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 45 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 46 is a protein called uS2 (SA).

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AA	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 47 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 48 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	CC	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	13	ASP	GLY	conflict	UNP O18789
CC	19	ILE	MET	conflict	UNP O18789

- Molecule 49 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	DD	224	Total	C	N	O	S	0	0
			1739	1108	313	311	7		

- Molecule 50 is a protein called eS4 (S4 X isoform).

Mol	Chain	Residues	Atoms					AltConf	Trace
50	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	25	GLY	SER	conflict	UNP G1TK17
EE	51	ARG	LYS	conflict	UNP G1TK17
EE	78	THR	ALA	conflict	UNP G1TK17
EE	156	VAL	MET	conflict	UNP G1TK17

- Molecule 51 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	FF	184	Total	C	N	O	S	0	0
			1460	915	273	265	7		

- Molecule 52 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	GG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 53 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	HH	185	Total	C	N	O	S	0	0
			1489	952	271	265	1		

- Molecule 54 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	II	198	Total	C	N	O	S	0	0
			1628	1021	322	280	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 55 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
55	JJ	181	Total	C	N	O	S	0	0
			1508	960	302	244	2		

- Molecule 56 is a protein called S10_ plectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	KK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 57 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 58 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	MM	112	Total	C	N	O	S	0	0
			871	551	155	158	7		

- Molecule 59 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	NN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 60 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	OO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 61 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	PP	129	Total	C	N	O	S	0	0
			1058	670	201	180	7		

- Molecule 62 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	QQ	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 63 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	RR	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 64 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 65 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	TT	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TT	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 66 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	UU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 67 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	VV	83	Total	C	N	O	S	0	0
			637	393	117	122	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	conflict	UNP G1TM82
VV	4	ASP	ASN	conflict	UNP G1TM82
VV	33	GLN	PRO	conflict	UNP G1TM82
VV	50	PHE	SER	conflict	UNP G1TM82
VV	75	ALA	SER	conflict	UNP G1TM82
VV	76	ASP	HIS	conflict	UNP G1TM82
VV	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 68 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	WW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 69 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	XX	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 70 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	YY	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 71 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	ZZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 72 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
aa	28	ARG	CYS	conflict	UNP G1TFE8
aa	56	ALA	VAL	conflict	UNP G1TFE8
aa	109	ARG	PRO	conflict	UNP G1TFE8

- Molecule 73 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	bb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 74 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	cc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 75 is a protein called eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	dd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 76 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	ee	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 77 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	ff	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 78 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	gg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 79 is a RNA chain called MF mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	10	11	Total	C	N	O	P	0	0
			234	105	41	77	11		

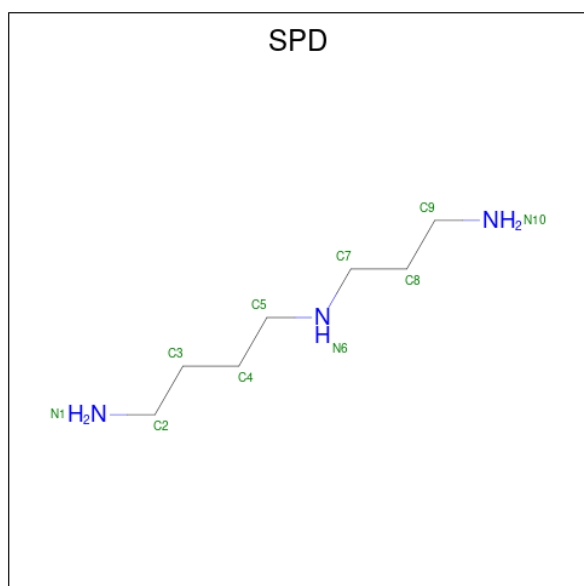
- Molecule 80 is a RNA chain called Met-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	13	74	Total	C	N	O	P	0	0
			1585	707	293	511	74		
80	11	74	Total	C	N	O	P	0	0
			1585	707	293	511	74		

- Molecule 81 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 82 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).

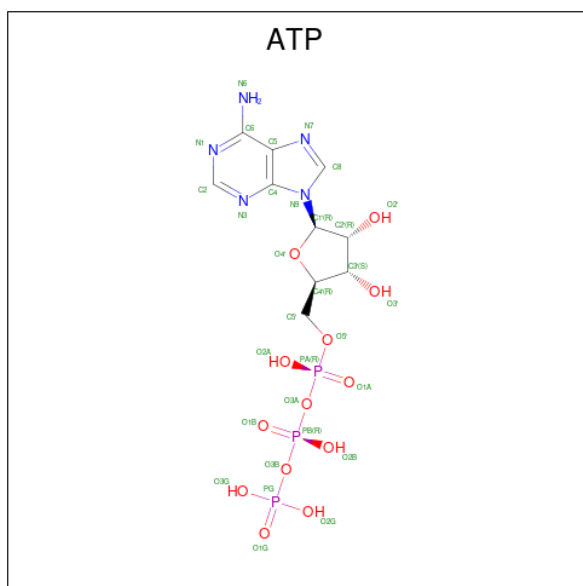


Mol	Chain	Residues	Atoms			AltConf
82	5	1	Total	C	N	0
			10	7	3	

- Molecule 83 is ZINC ION (CCD ID: ZN) (formula: Zn).

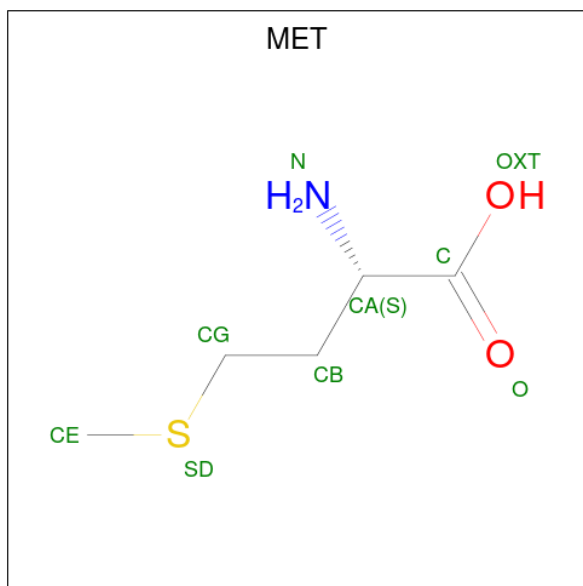
Mol	Chain	Residues	Atoms		AltConf
83	g	1	Total	Zn	0
			1	1	
83	m	1	Total	Zn	0
			1	1	
83	o	1	Total	Zn	0
			1	1	
83	p	1	Total	Zn	0
			1	1	
83	dd	1	Total	Zn	0
			1	1	
83	j	1	Total	Zn	0
			1	1	

- Molecule 84 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
84	13	1	Total	C	N	O	P	0
			31	10	5	13	3	
84	11	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 85 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).

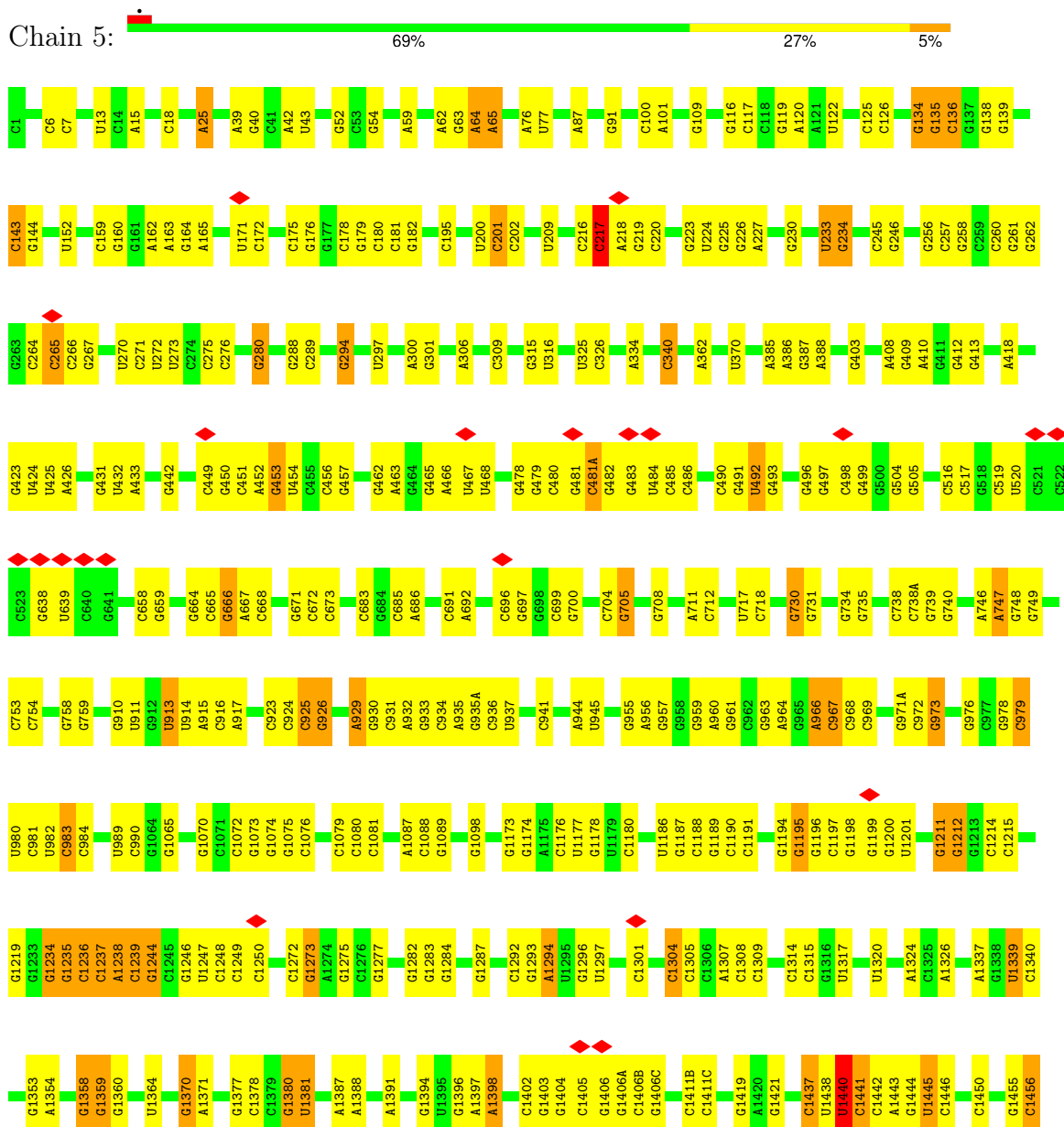


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
85	13	1	8	5	1	1	1	0

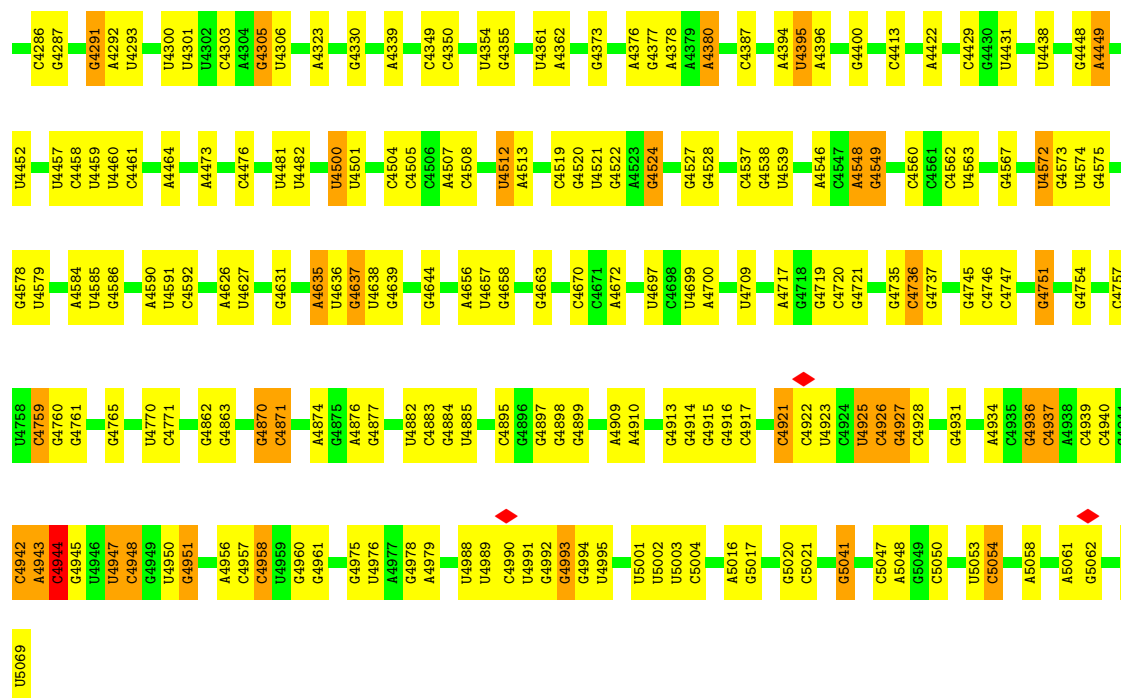
3 Residue-property plots

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

• Molecule 1: 28S ribosomal RNA

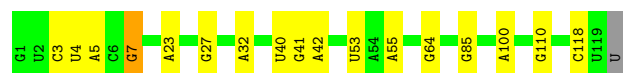


G1457	C1458	A1459	C1460	C1461	C1468	C1472	C1473	C1474	G1475	C1476	C1477	C1478	G1482	C1483	G1484	C1485	C1486	U1494	G1495	G1498	G1502	C1509	G1516	A1523	G1529	G1532	A1533	A1534	U1538	G1539	A1554	G1555	A1558	G1559	A1563	A1564	A1565	C1566	G1577	U1578	C1590	U1591																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
	U1596		U1602	G1603	G1604	G1605			U1612	A1613	C1614			A1631	A1632	G1633	A1634		G1641		G1654		C1661		G1670		C1676	U1677		G1691	C1692	U1693		G1724		G1733	G1734		G1741	A1742		G1750		C1755	U1756		G1761	C1762	C1763	G1764	A1765	A1766	A1767	C1768	G1769	A1770																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
U1771	C1772		A1773	C1774	A1775	A1776		U1779	A1780	A1786	A1787	A1788	C1789		A1802	G1803	A1804	A1805		G1818	G1819	U1820	G1821		U1834	G1835	G1836	A1837		G1842		G1846	C1847	G1854	G1855	C1859	U1860		U1866	A1867	A1868	G1869		C1884		G1890	A1891		A1897	C1898	G1899		G1916	A1917	U1918		C1921		G2001	A2002	G2003	U2004	G2005	U2006																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G1922		A1929	U1930	C1931		A1939	G1940	A1942	A1943		G1948		U1954	G1955		A1958		A1962	C1963	A1964		A1967	G1968	G1969	U1970	U1971	G1972	G1973	U1974		G1975		G1976	C1977	G1978	A1979	U1980	G1981	G1982	A1983	A1984	G1985	U1986		C1987		G1988	G1989	A1990	A1991	U1992	C1993		U1997	A1998		G2001	A2002	G2003	U2004	G2005	U2006																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
G2007	U2008	A2009	A2010	C2011	A2012	A2013	C2014	U2015	C2016	A2017	C2018	C2019	U2020	C2021	C2022	C2023	A2026		A2033		U2044	U2048	G2052		G2055	C2056	G2065	C2066	C2067	C2068	A2069	U2070	G2079	U2080	U2084	A2088	A2089	U2090	C2091	G2092	U2093	C2094		A2097	G2098	C2099	G2100	A2101	G2102	A2103	A2104	A2105																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G2106	A2107	G2108	A2109	G2110		G2259	C2260	G2261		C2266	U2267	A2268	C2269		A2276	C2277		C2289		U2293	G2294	A2300	G2301		A2313	G2314		G2326	A2332	G2333	C2334	G2335	G2336	G2348		C2351		A2395	A2396	G2397		A2404		G2407	U2408	U2409	C2410	C2411	A2412		G2421	C2422		A2428					U2570																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A2431	U2440	C2441		G2457		C2465		G2474	A2475	A2476	A2477	C2478	G2479		G2486	G2487		C2488	C2489		U2490	C2491		A2502	G2503	C2504	C2505	G2506	A2507		A2511	A2512	A2513		A2517		C2520		A2529		C2539	C2540		G2543	U2545		G2546	G2547		A2553	U2554	G2555		G2562	C2563	G2564	A2565	G2566	G2567				U2570																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
C2571	U2580	C2583		A2587		A2601	G2602		G2622		C2627	U2628		U2632	U2633	C2634	U2635		U2638	U2639	G2640		A2647		G2657		G2664		C2669		G2677		G2686	U2687		G2694	A2695	A2696	A2697		G2705	G2706		U2707	U2708		C2709		G2711	G2712		C2719		G2724	A2725	G2726		U2730	C2731																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
G2732	C2733		U2740	A2743	A2744	A2745		A2755		G2758	G2759	G2760	U2761	G2762	U2763	A2764	A2765		G2771	C2772		A2783		A2787	U2788	A2789	U2790		C2794	A2795	G2796		U2801		A2806		G2809		C2814		U2826	G2827	U2828		U2837		A2844		G2855		C2899	U2900	G2901	C3597	A3598	A3599	G3600																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G3603	A3604	C3605		A3611		G3614	G3615		A3621		G3625	G3626		A3635	U3641	A3642	A3643	U3644	U3645		A3646		A3653		A3656	U3657		A3662		G3672	G3673	G3674		A3682		G3696		U3707	C3708		U3709		A3710	A3711	A3712	U3713	G3714		A3717	A3718	A3723	A3724		A3727	A3728		A3732	A3733		A3736																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									</



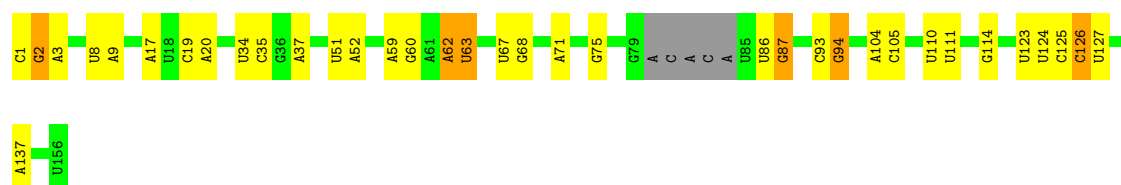
- Molecule 2: 5S ribosomal RNA

Chain 7: 85% 13% ..



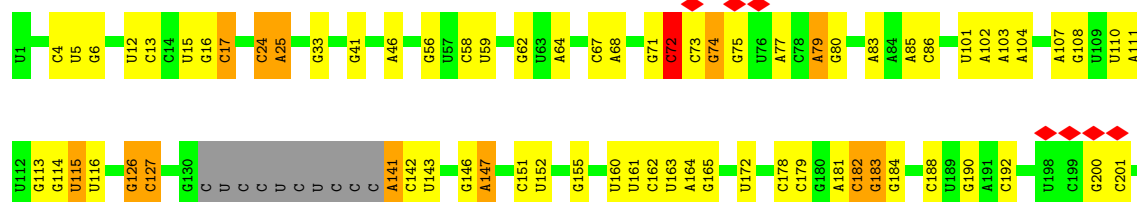
- Molecule 3: 5.8S ribosomal RNA

Chain 8: 74% 19% . .

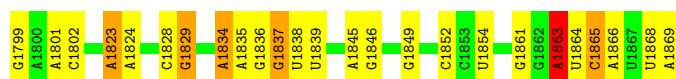


- Molecule 4: 18S ribosomal RNA

Chain 9: 62% 24% 9% .







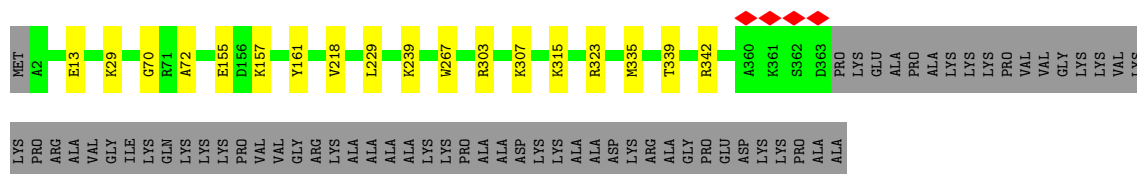
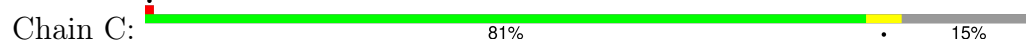
• Molecule 5: Ribosomal protein L8



• Molecule 6: Ribosomal protein L3



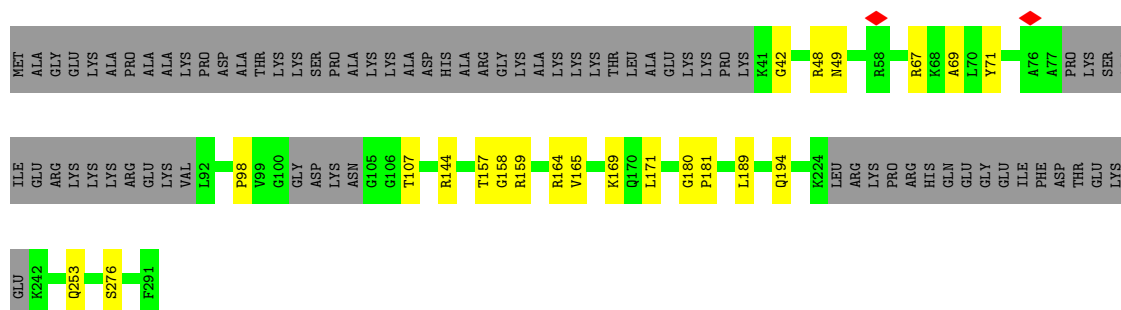
• Molecule 7: 60S ribosomal protein L4



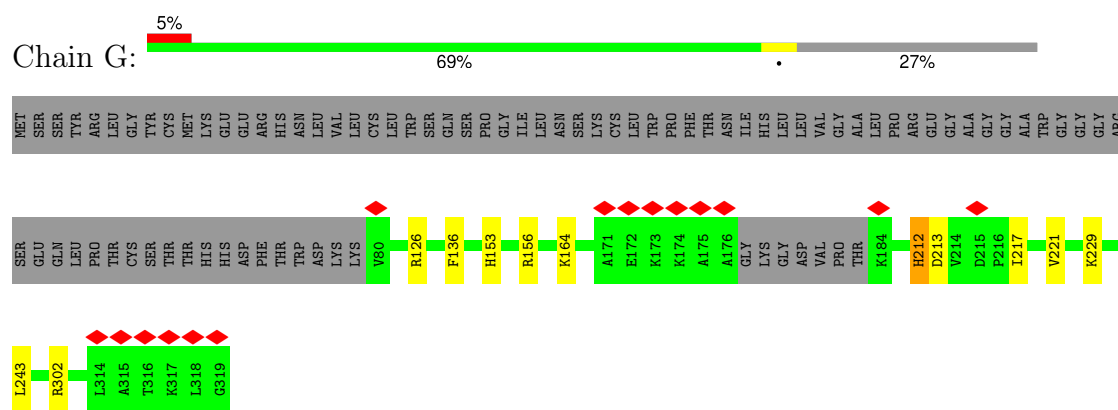
• Molecule 8: Large ribosomal subunit protein uL18



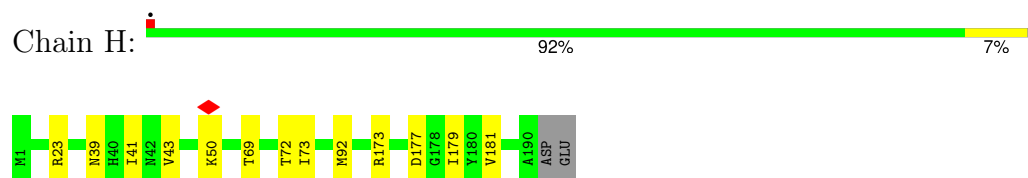
• Molecule 9: 60S ribosomal protein L6



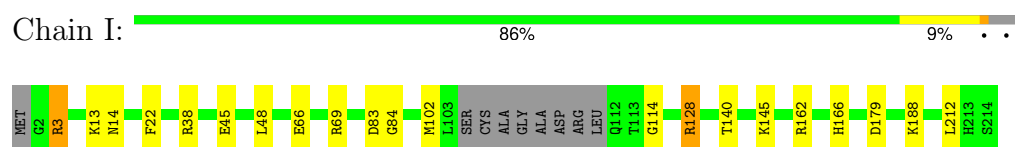
• Molecule 10: 60S ribosomal protein L7a



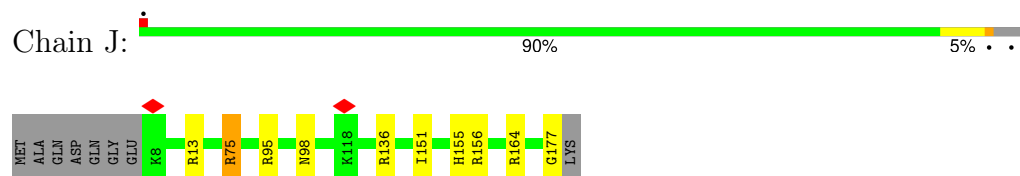
- Molecule 11: 60S ribosomal protein L9



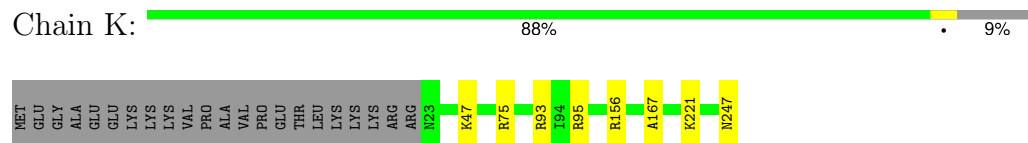
- Molecule 12: 60S ribosomal protein L10



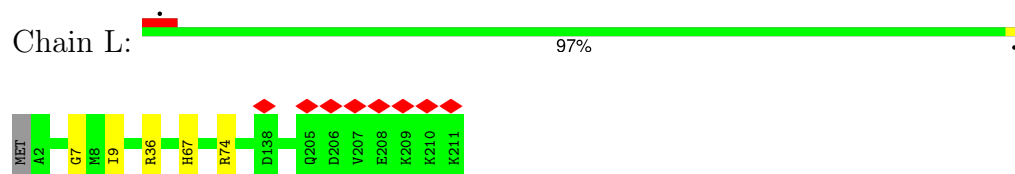
- Molecule 13: Ribosomal protein L11



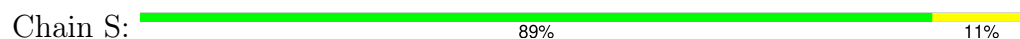
- Molecule 14: 60S ribosomal protein L7



- Molecule 15: 60S ribosomal protein L13



- Molecule 16: 60S ribosomal protein L14

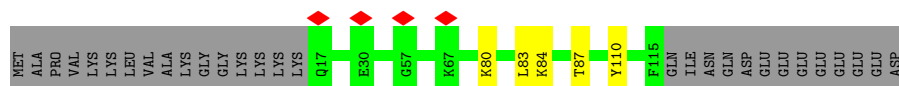




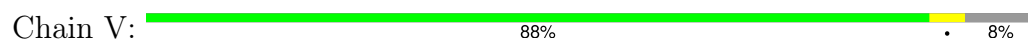
- Molecule 23: eL21



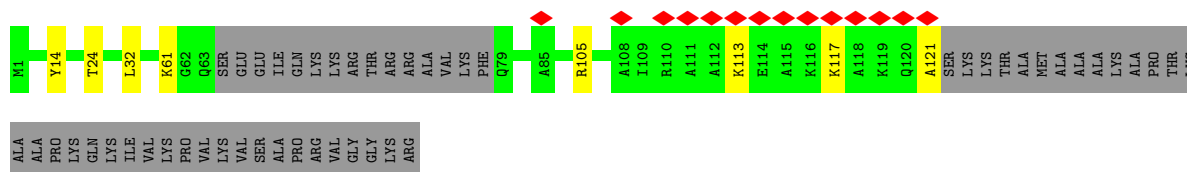
- Molecule 24: eL22



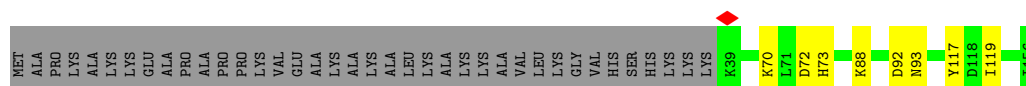
- Molecule 25: Ribosomal protein L23



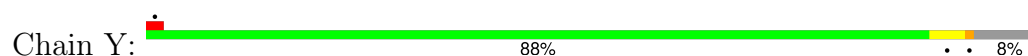
- Molecule 26: eL24



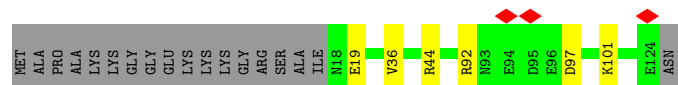
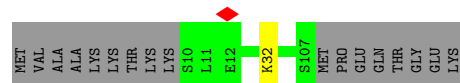
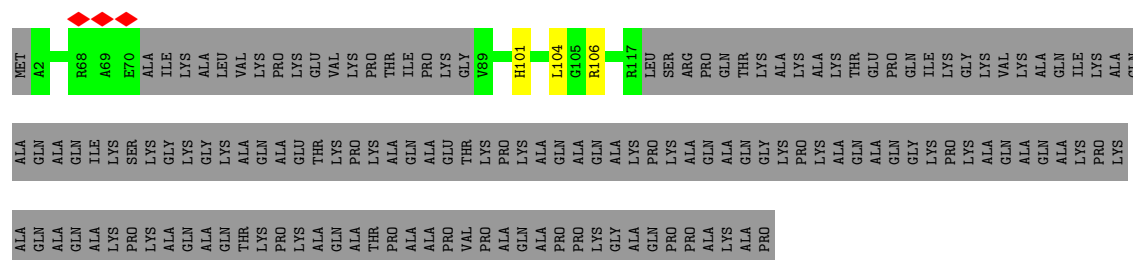
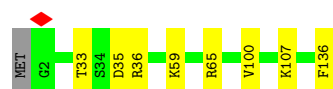
- Molecule 27: eL23




- Molecule 28: uL24



- Molecule 29: 60S ribosomal protein L27




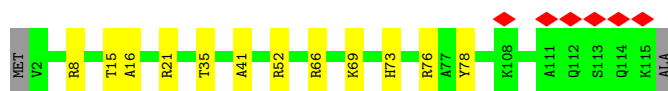
- 

Chain f:  92% 7%



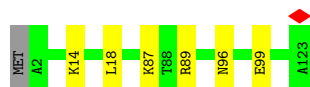
- Molecule 36: Large ribosomal subunit protein eL34

Chain g:  5% 88% 10%



- Molecule 37: eL35

Chain h:  94% 5%



- Molecule 38: 60S ribosomal protein L36

Chain i:  93%




- Molecule 39: eL38

Chain k:  91% 7%



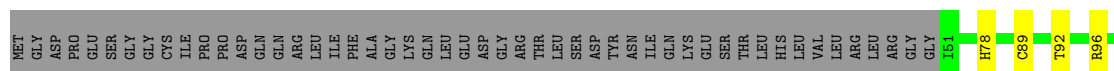
- Molecule 40: eL39

Chain l:  84% 14%



- Molecule 41: Ubiquitin A-52 residue ribosomal protein fusion product 1

Chain m:  46% 5% 49%





• Molecule 42: eL41

Chain n: 92% 8%



• Molecule 43: Large ribosomal subunit protein eL42

Chain o: 91% 8%



• Molecule 44: eL43

Chain p: 88% 11%



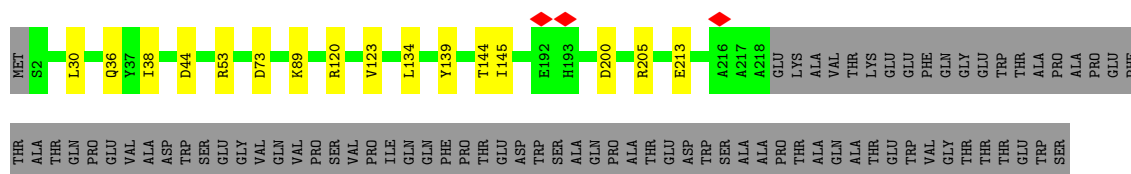
• Molecule 45: eL28

Chain r: 85% 6% 9%



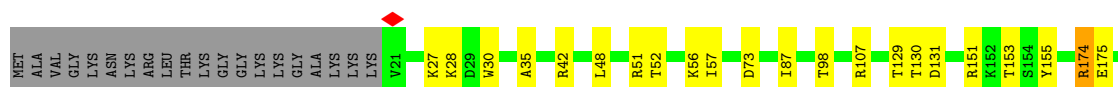
• Molecule 46: uS2 (SA)

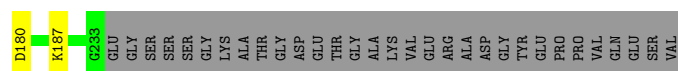
Chain AA: 68% 5% 26%



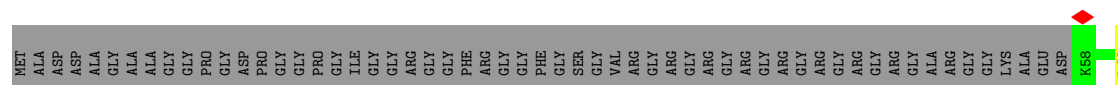
• Molecule 47: 40S ribosomal protein S3a

Chain BB: 72% 9% 19%

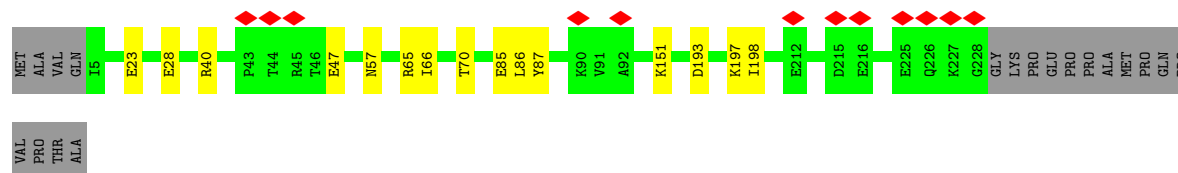
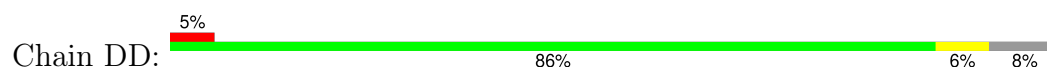




- Molecule 48: Small ribosomal subunit protein uS5



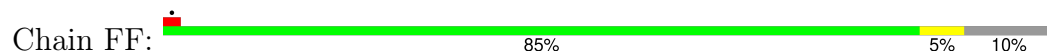
- Molecule 49: Ribosomal protein S3



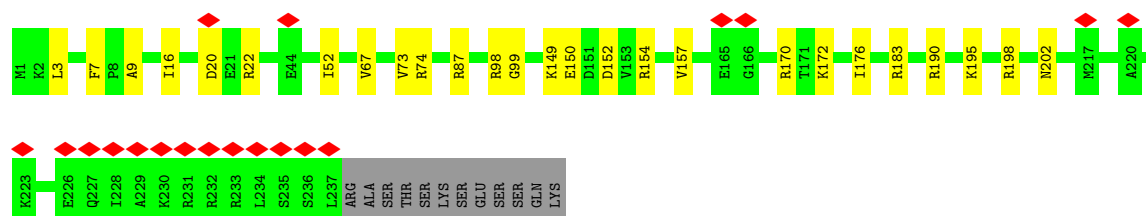
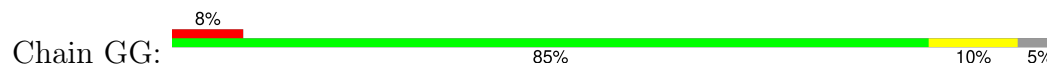
- Molecule 50: eS4 (S4 X isoform)



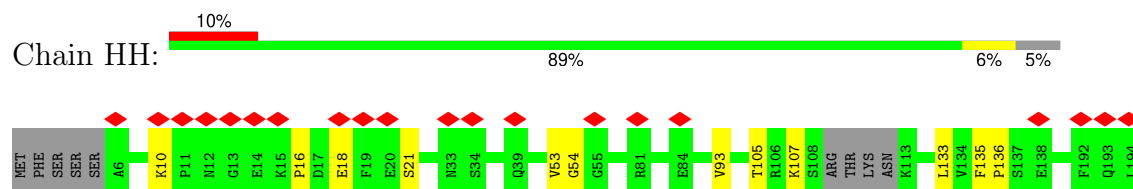
- Molecule 51: Ribosomal protein S5



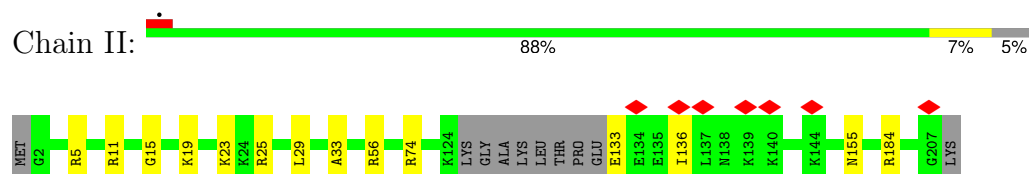
- Molecule 52: 40S ribosomal protein S6



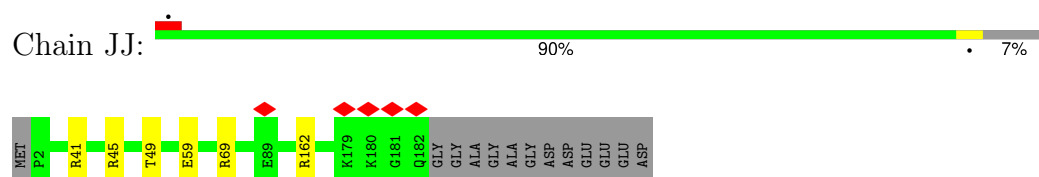
• Molecule 53: 40S ribosomal protein S7



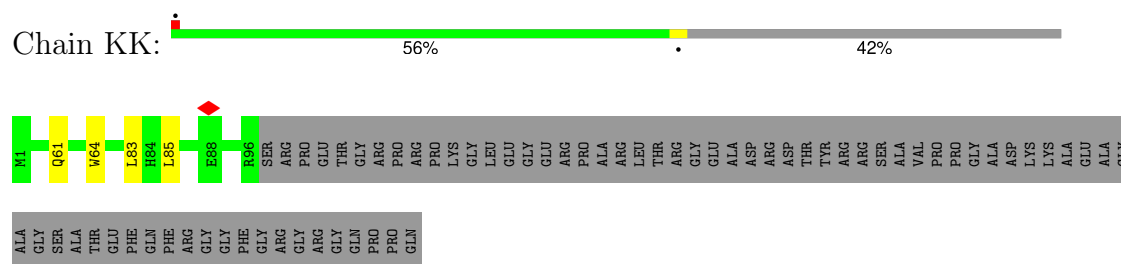
• Molecule 54: 40S ribosomal protein S8



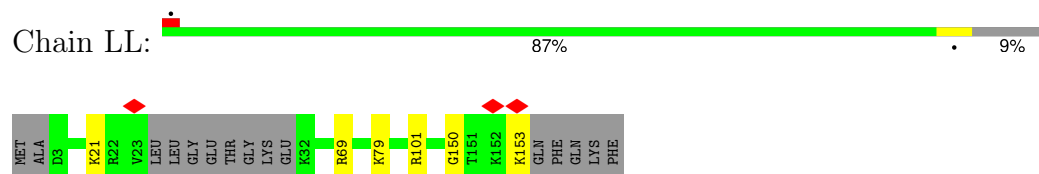
• Molecule 55: Ribosomal protein S9 (Predicted)



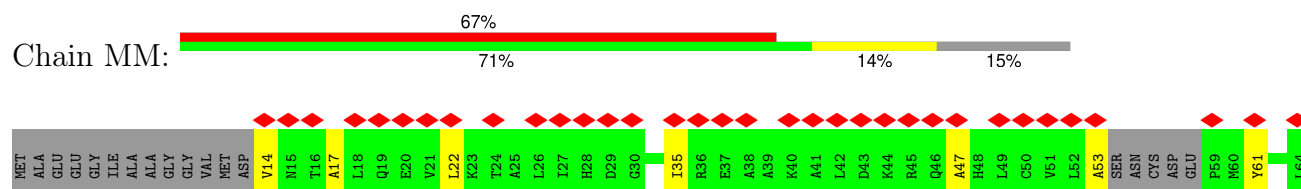
• Molecule 56: S10_pectin domain-containing protein

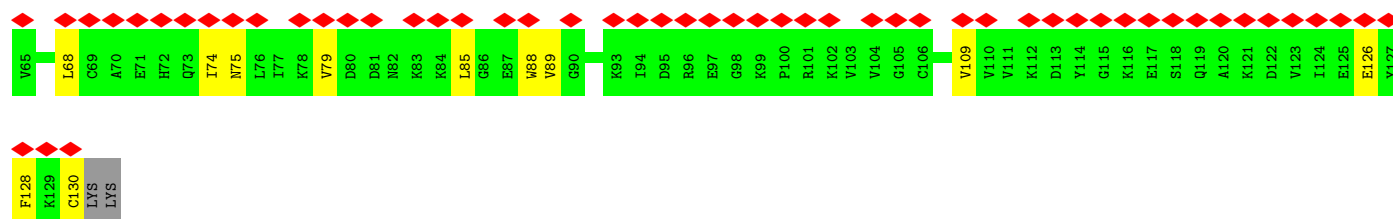


• Molecule 57: Ribosomal protein S11



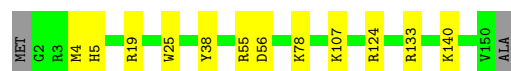
• Molecule 58: 40S ribosomal protein S12





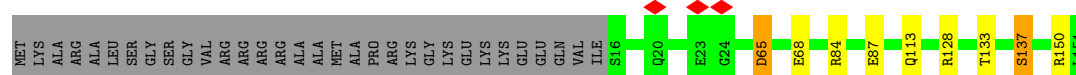
- Molecule 59: Ribosomal protein S13

Chain NN: 91% 8%



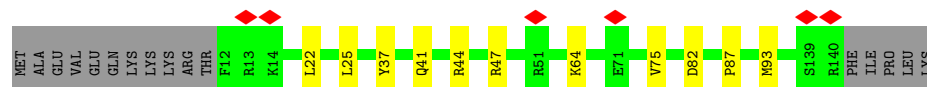
- Molecule 60: Small ribosomal subunit protein uS11

Chain OO: 76% 19%



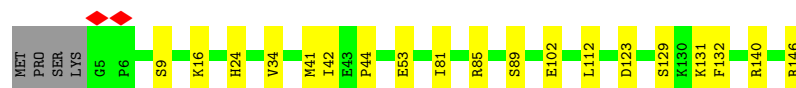
- Molecule 61: uS19

Chain PP: 81% 8% 11%



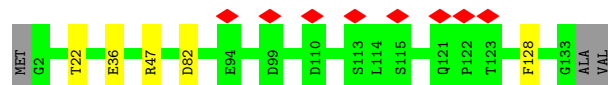
- Molecule 62: uS9

Chain QQ: 84% 13%



- Molecule 63: eS17

Chain RR: 6% 94%

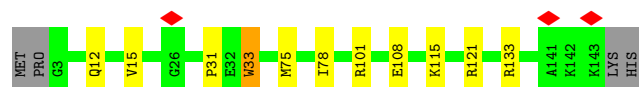
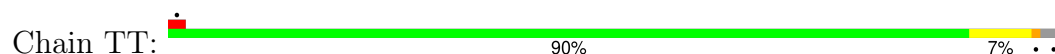


- Molecule 64: uS13

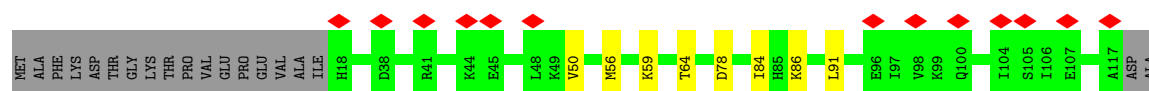
Chain SS: 86% 8% 5%



• Molecule 65: eS19



• Molecule 66: uS10



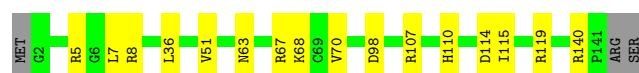
• Molecule 67: eS21



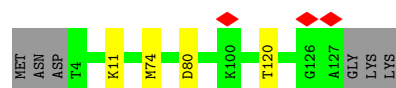
• Molecule 68: Ribosomal protein S15a



• Molecule 69: uS12

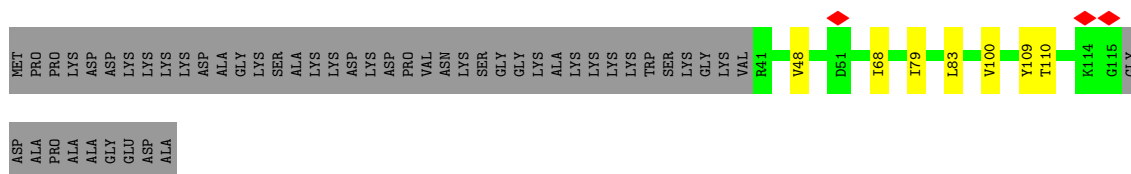


• Molecule 70: 40S ribosomal protein S24

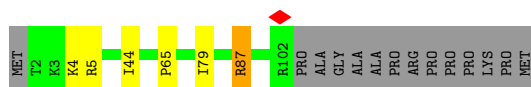
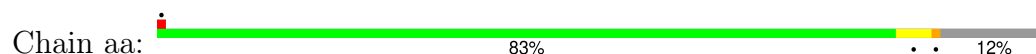


• Molecule 71: eS25

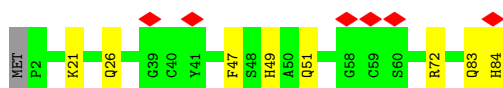
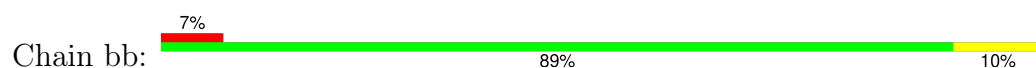




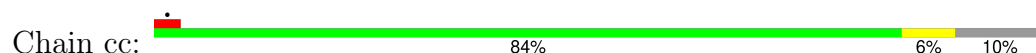
- Molecule 72: 40S ribosomal protein S26



- Molecule 73: 40S ribosomal protein S27



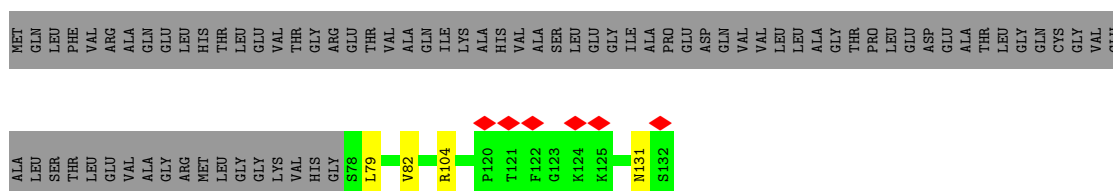
- Molecule 74: Ribosomal protein S28



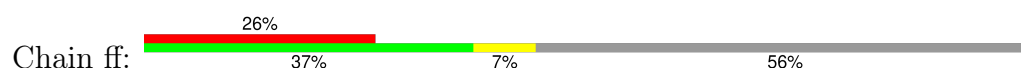
- Molecule 75: eS29



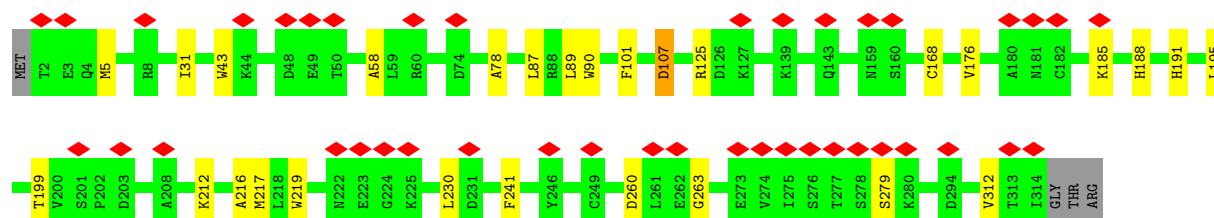
- Molecule 76: 40S ribosomal protein S30



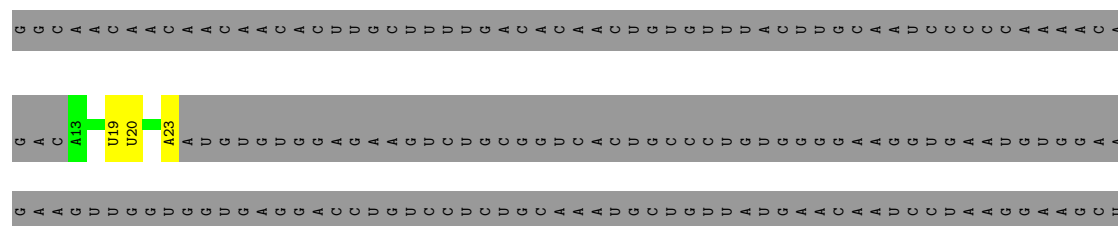
- Molecule 77: Ribosomal protein S27a



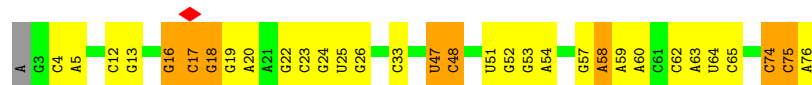
- Molecule 78: RACK1



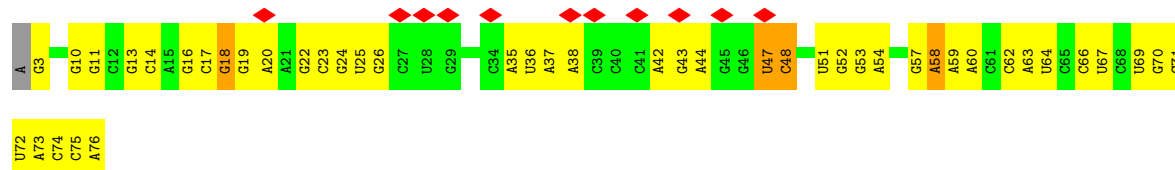
- Molecule 79: MF mRNA



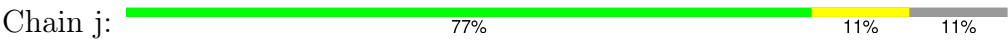
- Molecule 80: Met-tRNA



- Molecule 80: Met-tRNA



- Molecule 81: Ribosomal protein L37



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10267	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 ($e^-/\text{\AA}^2$)	30.0165	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.162, 1.162, 1.162	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP, SPD

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	5	0.47	0/86380	0.68	26/134721 (0.0%)
2	7	0.45	0/2836	0.62	0/4421
3	8	0.46	0/3581	0.64	0/5577
4	9	0.43	0/40509	0.67	5/63128 (0.0%)
5	A	0.37	0/1936	0.52	0/2596
6	B	0.35	0/3240	0.53	0/4339
7	C	0.37	0/2937	0.54	0/3946
8	D	0.31	0/2437	0.50	0/3264
9	E	0.31	0/1762	0.54	0/2362
10	G	0.31	0/1910	0.53	0/2569
11	H	0.34	0/1535	0.50	0/2063
12	I	0.34	0/1702	0.49	0/2272
13	J	0.30	0/1385	0.50	0/1852
14	K	0.37	0/1911	0.53	0/2549
15	L	0.33	0/1733	0.53	0/2316
16	M	0.33	0/1158	0.51	0/1547
17	N	0.40	0/1746	0.57	0/2338
18	O	0.38	0/1662	0.57	0/2222
19	P	0.38	0/1268	0.54	0/1700
20	Q	0.38	0/1539	0.55	0/2054
21	R	0.33	0/1524	0.52	0/2013
22	S	0.37	0/1501	0.51	0/2012
23	T	0.35	0/1326	0.51	0/1770
24	U	0.28	0/823	0.50	0/1104
25	V	0.35	0/983	0.52	0/1319
26	W	0.31	0/873	0.55	0/1158
27	X	0.33	0/984	0.48	0/1323
28	Y	0.33	0/1132	0.51	0/1504
29	Z	0.33	0/1130	0.49	0/1507
30	a	0.38	0/1191	0.56	0/1590
31	b	0.31	0/819	0.55	0/1081
32	c	0.35	0/771	0.49	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.35	0/903	0.53	0/1216
34	e	0.38	0/1071	0.54	0/1429
35	f	0.39	0/895	0.50	0/1198
36	g	0.37	0/916	0.57	0/1220
37	h	0.34	0/1021	0.55	0/1348
38	i	0.31	0/841	0.55	0/1112
39	k	0.30	0/575	0.51	0/761
40	l	0.38	0/459	0.54	0/608
41	m	0.34	0/435	0.47	0/575
42	n	0.39	0/241	0.57	0/305
43	o	0.33	0/864	0.52	0/1140
44	p	0.36	0/718	0.55	0/953
45	r	0.36	0/1010	0.54	0/1354
46	AA	0.30	0/1747	0.50	0/2374
47	BB	0.29	0/1756	0.52	0/2350
48	CC	0.32	0/1753	0.53	0/2369
49	DD	0.26	0/1767	0.47	0/2378
50	EE	0.29	0/2118	0.51	0/2849
51	FF	0.28	0/1481	0.55	0/1991
52	GG	0.27	0/1946	0.51	0/2590
53	HH	0.25	0/1511	0.49	0/2022
54	II	0.31	0/1655	0.51	0/2205
55	JJ	0.30	0/1533	0.49	0/2047
56	KK	0.25	0/834	0.45	0/1125
57	LL	0.34	0/1195	0.51	0/1597
58	MM	0.20	0/880	0.55	0/1179
59	NN	0.32	0/1226	0.53	0/1649
60	OO	0.33	0/1029	0.50	0/1380
61	PP	0.23	0/1079	0.53	0/1441
62	QQ	0.29	0/1146	0.51	0/1534
63	RR	0.27	0/1082	0.51	0/1452
64	SS	0.27	0/1208	0.47	0/1618
65	TT	0.27	0/1115	0.54	0/1493
66	UU	0.26	0/805	0.48	0/1081
67	VV	0.30	0/644	0.48	0/860
68	WW	0.36	0/1051	0.48	0/1406
69	XX	0.32	0/1105	0.49	0/1476
70	YY	0.26	0/1028	0.49	0/1366
71	ZZ	0.25	0/604	0.47	0/810
72	aa	0.34	0/828	0.46	0/1109
73	bb	0.27	0/665	0.55	0/891
74	cc	0.26	0/490	0.38	0/656
75	dd	0.30	0/470	0.52	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	ee	0.26	0/447	0.59	0/587
77	ff	0.17	0/567	0.49	0/753
78	gg	0.22	0/2493	0.46	0/3394
79	10	0.32	0/261	0.56	0/404
80	11	0.29	0/1773	0.70	0/2763
80	13	0.35	0/1773	0.66	0/2763
81	j	0.38	0/720	0.56	0/952
All	All	0.40	0/229958	0.62	31/338007 (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
1	5	0	2
5	A	0	1
6	B	0	1
7	C	0	1
8	D	0	2
12	I	0	2
13	J	0	2
17	N	0	1
20	Q	0	2
22	S	0	1
28	Y	0	1
35	f	0	1
36	g	0	1
44	p	0	1
47	BB	0	1
54	II	0	2
59	NN	0	1
60	OO	0	1
64	SS	0	1
65	TT	0	1
72	aa	0	1
73	bb	0	1
76	ee	0	1
All	All	0	29

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2544	G	C8-N9-C1'	-7.12	105.65	127.00
1	5	2546	G	C2'-C3'-O3'	6.59	119.38	109.50
4	9	1396	A	C2'-C3'-O3'	6.50	119.26	109.50
1	5	2544	G	C4-N9-C1'	6.37	145.60	126.50
1	5	1440	U	C2'-C3'-O3'	6.31	118.97	109.50
1	5	2068	C	C2'-C3'-O3'	6.18	118.78	109.50
1	5	4119	C	C2'-C3'-O3'	6.06	118.59	109.50
1	5	4944	C	C1'-O4'-C4'	-5.82	104.08	109.90
1	5	3888	G	C2'-C3'-O3'	5.80	122.40	113.70
4	9	1863	A	C1'-O4'-C4'	-5.73	103.97	109.70
1	5	929	A	C5'-C4'-O4'	5.59	118.18	109.80
1	5	4232	U	C2'-C3'-O3'	5.57	117.86	109.50
1	5	492	U	C4'-C3'-O3'	5.55	117.73	109.40
1	5	2546	G	C5'-C4'-O4'	5.55	117.42	109.10
4	9	72	C	P-O3'-C3'	5.55	128.52	120.20
1	5	1916	G	N9-C1'-C2'	5.54	120.31	112.00
1	5	2395	A	C2'-C3'-O3'	5.54	117.82	109.50
1	5	2089	G	C4'-C3'-O3'	5.39	117.48	109.40
1	5	1485	C	C2'-C3'-O3'	5.30	117.45	109.50
1	5	217	C	C2'-C3'-O3'	5.27	117.40	109.50
1	5	2089	G	C2'-C3'-O3'	5.25	117.38	109.50
1	5	2546	G	C4'-C3'-O3'	5.25	117.27	109.40
1	5	1236	C	C4'-C3'-O3'	5.21	120.81	113.00
1	5	2007	G	N9-C1'-C2'	5.19	119.79	112.00
1	5	1891	A	N9-C1'-C2'	5.11	119.67	112.00
1	5	3876	A	C2'-C3'-O3'	5.11	117.17	109.50
4	9	495	U	N1-C1'-C2'	5.09	119.63	112.00
1	5	1818	G	C2'-C3'-O3'	5.08	117.12	109.50
1	5	1477	C	C2'-C3'-O3'	5.05	121.28	113.70
4	9	532	C	C2'-C3'-O3'	5.04	121.26	113.70
1	5	2711	G	C1'-O4'-C4'	-5.00	104.70	109.70

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	5	1964	A	Sidechain
1	5	2544	G	Sidechain
5	A	123	ARG	Sidechain
6	B	200	ARG	Sidechain
47	BB	174	ARG	Sidechain
7	C	303	ARG	Sidechain
8	D	24	ARG	Sidechain

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Mol	Chain	Res	Type	Group
8	D	33	ARG	Sidechain
12	I	128	ARG	Sidechain
12	I	3	ARG	Sidechain
54	II	5	ARG	Sidechain
54	II	74	ARG	Sidechain
13	J	164	ARG	Sidechain
13	J	75	ARG	Sidechain
17	N	73	ARG	Sidechain
59	NN	124	ARG	Sidechain
60	OO	137	SER	Peptide
20	Q	108	ARG	Sidechain
20	Q	91	ARG	Sidechain
22	S	95	ARG	Sidechain
64	SS	132	ARG	Sidechain
65	TT	133	ARG	Sidechain
28	Y	115	ARG	Sidechain
72	aa	87	ARG	Sidechain
73	bb	72	ARG	Sidechain
76	ee	104	ARG	Sidechain
35	f	100	ARG	Sidechain
36	g	8	ARG	Sidechain
44	p	49	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	5	77221	0	39013	527	0
2	7	2538	0	1286	10	0
3	8	3208	0	1629	20	0
4	9	36229	0	18300	275	0
5	A	1898	0	1993	11	0
6	B	3172	0	3310	17	0
7	C	2883	0	3053	14	0
8	D	2391	0	2424	10	0
9	E	1729	0	1887	16	0
10	G	1879	0	2027	9	0
11	H	1516	0	1597	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	I	1664	0	1712	15	0
13	J	1362	0	1399	6	0
14	K	1875	0	1995	6	0
15	L	1702	0	1820	4	0
16	M	1137	0	1211	5	0
17	N	1701	0	1749	13	0
18	O	1630	0	1778	7	0
19	P	1242	0	1274	10	0
20	Q	1515	0	1634	9	0
21	R	1508	0	1664	12	0
22	S	1462	0	1508	11	0
23	T	1298	0	1366	8	0
24	U	809	0	833	4	0
25	V	969	0	1031	5	0
26	W	860	0	903	7	0
27	X	967	0	1040	5	0
28	Y	1115	0	1205	7	0
29	Z	1107	0	1182	7	0
30	a	1162	0	1209	10	0
31	b	806	0	866	3	0
32	c	761	0	794	1	0
33	d	888	0	930	3	0
34	e	1053	0	1147	8	0
35	f	876	0	912	6	0
36	g	906	0	998	8	0
37	h	1013	0	1147	4	0
38	i	830	0	916	3	0
39	k	569	0	637	3	0
40	l	447	0	480	9	0
41	m	429	0	465	5	0
42	n	240	0	289	1	0
43	o	851	0	920	4	0
44	p	708	0	756	10	0
45	r	994	0	1051	7	0
46	AA	1710	0	1708	11	0
47	BB	1729	0	1803	16	0
48	CC	1716	0	1806	9	0
49	DD	1739	0	1832	10	0
50	EE	2076	0	2177	18	0
51	FF	1460	0	1509	9	0
52	GG	1923	0	2089	20	0
53	HH	1489	0	1582	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	II	1628	0	1706	11	0
55	JJ	1508	0	1626	4	0
56	KK	810	0	836	3	0
57	LL	1175	0	1249	7	0
58	MM	871	0	913	11	0
59	NN	1202	0	1289	11	0
60	OO	1016	0	1039	8	0
61	PP	1058	0	1104	8	0
62	QQ	1128	0	1195	12	0
63	RR	1068	0	1121	4	0
64	SS	1190	0	1249	9	0
65	TT	1097	0	1132	7	0
66	UU	795	0	862	6	0
67	VV	637	0	637	1	0
68	WW	1034	0	1080	7	0
69	XX	1087	0	1154	14	0
70	YY	1011	0	1083	4	0
71	ZZ	598	0	656	6	0
72	aa	814	0	867	7	0
73	bb	651	0	672	5	0
74	cc	488	0	514	2	0
75	dd	459	0	448	3	0
76	ee	443	0	492	3	0
77	ff	555	0	567	8	0
78	gg	2436	0	2393	18	0
79	10	234	0	118	1	0
80	11	1585	0	804	31	0
80	13	1585	0	803	21	0
81	j	705	0	737	11	0
82	5	10	0	19	0	0
83	dd	1	0	0	0	0
83	g	1	0	0	0	0
83	j	1	0	0	0	0
83	m	1	0	0	0	0
83	o	1	0	0	0	0
83	p	1	0	0	0	0
84	11	31	0	11	2	0
84	13	31	0	11	0	0
85	13	8	0	8	0	0
All	All	213916	0	158241	1254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (1254) 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)
1:5:2638:G:N2	1:5:2697:A:N1	2.11	0.97
1:5:4099:G:H22	1:5:4109:G:H22	1.07	0.95
1:5:3692:A:H62	1:5:3823:G:H21	1.19	0.91
1:5:973:G:N2	1:5:1282:G:N7	2.20	0.90
26:W:117:LYS:HA	26:W:121:ALA:HB3	1.53	0.87
4:9:925:G:H1	4:9:1017:U:H3	1.21	0.85
4:9:830:A:H62	4:9:845:G:H21	1.27	0.83
1:5:4099:G:H22	1:5:4109:G:N2	1.80	0.80
1:5:978:G:N2	1:5:1277:G:H1	1.78	0.80
1:5:4992:G:H2'	1:5:4993:G:C8	2.17	0.79
4:9:1834:A:H2	4:9:1837:G:H1	1.32	0.78
66:UU:59:LYS:HD2	66:UU:84:ILE:HD11	1.65	0.77
4:9:64:A:H2	4:9:83:A:H62	1.33	0.76
4:9:1272:C:O2'	4:9:1274:G:N2	2.17	0.76
1:5:2562:G:N2	1:5:2565:A:OP2	2.18	0.76
4:9:114:G:OP1	57:LL:69:ARG:NH1	2.18	0.76
1:5:2457:G:H21	1:5:3672:G:H21	1.34	0.75
1:5:2395:A:O2'	1:5:2806:A:H1'	1.86	0.74
62:QQ:146:ARG:NH2	80:13:33:C:OP2	2.19	0.74
4:9:79:A:OP1	52:GG:172:LYS:NZ	2.20	0.74
1:5:2520:C:O2	1:5:2640:G:N2	2.21	0.73
1:5:691:C:H2'	1:5:692:A:C8	2.23	0.73
1:5:978:G:H22	1:5:1277:G:H1	1.35	0.72
1:5:4431:U:OP2	12:I:3:ARG:NH2	2.22	0.72
4:9:1228:A:H2'	4:9:1229:G:C8	2.23	0.72
1:5:4413:C:H5	1:5:4429:C:H42	1.37	0.72
1:5:4770:U:OP1	18:O:176:ARG:NH1	2.21	0.72
80:11:62:C:H2'	80:11:63:A:C8	2.24	0.72
1:5:1317:U:OP1	30:a:21:ARG:NH2	2.22	0.72
22:S:77:ASN:ND2	22:S:137:CYS:SG	2.63	0.71
1:5:2457:G:H21	1:5:3672:G:N2	1.88	0.71
33:d:97:ASP:OD1	33:d:101:LYS:NZ	2.23	0.71
1:5:2477:A:H2'	1:5:2478:C:C6	2.26	0.71
74:cc:44:ARG:NH2	74:cc:60:GLU:O	2.24	0.71
53:HH:93:VAL:HG21	53:HH:133:LEU:HD12	1.74	0.70
8:D:107:ARG:NH2	8:D:116:ASP:OD1	2.25	0.70
44:p:42:CYS:HB3	44:p:60:CYS:SG	2.31	0.70
1:5:4751:G:H1	1:5:4948:C:H5	1.39	0.70
1:5:4099:G:N2	1:5:4109:G:H22	1.87	0.70
80:11:62:C:H2'	80:11:63:A:H8	1.54	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3860:A:H61	1:5:4560:C:H5	1.38	0.69
4:9:1263:U:O2	75:dd:16:GLN:NE2	2.25	0.69
1:5:4077:A:N1	1:5:4171:C:N4	2.38	0.69
4:9:1563:G:OP1	65:TT:121:ARG:NH1	2.26	0.69
4:9:568:C:O2'	4:9:569:A:N3	2.26	0.69
1:5:2758:G:O2'	1:5:2765:A:N3	2.26	0.69
1:5:2706:G:O6	21:R:46:LYS:NZ	2.26	0.69
80:11:51:U:H2'	80:11:52:G:H8	1.58	0.68
80:11:51:U:H2'	80:11:52:G:C8	2.27	0.68
1:5:1441:C:H2'	1:5:1442:C:C6	2.29	0.68
4:9:1693:G:H21	4:9:1834:A:H8	1.40	0.68
16:M:52:PHE:O	22:S:157:ARG:NH2	2.27	0.68
80:13:62:C:H2'	80:13:63:A:C8	2.29	0.68
4:9:981:A:H2'	4:9:982:G:C8	2.28	0.68
4:9:743:U:O4	4:9:798:G:N2	2.26	0.67
4:9:830:A:H62	4:9:845:G:N2	1.92	0.67
4:9:1308:U:H2'	4:9:1309:C:C6	2.29	0.67
80:13:51:U:H2'	80:13:52:G:C8	2.30	0.67
1:5:3751:G:H21	1:5:3775:A:H8	1.41	0.67
60:OO:113:GLN:NE2	72:aa:44:ILE:O	2.25	0.67
80:13:51:U:H2'	80:13:52:G:H8	1.58	0.67
1:5:2601:A:N6	1:5:2744:A:OP2	2.28	0.67
4:9:126:G:OP1	52:GG:198:ARG:NH1	2.27	0.67
1:5:2478:C:H2'	1:5:2479:G:C8	2.29	0.67
1:5:1075:G:H1	1:5:1235:G:H22	1.42	0.66
61:PP:44:ARG:NH1	61:PP:82:ASP:O	2.29	0.66
1:5:2478:C:H2'	1:5:2479:G:H8	1.60	0.66
1:5:1380:G:H4'	1:5:1381:U:O2	1.95	0.66
50:EE:148:ARG:NH2	52:GG:202:ASN:OD1	2.26	0.66
4:9:928:G:H2'	4:9:929:G:C8	2.31	0.66
6:B:218:ASP:HB3	6:B:280:ILE:HA	1.78	0.66
1:5:4099:G:H1	1:5:4109:G:H1	1.43	0.66
50:EE:174:LYS:O	50:EE:179:ASN:ND2	2.28	0.66
1:5:4039:G:N7	1:5:4041:C:N4	2.44	0.65
1:5:2489:C:O2'	1:5:2491:C:N4	2.28	0.65
4:9:1407:U:H2'	4:9:1408:U:C6	2.32	0.65
1:5:1234:G:HO2'	1:5:1235:G:H8	1.42	0.65
1:5:2262:G:OP2	45:r:98:ARG:NH2	2.25	0.65
4:9:439:A:OP2	54:II:23:LYS:NZ	2.29	0.65
4:9:1091:C:HO2'	68:WW:2:VAL:N	1.95	0.65
4:9:830:A:N6	4:9:845:G:H21	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:36:GLU:OE1	5:A:163:ARG:NH1	2.27	0.65
57:LL:101:ARG:NH1	69:XX:5:ARG:O	2.30	0.65
1:5:294:G:O2'	30:a:59:ARG:NH2	2.30	0.65
1:5:1075:G:H1	1:5:1235:G:N2	1.95	0.65
4:9:1611:G:OP2	64:SS:121:ARG:NH2	2.25	0.64
4:9:1619:A:OP2	61:PP:47:ARG:NH1	2.29	0.64
1:5:4899:G:N2	1:5:4921:C:C2	2.65	0.64
80:11:43:G:H2'	80:11:44:A:C8	2.32	0.64
1:5:976:G:H21	7:C:323:ARG:NE	1.96	0.64
4:9:1693:G:N2	4:9:1834:A:H8	1.96	0.64
4:9:101:U:H5''	54:II:19:LYS:HE2	1.78	0.64
4:9:1667:U:H2'	4:9:1668:U:C6	2.33	0.64
57:LL:150:GLY:O	59:NN:133:ARG:NH1	2.31	0.63
34:e:40:GLY:O	34:e:46:ARG:NH1	2.30	0.63
1:5:980:U:H3	1:5:1275:G:H1	1.46	0.63
1:5:4206:C:OP1	23:T:5:LYS:NZ	2.26	0.63
12:I:66:GLU:OE1	12:I:69:ARG:NH1	2.31	0.63
1:5:1555:G:O6	44:p:4:ARG:NH2	2.31	0.63
9:E:48:ARG:O	9:E:67:ARG:NH1	2.30	0.63
4:9:1310:U:H2'	4:9:1311:C:C6	2.34	0.63
10:G:229:LYS:HG2	38:i:43:MET:HE1	1.81	0.63
49:DD:193:ASP:OD2	49:DD:197:LYS:N	2.32	0.63
80:13:63:A:H2'	80:13:64:U:C6	2.34	0.63
1:5:976:G:H21	7:C:323:ARG:HE	1.47	0.62
62:QQ:53:GLU:OE1	62:QQ:85:ARG:NH1	2.23	0.62
1:5:1970:A:H1'	1:5:2017:A:H61	1.65	0.62
4:9:1588:A:H2'	4:9:1589:A:C8	2.35	0.62
1:5:4460:U:OP1	6:B:10:ARG:NH1	2.33	0.62
17:N:68:ARG:NH1	17:N:124:ASP:O	2.30	0.62
4:9:1616:U:H3	4:9:1620:A:H2	1.48	0.62
21:R:3:MET:HE1	21:R:5:ARG:CZ	2.30	0.62
43:o:71:GLU:OE2	43:o:78:ARG:NH2	2.29	0.62
1:5:671:G:H2'	1:5:672:C:C6	2.35	0.61
1:5:3653:A:H4'	5:A:179:ILE:O	2.00	0.61
1:5:2639:U:O2'	1:5:2694:G:N1	2.29	0.61
49:DD:70:THR:HG22	49:DD:86:LEU:HD13	1.81	0.61
1:5:3910:C:H2'	1:5:3911:C:C6	2.34	0.61
9:E:165:VAL:HG13	9:E:180:GLY:H	1.65	0.61
1:5:1468:C:OP1	30:a:132:ARG:NH2	2.33	0.61
1:5:2517:A:O2'	36:g:66:ARG:NH2	2.33	0.61
1:5:76:A:OP2	15:L:74:ARG:NH1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2583:C:OP2	36:g:76:ARG:NH1	2.27	0.61
4:9:1410:C:H2'	4:9:1411:G:H8	1.66	0.61
4:9:303:C:O2	54:II:184:ARG:NH2	2.33	0.61
4:9:1144:A:H2'	4:9:1145:A:C8	2.36	0.61
1:5:175:C:H2'	1:5:176:G:C8	2.35	0.61
50:EE:51:ARG:HG2	50:EE:51:ARG:HH11	1.66	0.61
1:5:3692:A:H62	1:5:3823:G:N2	1.94	0.60
1:5:1197:C:H2'	1:5:1198:G:C8	2.36	0.60
4:9:1192:U:OP2	69:XX:119:ARG:NH2	2.30	0.60
4:9:115:U:H2'	4:9:116:U:C6	2.36	0.60
4:9:1395:C:O2'	4:9:1396:A:OP1	2.18	0.60
59:NN:55:ARG:NH2	73:bb:51:GLN:OE1	2.26	0.60
1:5:3736:A:H2'	1:5:3737:A:C8	2.36	0.60
4:9:1228:A:H2'	4:9:1229:G:H8	1.65	0.60
12:I:38:ARG:HD2	12:I:83:ASP:HB2	1.84	0.60
17:N:135:ILE:HG23	17:N:142:ILE:HD13	1.83	0.60
46:AA:205:ARG:NH2	46:AA:213:GLU:OE1	2.34	0.60
58:MM:22:LEU:HD13	58:MM:88:TRP:HB3	1.83	0.60
1:5:2019:C:H2'	1:5:2020:U:C6	2.36	0.60
1:5:3717:A:H2'	1:5:3718:A:C8	2.36	0.60
1:5:979:C:OP1	9:E:49:ASN:ND2	2.34	0.60
1:5:1370:G:O6	7:C:239:LYS:NZ	2.28	0.60
4:9:141:A:OP2	52:GG:149:LYS:NZ	2.35	0.60
9:E:189:LEU:H	9:E:253:GLN:HE22	1.50	0.60
1:5:4925:U:H4'	1:5:4926:C:C5'	2.32	0.60
4:9:79:A:H3'	4:9:80:G:H8	1.66	0.60
19:P:30:ARG:NH1	19:P:31:GLU:OE1	2.33	0.59
1:5:2695:A:OP1	39:k:35:LYS:NZ	2.34	0.59
1:5:4291:G:H5''	1:5:4293:U:C6	2.37	0.59
64:SS:23:ARG:HB3	71:ZZ:48:VAL:HG11	1.84	0.59
1:5:1358:G:H2'	1:5:1360:G:O6	2.02	0.59
17:N:178:HIS:HA	17:N:181:HIS:NE2	2.17	0.59
59:NN:55:ARG:NH1	59:NN:56:ASP:OD1	2.36	0.59
4:9:903:A:H2'	4:9:904:A:H8	1.67	0.59
62:QQ:132:PHE:O	62:QQ:140:ARG:NH2	2.34	0.59
66:UU:78:ASP:OD2	75:dd:44:ARG:NH1	2.34	0.59
1:5:4950:U:O2'	1:5:4951:G:OP1	2.19	0.59
43:o:63:THR:O	43:o:87:ARG:NH1	2.36	0.59
4:9:1060:A:O2'	4:9:1062:A:N7	2.36	0.59
47:BB:130:THR:OG1	47:BB:180:ASP:OD1	2.17	0.59
1:5:2638:G:H22	1:5:2697:A:N6	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:67:U:H2'	3:8:68:G:H8	1.67	0.59
1:5:2638:G:H22	1:5:2697:A:H61	1.51	0.59
1:5:260:C:H2'	1:5:261:G:C8	2.38	0.58
12:I:166:HIS:CE1	23:T:160:ALA:HB3	2.37	0.58
1:5:2503:G:H5''	1:5:2503:G:H8	1.67	0.58
51:FF:102:LEU:HD11	71:ZZ:100:VAL:HG11	1.84	0.58
5:A:29:LEU:O	5:A:123:ARG:NH1	2.35	0.58
7:C:315:LYS:HD2	14:K:167:ALA:HB1	1.84	0.58
1:5:3904:G:O2'	1:5:3905:A:OP1	2.18	0.58
64:SS:108:ARG:NH1	64:SS:112:GLU:OE2	2.34	0.58
1:5:4303:C:H2'	1:5:4305:G:C8	2.38	0.58
4:9:857:U:H2'	4:9:858:A:C8	2.38	0.58
50:EE:11:ARG:NH1	50:EE:24:THR:OG1	2.35	0.58
1:5:1450:C:O2'	1:5:2104:A:H1'	2.04	0.58
1:5:4635:A:H8	1:5:5048:A:H61	1.50	0.58
2:7:85:G:OP1	14:K:221:LYS:NZ	2.35	0.58
1:5:717:U:H2'	1:5:718:C:C6	2.39	0.58
11:H:41:ILE:HG21	11:H:73:ILE:HD11	1.85	0.58
4:9:533:A:H2'	4:9:534:G:C8	2.39	0.58
4:9:1736:G:H2'	4:9:1737:G:C8	2.38	0.58
80:11:42:A:H2'	80:11:43:G:H8	1.68	0.58
1:5:1198:G:H2'	1:5:1199:G:C8	2.38	0.57
1:5:3932:U:H2'	1:5:3933:G:H8	1.69	0.57
4:9:582:U:OP1	55:JJ:162:ARG:NH1	2.37	0.57
1:5:1406:G:H2'	1:5:1406(A):G:H8	1.69	0.57
1:5:3799:A:OP1	25:V:64:THR:HG21	2.03	0.57
4:9:1289:U:OP2	77:ff:95:ARG:NH1	2.35	0.57
5:A:117:GLU:HA	5:A:124:GLY:HA2	1.86	0.57
1:5:3641:U:H5	1:5:3646:A:N7	2.02	0.57
17:N:124:ASP:OD1	17:N:125:SER:N	2.37	0.57
50:EE:11:ARG:HH12	50:EE:24:THR:HG1	1.52	0.57
69:XX:68:LYS:HE2	76:ee:82:VAL:HG22	1.85	0.57
1:5:280:G:H5''	17:N:14:LYS:HE2	1.86	0.57
1:5:3635:A:N6	44:p:17:ARG:O	2.34	0.57
65:TT:108:GLU:OE1	65:TT:115:LYS:NZ	2.34	0.57
1:5:4936:G:O2'	1:5:4937:C:OP1	2.22	0.57
52:GG:98:ARG:NH1	52:GG:99:GLY:O	2.37	0.57
1:5:424:U:H2'	1:5:425:U:C6	2.39	0.57
1:5:2465:C:H1'	1:5:3672:G:H22	1.69	0.57
1:5:4047:A:O2'	1:5:4048:A:OP1	2.22	0.57
4:9:107:A:H2'	4:9:108:G:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:165:VAL:HG13	9:E:180:GLY:N	2.19	0.57
1:5:2647:A:H62	1:5:2686:G:H8	1.52	0.57
1:5:4942:C:H4'	1:5:4943:A:OP1	2.03	0.57
34:e:67:LYS:O	34:e:75:ARG:NH1	2.37	0.57
3:8:37:A:OP2	37:h:89:ARG:NH1	2.35	0.57
54:II:155:ASN:O	57:LL:21:LYS:NZ	2.33	0.57
80:11:35:A:H2'	80:11:36:U:C6	2.40	0.57
1:5:1577:G:OP1	44:p:17:ARG:NH1	2.34	0.56
1:5:4944:C:N4	35:f:58:VAL:O	2.37	0.56
4:9:71:G:N7	52:GG:170:ARG:NH2	2.49	0.56
49:DD:40:ARG:NH1	49:DD:47:GLU:OE2	2.38	0.56
1:5:4274:A:H2'	1:5:4275:G:C8	2.40	0.56
17:N:80:THR:HB	17:N:87:HIS:CB	2.34	0.56
1:5:62:A:N3	1:5:77:U:O2'	2.34	0.56
1:5:462:G:H2'	1:5:463:A:C8	2.40	0.56
1:5:4076:G:OP1	10:G:126:ARG:NH1	2.33	0.56
1:5:4260:U:H2'	1:5:4261:C:C6	2.40	0.56
78:gg:168:CYS:HB2	78:gg:195:LEU:HD13	1.86	0.56
1:5:3635:A:H61	44:p:18:TYR:HA	1.71	0.56
11:H:23:ARG:NH1	11:H:39:ASN:O	2.39	0.56
4:9:744:G:N2	4:9:797:C:O2	2.32	0.56
37:h:87:LYS:NZ	81:j:80:GLU:OE2	2.24	0.56
1:5:4916:G:H2'	1:5:4917:C:C6	2.41	0.56
4:9:1075:C:OP1	59:NN:107:LYS:NZ	2.35	0.56
8:D:94:ASN:HD21	8:D:204:VAL:HG21	1.68	0.56
1:5:87:A:OP2	20:Q:173:LYS:NZ	2.38	0.56
1:5:4940:C:OP1	9:E:159:ARG:NH1	2.39	0.56
17:N:80:THR:HB	17:N:87:HIS:HB3	1.88	0.56
4:9:886:A:H3'	4:9:887:U:H5''	1.88	0.56
25:V:107:ASN:HD21	25:V:111:GLU:HB3	1.70	0.56
54:II:56:ARG:HH11	54:II:56:ARG:HG3	1.71	0.56
4:9:1101:U:H2'	4:9:1102:G:C8	2.41	0.56
80:11:43:G:H2'	80:11:44:A:H8	1.70	0.56
4:9:396:U:OP2	57:LL:79:LYS:NZ	2.37	0.56
4:9:692:G:H2'	4:9:693:A:H8	1.70	0.56
63:RR:36:GLU:OE1	63:RR:47:ARG:NH1	2.38	0.56
1:5:143:C:OP2	10:G:164:LYS:NZ	2.32	0.55
1:5:4053:A:H2'	1:5:4054:C:C6	2.41	0.55
4:9:178:C:H2'	4:9:179:C:C6	2.40	0.55
4:9:1438:A:H2'	4:9:1439:A:C8	2.41	0.55
4:9:1489:A:H4'	4:9:1490:G:OP2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:OO:65:ASP:OD1	60:OO:65:ASP:N	2.39	0.55
1:5:691:C:H2'	1:5:692:A:H8	1.68	0.55
1:5:1406:G:H2'	1:5:1406(A):G:C8	2.41	0.55
1:5:4303:C:H2'	1:5:4305:G:H8	1.72	0.55
1:5:1402:C:H2'	1:5:1403:G:H8	1.72	0.55
1:5:4458:C:H2'	1:5:4459:U:C6	2.41	0.55
66:UU:56:MET:HG3	66:UU:86:LYS:HE3	1.87	0.55
1:5:1339:U:H2'	1:5:1340:C:C6	2.42	0.55
4:9:1565:C:OP2	65:TT:101:ARG:NH1	2.39	0.55
68:WW:11:LEU:HD22	68:WW:72:CYS:SG	2.46	0.55
80:11:63:A:H2'	80:11:64:U:C6	2.41	0.55
1:5:1391:A:P	20:Q:181:ARG:HH22	2.29	0.55
1:5:2632:U:H2'	1:5:2633:U:C6	2.42	0.55
4:9:317:C:OP2	52:GG:183:ARG:NH2	2.34	0.55
78:gg:107:ASP:OD2	78:gg:125:ARG:NH1	2.38	0.55
1:5:1238:A:O2'	1:5:1239:C:OP1	2.23	0.55
4:9:695:C:H2'	4:9:696:G:C8	2.41	0.55
16:M:89:THR:HG22	16:M:91:TRP:H	1.71	0.55
1:5:1398:A:H61	1:5:1419:G:H2'	1.71	0.55
1:5:1963:C:H5''	1:5:1964:A:OP2	2.07	0.55
38:i:68:ARG:NH1	38:i:71:LYS:HD3	2.21	0.55
50:EE:100:ARG:HH21	50:EE:118:GLU:HG2	1.72	0.55
1:5:1237:C:H4'	1:5:1238:A:O5'	2.05	0.55
1:5:1967:A:C6	1:5:2021:G:C6	2.94	0.55
1:5:3932:U:H2'	1:5:3933:G:C8	2.42	0.55
1:5:4546:A:N7	5:A:215:ASN:ND2	2.55	0.55
4:9:126:G:OP2	52:GG:195:LYS:NZ	2.38	0.55
17:N:84:PRO:HA	17:N:87:HIS:NE2	2.22	0.54
80:13:62:C:H2'	80:13:63:A:H8	1.72	0.54
2:7:40:U:O2	13:J:75:ARG:NH1	2.40	0.54
4:9:907:G:H2'	4:9:908:A:C8	2.42	0.54
49:DD:28:GLU:OE1	56:KK:61:GLN:NE2	2.28	0.54
69:XX:63:ASN:ND2	69:XX:114:ASP:OD1	2.37	0.54
4:9:1736:G:H2'	4:9:1737:G:H8	1.73	0.54
7:C:335:MET:O	7:C:339:THR:HG23	2.07	0.54
13:J:151:ILE:HD11	13:J:156:ARG:HG2	1.88	0.54
9:E:164:ARG:NH2	9:E:276:SER:OG	2.41	0.54
30:a:72:THR:HG22	30:a:110:LYS:HB3	1.89	0.54
1:5:1075:G:H22	1:5:1235:G:N2	2.06	0.54
1:5:1509:C:H5''	30:a:2:PRO:HD2	1.89	0.54
1:5:2566:G:H2'	1:5:2567:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3961:G:C6	1:5:3963:A:H2'	2.42	0.54
3:8:52:A:H62	40:l:27:ILE:HD13	1.71	0.54
12:I:14:ASN:O	12:I:128:ARG:NH2	2.31	0.54
58:MM:75:ASN:HB3	58:MM:128:PHE:CZ	2.43	0.54
1:5:1188:C:H2'	1:5:1189:G:H8	1.72	0.54
1:5:1195:G:H2'	1:5:1196:G:C8	2.43	0.54
1:5:1973:G:H2'	1:5:1974:U:C5	2.43	0.54
1:5:2755:A:P	29:Z:65:ARG:HH22	2.31	0.54
1:5:4925:U:H4'	1:5:4926:C:H5''	1.89	0.54
4:9:102:A:OP2	54:II:19:LYS:NZ	2.35	0.54
37:h:14:LYS:HE2	37:h:18:LEU:HD11	1.90	0.54
1:5:270:U:H2'	1:5:271:C:C6	2.43	0.53
1:5:1440:U:H2'	1:5:1441:C:C6	2.44	0.53
1:5:3707:U:H2'	1:5:3708:C:C6	2.43	0.53
4:9:1113:A:H2'	4:9:1114:U:C6	2.43	0.53
54:II:11:ARG:NH1	54:II:15:GLY:O	2.39	0.53
1:5:325:U:H2'	1:5:326:C:C6	2.43	0.53
1:5:2313:A:O2'	1:5:2314:G:OP1	2.23	0.53
59:NN:38:TYR:CZ	59:NN:78:LYS:HG3	2.42	0.53
1:5:753:C:H2'	1:5:754:C:H6	1.74	0.53
3:8:8:U:H2'	3:8:9:A:C8	2.44	0.53
4:9:874:G:H5'	4:9:874:G:H8	1.73	0.53
4:9:903:A:H2'	4:9:904:A:C8	2.43	0.53
44:p:84:ARG:NH1	44:p:88:GLU:OE2	2.40	0.53
1:5:519:C:H2'	1:5:520:U:C6	2.44	0.53
1:5:5068:G:N2	1:5:5069:U:O4	2.33	0.53
4:9:693:A:H2'	4:9:694:G:H8	1.73	0.53
4:9:1410:C:H2'	4:9:1411:G:C8	2.43	0.53
77:ff:100:LEU:HG	77:ff:103:LEU:HD13	1.90	0.53
1:5:100:C:H2'	1:5:101:A:H8	1.72	0.53
1:5:672:C:H2'	1:5:673:C:C6	2.44	0.53
4:9:24:C:O2'	4:9:25:A:OP1	2.26	0.53
1:5:982:U:H3	1:5:1273:G:H1	1.56	0.53
1:5:2431:A:OP1	40:l:41:ARG:NH1	2.42	0.53
1:5:3732:A:H2'	1:5:3733:A:C8	2.43	0.53
1:5:4578:G:H2'	1:5:4579:U:C6	2.43	0.53
4:9:1182:A:C5	4:9:1183:A:H1'	2.44	0.53
4:9:1834:A:H2	4:9:1837:G:N1	2.02	0.53
71:ZZ:100:VAL:HG21	71:ZZ:110:THR:HG23	1.91	0.53
1:5:257:C:H2'	1:5:258:G:C8	2.44	0.53
1:5:1786:A:H2'	1:5:1789:C:C5	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4537:C:H2'	1:5:4538:G:C8	2.44	0.53
11:H:173:ARG:HD2	41:m:101:VAL:HG13	1.90	0.53
4:9:1628:C:H2'	4:9:1629:C:C6	2.44	0.53
58:MM:68:LEU:HD13	77:ff:114:ILE:HD13	1.91	0.53
1:5:4108:G:H2'	1:5:4109:G:C8	2.43	0.53
62:QQ:9:SER:HB2	62:QQ:24:HIS:HE1	1.74	0.53
74:cc:18:LEU:HD12	74:cc:29:GLN:HG2	1.90	0.53
80:11:69:U:H2'	80:11:70:G:H8	1.73	0.53
1:5:1985:G:H1'	1:5:2003:G:H2'	1.90	0.52
14:K:93:ARG:NH1	14:K:95:ARG:O	2.42	0.52
31:b:101:HIS:CD2	31:b:104:LEU:H	2.28	0.52
1:5:2016:C:C2	1:5:2017:A:C8	2.97	0.52
1:5:4591:U:H2'	1:5:4592:C:C6	2.44	0.52
51:FF:44:LYS:HE3	51:FF:45:TYR:CZ	2.44	0.52
1:5:1308:C:H2'	1:5:1309:C:C6	2.44	0.52
4:9:1252:C:N4	62:QQ:146:ARG:OXT	2.41	0.52
28:Y:31:SER:HA	28:Y:48:PRO:HA	1.90	0.52
1:5:2033:A:P	12:I:162:ARG:HH22	2.31	0.52
1:5:4395:U:H6	1:5:4395:U:H5'	1.74	0.52
1:5:5053:U:H5'	1:5:5054:C:C5	2.44	0.52
6:B:261:ARG:HB2	18:O:64:THR:HG21	1.92	0.52
68:WW:69:LEU:HD21	68:WW:72:CYS:HB2	1.89	0.52
1:5:1846:G:H2'	1:5:1847:C:C6	2.44	0.52
1:5:2787:A:N3	1:5:2787:A:H2'	2.24	0.52
1:5:3723:A:H2'	1:5:3724:A:C8	2.45	0.52
80:13:23:C:H2'	80:13:24:G:H8	1.74	0.52
3:8:8:U:H2'	3:8:9:A:H8	1.75	0.52
8:D:94:ASN:ND2	8:D:204:VAL:HG21	2.24	0.52
1:5:2570:U:H2'	1:5:2571:C:C6	2.44	0.52
1:5:4899:G:H22	1:5:4921:C:H2'	1.74	0.52
2:7:7:G:OP1	8:D:33:ARG:NE	2.36	0.52
1:5:178:C:H2'	1:5:179:G:C8	2.45	0.52
4:9:5:U:H2'	4:9:6:G:H8	1.75	0.52
80:13:47:U:H3'	80:13:48:C:H5'	1.92	0.52
1:5:3923:A:H2'	1:5:3924:C:C6	2.45	0.52
1:5:4065:G:H2'	1:5:4066:U:C6	2.45	0.52
18:O:37:ARG:HD2	18:O:108:ILE:HD11	1.91	0.52
21:R:105:LEU:HD22	21:R:135:LYS:HG3	1.91	0.52
1:5:1364:U:OP2	15:L:36:ARG:NH2	2.38	0.52
4:9:1013:U:OP1	4:9:1129:G:O2'	2.25	0.52
4:9:1698:C:O2'	4:9:1699:A:OP1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:339:THR:HG22	7:C:342:ARG:HH22	1.75	0.52
1:5:456:C:H2'	1:5:457:G:H8	1.74	0.51
2:7:55:A:H4'	13:J:155:HIS:HB2	1.92	0.51
52:GG:67:VAL:HB	52:GG:99:GLY:HA2	1.92	0.51
80:13:23:C:H2'	80:13:24:G:C8	2.45	0.51
80:11:42:A:H2'	80:11:43:G:C8	2.44	0.51
4:9:465:A:H5'	4:9:465:A:H8	1.75	0.51
6:B:381:THR:HG23	6:B:384:GLU:H	1.74	0.51
10:G:136:PHE:HA	10:G:236:ILE:HD13	1.92	0.51
27:X:92:ASP:C	27:X:93:ASN:HD22	2.18	0.51
1:5:1080:C:H2'	1:5:1081:C:C6	2.46	0.51
1:5:4638:U:H2'	1:5:4639:G:N3	2.25	0.51
1:5:4746:C:H2'	1:5:4747:C:C6	2.46	0.51
1:5:4944:C:H4'	1:5:4944:C:OP1	2.10	0.51
3:8:60:G:OP1	27:X:70:LYS:NZ	2.43	0.51
4:9:804:U:H2'	4:9:805:U:C6	2.44	0.51
26:W:105:ARG:NH1	52:GG:150:GLU:OE1	2.43	0.51
34:e:10:PRO:HD2	34:e:69:MET:HE1	1.91	0.51
34:e:84:GLU:CD	45:r:20:ARG:HH22	2.18	0.51
80:11:53:G:H2'	80:11:54:A:H8	1.75	0.51
1:5:1472:C:H2'	1:5:1473:U:C6	2.46	0.51
1:5:2730:U:H2'	1:5:2731:C:C6	2.45	0.51
1:5:4994:G:H2'	1:5:4995:U:C6	2.45	0.51
4:9:533:A:H2'	4:9:534:G:H8	1.74	0.51
4:9:1286:G:OP2	77:ff:99:LYS:HD3	2.10	0.51
4:9:1351:G:O2'	4:9:1378:A:N1	2.43	0.51
4:9:1653:U:H2'	4:9:1654:G:C8	2.46	0.51
48:CC:209:VAL:HG21	48:CC:233:LEU:HD22	1.92	0.51
49:DD:193:ASP:OD2	49:DD:198:ILE:N	2.39	0.51
59:NN:55:ARG:HG2	59:NN:55:ARG:HH11	1.75	0.51
1:5:230:G:OP1	28:Y:15:ARG:NH1	2.39	0.51
1:5:1617:G:H1'	1:5:2513:A:N6	2.25	0.51
1:5:3911:C:H2'	1:5:3912:U:H6	1.74	0.51
4:9:841:G:H2'	4:9:842:C:H4'	1.92	0.51
69:XX:98:ASP:OD2	69:XX:140:ARG:NH1	2.39	0.51
4:9:791:C:H2'	4:9:792:C:C6	2.45	0.51
4:9:986:G:C8	60:OO:137:SER:O	2.64	0.51
36:g:69:LYS:HG2	36:g:73:HIS:CD2	2.45	0.51
1:5:753:C:H2'	1:5:754:C:C6	2.46	0.51
1:5:2539:C:H2'	1:5:2540:C:C6	2.44	0.51
4:9:190:G:H1'	4:9:209:A:N6	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1305:C:OP2	77:ff:93:HIS:ND1	2.39	0.51
47:BB:129:THR:OG1	47:BB:131:ASP:OD1	2.24	0.51
1:5:2440:U:O2'	1:5:2441:C:OP1	2.28	0.51
1:5:3597:G:OP2	21:R:114:LYS:NZ	2.41	0.51
1:5:4114:C:H3'	1:5:4115:G:N2	2.25	0.51
28:Y:115:ARG:HG3	28:Y:115:ARG:HH11	1.75	0.51
48:CC:169:TYR:OH	48:CC:175:GLY:O	2.28	0.51
1:5:134:G:C8	1:5:134:G:H5'	2.45	0.51
1:5:1563:A:N6	4:9:1028:A:N1	2.59	0.51
1:5:2293:U:H2'	1:5:2294:G:C8	2.46	0.51
4:9:1865:C:OP2	72:aa:5:ARG:NH1	2.42	0.51
1:5:63:G:P	17:N:169:ARG:HH22	2.34	0.51
1:5:1320:U:O2'	1:5:1891:A:N1	2.31	0.51
78:gg:5:MET:HG2	78:gg:312:VAL:HG12	1.93	0.51
1:5:1402:C:H2'	1:5:1403:G:C8	2.46	0.50
39:k:8:ILE:HD11	39:k:56:LEU:HD13	1.93	0.50
68:WW:90:GLN:HG3	68:WW:94:LEU:HD12	1.93	0.50
1:5:1353:G:N7	20:Q:104:ARG:NH2	2.57	0.50
4:9:465:A:H5'	4:9:465:A:C8	2.45	0.50
50:EE:259:LYS:O	50:EE:263:GLY:N	2.43	0.50
62:QQ:16:LYS:NZ	62:QQ:123:ASP:OD2	2.44	0.50
1:5:424:U:H2'	1:5:425:U:H6	1.76	0.50
2:7:32:A:O2'	2:7:41:G:N7	2.40	0.50
4:9:1101:U:H2'	4:9:1102:G:H8	1.77	0.50
1:5:1080:C:H2'	1:5:1081:C:H6	1.76	0.50
1:5:1177:U:H2'	1:5:1178:G:H8	1.77	0.50
4:9:1458:G:OP1	78:gg:279:SER:OG	2.29	0.50
48:CC:169:TYR:CG	48:CC:173:LYS:HA	2.47	0.50
4:9:416:U:H2'	4:9:417:C:O4'	2.12	0.50
47:BB:107:ARG:NH1	60:OO:133:THR:O	2.29	0.50
50:EE:212:ASP:OD1	50:EE:213:ALA:N	2.45	0.50
1:5:1802:A:H5''	1:5:1803:G:H5'	1.94	0.50
1:5:4039:G:H5'	1:5:4042:G:O6	2.11	0.50
1:5:4751:G:N1	1:5:4948:C:H5	2.09	0.50
78:gg:191:HIS:CD2	78:gg:195:LEU:HD21	2.47	0.50
1:5:989:U:H2'	1:5:990:C:C6	2.47	0.50
1:5:1930:U:OP2	18:O:49:ARG:HD2	2.11	0.50
1:5:2431:A:P	40:I:41:ARG:HH12	2.34	0.50
1:5:2837:U:OP1	6:B:249:ARG:NH1	2.41	0.50
1:5:3868:G:H22	1:5:3900:G:H1'	1.76	0.50
4:9:5:U:H2'	4:9:6:G:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:116:ASP:OD2	21:R:149:LYS:NZ	2.44	0.50
46:AA:44:ASP:HA	63:RR:128:PHE:HB3	1.93	0.50
1:5:2474:G:N2	1:5:2502:A:H2'	2.27	0.50
1:5:4188:U:H2'	1:5:4189:U:C6	2.47	0.50
4:9:1277:C:H2'	4:9:1278:A:H8	1.76	0.50
46:AA:73:ASP:HB3	46:AA:120:ARG:HB2	1.94	0.50
61:PP:22:LEU:HA	61:PP:25:LEU:HD12	1.93	0.50
1:5:956:A:H8	1:5:957:G:C8	2.29	0.50
1:5:2504:C:O2'	1:5:2505:C:O2	2.22	0.50
1:5:2900:U:H2'	1:5:2901:G:C8	2.46	0.50
1:5:4233:A:C8	1:5:4235:G:C8	3.00	0.50
4:9:1412:C:H2'	4:9:1413:G:H8	1.77	0.50
4:9:1524:G:OP2	64:SS:141:ARG:NH2	2.27	0.50
29:Z:33:THR:HG22	29:Z:35:ASP:H	1.77	0.50
45:r:105:ASP:OD1	45:r:105:ASP:N	2.44	0.50
53:HH:18:GLU:O	53:HH:21:SER:OG	2.28	0.50
61:PP:75:VAL:HG22	61:PP:93:MET:HB3	1.94	0.50
78:gg:87:LEU:HB3	78:gg:101:PHE:HB2	1.93	0.50
4:9:379:C:H5'	54:II:33:ALA:HA	1.93	0.49
4:9:626:G:N3	4:9:626:G:H2'	2.27	0.49
1:5:1088:C:H2'	1:5:1089:G:H8	1.77	0.49
7:C:29:LYS:HB2	7:C:267:TRP:HH2	1.77	0.49
1:5:180:C:H2'	1:5:181:C:C6	2.47	0.49
1:5:516:C:H2'	1:5:517:C:C6	2.48	0.49
1:5:4049:U:H3'	1:5:4050:A:H8	1.77	0.49
22:S:3:ALA:O	22:S:111:ARG:NH2	2.43	0.49
34:e:35:TRP:CZ2	34:e:56:PRO:HD2	2.47	0.49
47:BB:73:ASP:OD1	60:OO:128:ARG:NH1	2.45	0.49
1:5:442:G:OP1	35:f:68:ARG:NH1	2.35	0.49
1:5:1475:G:H2'	1:5:1476:C:C6	2.48	0.49
2:7:3:C:H2'	2:7:4:U:H6	1.77	0.49
40:l:24:PRO:HD2	40:l:27:ILE:HD12	1.94	0.49
46:AA:134:LEU:HD13	46:AA:144:THR:HG21	1.95	0.49
1:5:3911:C:H2'	1:5:3912:U:C6	2.48	0.49
1:5:4088:C:OP1	5:A:37:ARG:NH1	2.45	0.49
3:8:93:C:OP1	81:j:76:HIS:HE1	1.96	0.49
29:Z:136:PHE:O	36:g:78:TYR:OH	2.25	0.49
1:5:3611:A:H2	1:5:5016:A:H8	1.60	0.49
1:5:3905:A:O3'	7:C:70:GLY:HA2	2.12	0.49
1:5:3948:C:H5''	1:5:3949:A:OP2	2.13	0.49
1:5:4068:U:H2'	1:5:4069:U:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:217:ILE:O	10:G:221:VAL:HG13	2.12	0.49
1:5:1483:C:H5''	1:5:1483:C:O2	2.13	0.49
4:9:1329:U:O2'	4:9:1332:A:OP2	2.26	0.49
1:5:481(A):C:H2'	1:5:481(A):C:O2	2.12	0.49
4:9:874:G:H5'	4:9:874:G:C8	2.48	0.49
4:9:1292:C:O2	77:ff:138:ARG:NE	2.34	0.49
4:9:1839:U:H1'	4:9:1863:A:H2	1.78	0.49
21:R:105:LEU:HD23	21:R:138:LEU:HD23	1.95	0.49
64:SS:89:ASP:HB3	64:SS:92:ASP:O	2.12	0.49
80:13:16:G:OP2	80:13:17:C:N4	2.46	0.49
4:9:200:G:H2'	4:9:201:C:C6	2.47	0.49
4:9:562:U:H2'	4:9:563:G:C8	2.47	0.49
4:9:1692:U:H2'	4:9:1693:G:C8	2.48	0.49
21:R:39:GLN:OE1	21:R:42:ARG:NH1	2.46	0.49
1:5:2553:A:H2	1:5:2765:A:H62	1.60	0.49
1:5:4274:A:H2'	1:5:4275:G:H8	1.77	0.49
4:9:1547:C:H5'	4:9:1548:G:OP2	2.13	0.49
78:gg:107:ASP:OD1	78:gg:107:ASP:N	2.46	0.49
1:5:699:C:H2'	1:5:700:G:H8	1.78	0.48
1:5:2404:A:OP2	40:l:2:SER:OG	2.22	0.48
4:9:910:G:OP2	21:R:173:ARG:NH1	2.45	0.48
4:9:1277:C:H2'	4:9:1278:A:C8	2.48	0.48
48:CC:168:GLY:N	48:CC:179:THR:O	2.39	0.48
1:5:1246:G:H2'	1:5:1247:U:C6	2.48	0.48
4:9:831:G:H1	4:9:844:U:H3	1.61	0.48
19:P:94:MET:HE1	19:P:146:ILE:HB	1.95	0.48
29:Z:100:VAL:HG13	29:Z:107:LYS:HA	1.95	0.48
48:CC:272:HIS:CE1	48:CC:276:THR:HG21	2.48	0.48
4:9:455:A:H2'	4:9:456:C:C6	2.49	0.48
4:9:1397:U:H2'	4:9:1397:U:O2	2.14	0.48
47:BB:174:ARG:NH1	47:BB:175:GLU:OE2	2.45	0.48
1:5:135:G:O2'	1:5:136:C:OP1	2.27	0.48
1:5:4250:G:OP1	13:J:98:ASN:ND2	2.45	0.48
80:13:74:C:O2'	80:13:75:C:OP1	2.25	0.48
80:11:69:U:H2'	80:11:70:G:C8	2.48	0.48
1:5:2404:A:H61	1:5:2787:A:N6	2.11	0.48
4:9:368:U:O2'	4:9:369:C:OP1	2.30	0.48
4:9:942:G:H2'	4:9:943:U:C6	2.48	0.48
47:BB:175:GLU:OE1	47:BB:187:LYS:NZ	2.44	0.48
1:5:1502:G:H5''	1:5:1502:G:H8	1.78	0.48
1:5:3599:A:H2'	1:5:3600:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3968:U:O2'	1:5:3969:G:OP1	2.29	0.48
1:5:4114:C:H3'	1:5:4115:G:H21	1.79	0.48
4:9:1553:C:H2'	4:9:1554:C:C5	2.49	0.48
39:k:37:ARG:HD3	39:k:38:CYS:O	2.14	0.48
1:5:388:A:H1'	1:5:403:G:N2	2.29	0.48
3:8:94:G:OP2	81:j:72:ARG:NH1	2.46	0.48
4:9:1651:A:H1'	51:FF:83:ASN:HD22	1.79	0.48
7:C:339:THR:HG22	7:C:342:ARG:NH2	2.29	0.48
78:gg:31:ILE:O	78:gg:43:TRP:N	2.42	0.48
1:5:2487:G:O6	1:5:2489:C:O2'	2.20	0.48
1:5:3958:G:H2'	1:5:3959:U:C5	2.48	0.48
1:5:4305:G:H22	23:T:87:LYS:NZ	2.12	0.48
9:E:69:ALA:HA	9:E:71:TYR:CE2	2.48	0.48
50:EE:124:CYS:HB3	50:EE:141:THR:HB	1.95	0.48
80:13:18:G:H1'	80:13:57:G:N2	2.29	0.48
1:5:40:G:N2	1:5:4380:A:H62	2.12	0.48
1:5:2809:G:O2'	1:5:4644:G:OP1	2.28	0.48
1:5:4897:G:C6	1:5:4898:G:C6	3.02	0.48
4:9:333:G:OP2	52:GG:190:ARG:NH1	2.45	0.48
4:9:669:A:H2'	4:9:670:A:C8	2.49	0.48
1:5:497:G:O6	1:5:658:C:N4	2.46	0.48
1:5:4066:U:H2'	1:5:4067:U:H6	1.79	0.48
4:9:527:C:H2'	4:9:528:A:H8	1.79	0.48
4:9:830:A:OP2	4:9:846:G:N2	2.47	0.48
4:9:1863:A:OP2	72:aa:4:LYS:NZ	2.41	0.48
6:B:222:VAL:O	6:B:343:ARG:NH1	2.46	0.48
17:N:84:PRO:HA	17:N:87:HIS:CD2	2.48	0.48
58:MM:85:LEU:HD21	58:MM:109:VAL:HG23	1.94	0.48
1:5:181:C:H2'	1:5:182:G:C8	2.48	0.47
1:5:983:C:H2'	1:5:984:C:C6	2.48	0.47
47:BB:153:THR:HB	47:BB:155:TYR:CE2	2.49	0.47
64:SS:26:ILE:HD11	64:SS:54:LYS:HB2	1.96	0.47
1:5:223:G:H4'	1:5:225:G:N7	2.29	0.47
1:5:264:C:H5''	1:5:265:C:OP2	2.14	0.47
4:9:164:A:H3'	4:9:165:G:H21	1.79	0.47
41:m:89:CYS:O	41:m:92:THR:HG23	2.13	0.47
57:LL:101:ARG:HB2	69:XX:7:LEU:O	2.13	0.47
80:13:58:A:H1'	80:13:60:A:N7	2.29	0.47
1:5:1444:G:H21	1:5:2110:G:H1	1.61	0.47
1:5:3873:G:H2'	1:5:3874:G:C8	2.48	0.47
1:5:3965:A:N1	1:5:4047:A:H2'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4266:G:N3	1:5:4266:G:H2'	2.29	0.47
1:5:4562:C:H2'	1:5:4563:U:C6	2.49	0.47
1:5:4870:G:H2'	16:M:91:TRP:CZ2	2.48	0.47
4:9:945:U:H2'	4:9:946:U:C6	2.49	0.47
4:9:1253:A:H4'	4:9:1254:C:H5''	1.96	0.47
17:N:155:VAL:O	17:N:162:ARG:NH2	2.48	0.47
72:aa:44:ILE:HD12	72:aa:65:PRO:HG2	1.96	0.47
1:5:1190:C:H2'	1:5:1191:C:C6	2.49	0.47
1:5:4301:U:H4'	23:T:54:HIS:CD2	2.49	0.47
4:9:958:G:H2'	4:9:959:G:C8	2.50	0.47
4:9:1597:C:H4'	4:9:1603:G:O6	2.14	0.47
21:R:44:LEU:HD22	21:R:49:LEU:HD12	1.96	0.47
37:h:96:ASN:HB2	37:h:99:GLU:H	1.79	0.47
1:5:465:G:H2'	1:5:466:A:C8	2.49	0.47
1:5:1177:U:H2'	1:5:1178:G:C8	2.50	0.47
1:5:2407:G:O6	40:l:2:SER:N	2.47	0.47
1:5:4572:U:HO2'	1:5:4573:G:H8	1.59	0.47
4:9:1305:C:H2'	4:9:1306:U:C6	2.49	0.47
4:9:1462:U:H2'	4:9:1464:C:C5	2.50	0.47
18:O:81:TRP:HB2	18:O:104:VAL:HG21	1.95	0.47
19:P:40:HIS:HE1	19:P:42:ARG:HG2	1.79	0.47
47:BB:28:LYS:HB3	47:BB:48:LEU:HD11	1.96	0.47
1:5:4300:U:OP1	23:T:87:LYS:NZ	2.46	0.47
4:9:640:A:H2'	4:9:641:A:C8	2.50	0.47
4:9:1610:G:OP2	64:SS:132:ARG:NH1	2.43	0.47
14:K:156:ARG:NH1	14:K:247:ASN:OXT	2.46	0.47
53:HH:105:THR:HG22	53:HH:107:LYS:H	1.80	0.47
1:5:708:G:OP1	35:f:89:ARG:NH2	2.48	0.47
1:5:1769:G:H2'	1:5:1770:A:C8	2.49	0.47
1:5:2899:C:P	21:R:108:ARG:HH22	2.38	0.47
1:5:4573:G:H2'	1:5:4574:U:C6	2.49	0.47
4:9:12:U:H2'	4:9:13:C:C6	2.49	0.47
4:9:682:U:OP2	69:XX:8:ARG:NH1	2.42	0.47
13:J:13:ARG:O	13:J:136:ARG:NH1	2.39	0.47
68:WW:30:CYS:SG	68:WW:31:SER:N	2.87	0.47
1:5:1437:C:N3	31:b:106:ARG:HD2	2.30	0.47
1:5:1444:G:N2	1:5:1445:U:O4	2.47	0.47
1:5:4520:G:H2'	1:5:4521:U:O4'	2.14	0.47
2:7:4:U:H2'	2:7:5:A:H8	1.79	0.47
4:9:691:G:H2'	4:9:692:G:H8	1.80	0.47
4:9:1619:A:P	61:PP:47:ARG:HH11	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:981:C:P	9:E:48:ARG:HH22	2.38	0.47
1:5:1982:G:H5'	1:5:1982:G:C8	2.49	0.47
1:5:2079:G:H2'	1:5:2080:U:C6	2.50	0.47
1:5:3598:C:H2'	1:5:3599:A:C8	2.49	0.47
4:9:952:G:OP1	47:BB:56:LYS:NZ	2.31	0.47
8:D:146:LEU:HD21	8:D:159:VAL:HG12	1.96	0.47
61:PP:37:TYR:OH	61:PP:87:PRO:HD3	2.14	0.47
62:QQ:34:VAL:HB	62:QQ:42:ILE:HD11	1.97	0.47
4:9:1597:C:H4'	4:9:1603:G:C6	2.50	0.47
4:9:1845:A:H2'	4:9:1846:G:C8	2.50	0.47
44:p:38:THR:HA	44:p:45:THR:HA	1.97	0.47
1:5:981:C:OP2	9:E:48:ARG:NH2	2.44	0.46
1:5:1554:A:OP2	44:p:4:ARG:NH1	2.42	0.46
3:8:86:U:O2'	3:8:87:G:OP1	2.32	0.46
7:C:218:VAL:HA	7:C:229:LEU:CD1	2.45	0.46
46:AA:36:GLN:O	46:AA:53:ARG:NH1	2.48	0.46
1:5:179:G:H2'	1:5:180:C:C6	2.50	0.46
1:5:433:A:C2	1:5:3867:A:H4'	2.50	0.46
1:5:3959:U:O2'	1:5:3960:A:C8	2.65	0.46
4:9:1485:U:OP1	49:DD:151:LYS:NZ	2.47	0.46
61:PP:37:TYR:HB3	61:PP:41:GLN:HB2	1.97	0.46
80:11:66:C:H2'	80:11:67:U:H6	1.81	0.46
1:5:456:C:H2'	1:5:457:G:C8	2.50	0.46
1:5:1198:G:N2	1:5:1199:G:O6	2.48	0.46
1:5:2335:C:H2'	1:5:2336:G:H8	1.81	0.46
1:5:4064:C:H2'	1:5:4065:G:C8	2.50	0.46
1:5:4457:U:H1'	6:B:252:ALA:HB3	1.98	0.46
3:8:19:C:H2'	3:8:20:A:C8	2.50	0.46
10:G:212:HIS:CE1	10:G:213:ASP:HB3	2.51	0.46
62:QQ:44:PRO:HD2	62:QQ:81:ILE:HD11	1.97	0.46
1:5:1237:C:O2'	14:K:47:LYS:HE3	2.15	0.46
1:5:3973:G:O6	1:5:4039:G:N1	2.49	0.46
1:5:4862:G:H2'	1:5:4863:G:C8	2.51	0.46
4:9:501:C:H2'	4:9:502:C:H5''	1.96	0.46
33:d:36:VAL:HG21	33:d:44:ARG:HG2	1.96	0.46
1:5:100:C:H2'	1:5:101:A:C8	2.51	0.46
1:5:162:A:H2'	1:5:163:A:C8	2.50	0.46
1:5:175:C:H2'	1:5:176:G:H8	1.80	0.46
1:5:1211:G:O2'	1:5:1212:G:OP1	2.26	0.46
1:5:2396:A:N6	1:5:2814:C:O2	2.48	0.46
1:5:4148:C:OP1	29:Z:59:LYS:NZ	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4239:A:H2'	1:5:4240:G:C8	2.51	0.46
1:5:4548:A:H4'	1:5:4549:G:O5'	2.16	0.46
4:9:146:G:O2'	4:9:147:A:O5'	2.32	0.46
1:5:490:C:H2'	1:5:491:G:C8	2.51	0.46
1:5:2486:G:H2'	1:5:2487:G:C8	2.51	0.46
1:5:2634:C:H2'	1:5:2635:U:C6	2.50	0.46
2:7:3:C:H2'	2:7:4:U:C6	2.50	0.46
50:EE:64:ILE:HG22	50:EE:70:ILE:HD11	1.97	0.46
1:5:1534:A:C8	81:j:15:THR:HG23	2.51	0.46
1:5:4960:G:H2'	1:5:4961:G:H8	1.79	0.46
4:9:552:G:H2'	4:9:553:U:C6	2.51	0.46
4:9:1664:A:H4'	4:9:1665:G:OP1	2.16	0.46
4:9:1674:G:OP1	51:FF:51:HIS:NE2	2.42	0.46
12:I:38:ARG:HH22	12:I:45:GLU:CD	2.24	0.46
80:13:4:C:H2'	80:13:5:A:H8	1.81	0.46
80:13:64:U:H2'	80:13:65:C:H6	1.80	0.46
1:5:152:U:P	17:N:49:ARG:HH12	2.39	0.46
1:5:1772:C:H2'	1:5:1773:U:O4'	2.15	0.46
1:5:2396:A:C6	1:5:2814:C:O2	2.68	0.46
3:8:62:A:H4'	3:8:63:U:O5'	2.16	0.46
4:9:1462:U:H2'	4:9:1464:C:C4	2.51	0.46
4:9:1482:C:OP1	75:dd:54:LYS:NZ	2.47	0.46
50:EE:45:ILE:HG13	50:EE:61:VAL:HG21	1.97	0.46
66:UU:64:THR:HA	66:UU:78:ASP:O	2.16	0.46
1:5:1307:A:H2'	1:5:1308:C:C6	2.51	0.46
1:5:1771:U:H2'	1:5:1772:C:C6	2.51	0.46
1:5:2744:A:H2'	1:5:2745:A:C8	2.51	0.46
1:5:4635:A:H2	1:5:4663:G:H21	1.64	0.46
4:9:1227:G:C2	4:9:1228:A:C8	3.03	0.46
11:H:41:ILE:HG22	11:H:43:VAL:HG13	1.97	0.46
20:Q:14:ARG:HH11	20:Q:14:ARG:HB3	1.80	0.46
80:13:4:C:H2'	80:13:5:A:C8	2.50	0.46
1:5:1457:G:O2'	1:5:1458:C:H5''	2.16	0.46
1:5:3865:A:H61	1:5:3881:G:H1	1.63	0.46
1:5:4572:U:O2'	1:5:4573:G:O4'	2.33	0.46
3:8:52:A:N6	40:l:27:ILE:HD13	2.31	0.46
4:9:674:C:H2'	4:9:675:U:C6	2.51	0.46
13:J:95:ARG:HH21	13:J:177:GLY:C	2.24	0.46
25:V:99:GLU:HB3	26:W:24:THR:HG23	1.98	0.46
36:g:15:THR:HG22	36:g:16:ALA:H	1.81	0.46
80:11:36:U:H2'	80:11:37:A:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:326:C:OP2	38:i:28:ARG:NH2	2.41	0.45
1:5:1975:G:H22	1:5:1983:A:P	2.37	0.45
1:5:3947:A:H2'	1:5:3948:C:C6	2.51	0.45
4:9:730:C:H2'	4:9:731:G:C8	2.51	0.45
8:D:94:ASN:OD1	8:D:95:TYR:N	2.49	0.45
65:TT:75:MET:HA	65:TT:78:ILE:HG22	1.98	0.45
79:10:23:A:C8	79:10:23:A:H5''	2.51	0.45
1:5:664:G:H2'	1:5:665:C:C6	2.51	0.45
1:5:1766:A:C8	1:5:1767:A:C2	3.04	0.45
1:5:2276:A:H2'	1:5:2277:C:O4'	2.16	0.45
1:5:2422:C:P	19:P:127:ARG:HH22	2.34	0.45
1:5:4960:G:H2'	1:5:4961:G:C8	2.51	0.45
4:9:72:C:O2'	4:9:74:G:OP2	2.33	0.45
4:9:841:G:H2'	4:9:842:C:C4'	2.46	0.45
4:9:1353:A:OP1	46:AA:139:TYR:OH	2.25	0.45
4:9:1656:G:H2'	4:9:1657:G:H8	1.80	0.45
80:13:64:U:H2'	80:13:65:C:C6	2.51	0.45
1:5:52:G:H4'	1:5:1529:G:H4'	1.97	0.45
1:5:4065:G:H2'	1:5:4066:U:H6	1.80	0.45
4:9:151:C:H2'	4:9:152:U:H6	1.80	0.45
4:9:429:C:O2'	4:9:811:A:N1	2.49	0.45
4:9:898:U:H2'	4:9:899:U:C6	2.51	0.45
4:9:1491:G:H2'	4:9:1492:U:C6	2.52	0.45
9:E:157:THR:HG23	9:E:158:GLY:N	2.32	0.45
71:ZZ:79:ILE:HB	71:ZZ:83:LEU:HD23	1.97	0.45
78:gg:191:HIS:HA	78:gg:217:MET:HE1	1.98	0.45
1:5:1604:G:H2'	1:5:1605:G:C8	2.52	0.45
1:5:2007:G:C2	1:5:2013:A:N6	2.85	0.45
1:5:2711:G:OP2	21:R:39:GLN:NE2	2.49	0.45
1:5:4927:G:H3'	1:5:4928:C:O2	2.17	0.45
1:5:223:G:H4'	1:5:225:G:C8	2.51	0.45
1:5:1304:C:H2'	1:5:1305:C:C6	2.51	0.45
1:5:2099:C:H4'	1:5:2100:G:OP2	2.16	0.45
1:5:2771:G:H2'	1:5:2772:C:O4'	2.17	0.45
3:8:75:G:OP2	28:Y:74:TYR:OH	2.28	0.45
4:9:563:G:N3	4:9:564:A:C8	2.84	0.45
18:O:10:ASP:OD1	18:O:37:ARG:HD3	2.16	0.45
52:GG:7:PHE:CZ	52:GG:9:ALA:HB3	2.51	0.45
4:9:1693:G:N2	4:9:1834:A:C8	2.82	0.45
24:U:80:LYS:HG2	24:U:110:TYR:CE2	2.51	0.45
1:5:3908:A:N7	1:5:4449:A:N6	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4537:C:H2'	1:5:4538:G:H8	1.82	0.45
4:9:847:A:H8	4:9:847:A:H5''	1.81	0.45
4:9:873:G:C2	57:LL:153:LYS:HE2	2.52	0.45
4:9:1395:C:H1'	4:9:1474:A:C5	2.52	0.45
47:BB:87:ILE:O	47:BB:98:THR:HA	2.17	0.45
49:DD:66:ILE:O	49:DD:70:THR:HG23	2.15	0.45
1:5:1456:C:H4'	20:Q:73:PRO:HG2	1.99	0.45
1:5:2022:C:C4	1:5:2023:C:C4	3.05	0.45
4:9:546:G:H2'	4:9:547:G:C8	2.52	0.45
26:W:113:LYS:O	26:W:117:LYS:HB2	2.17	0.45
40:l:44:TRP:O	40:l:48:LYS:NZ	2.42	0.45
1:5:1867:A:OP1	12:I:13:LYS:HE2	2.17	0.45
1:5:1973:G:H2'	1:5:1974:U:C6	2.52	0.45
1:5:2758:G:H2'	1:5:2759:G:C8	2.52	0.45
4:9:815:U:H2'	4:9:816:A:C8	2.52	0.45
4:9:1520:G:H2'	4:9:1520:G:N3	2.32	0.45
80:11:23:C:H2'	80:11:24:G:H8	1.82	0.45
80:11:37:A:H2'	80:11:38:A:O4'	2.17	0.45
1:5:1081:C:N3	1:5:1219:G:N1	2.65	0.45
1:5:4871:C:OP1	16:M:94:LYS:NZ	2.34	0.45
3:8:67:U:H2'	3:8:68:G:C8	2.48	0.45
4:9:182:C:H5'	4:9:183:G:C8	2.51	0.45
4:9:517:C:H2'	4:9:518:G:O4'	2.17	0.45
4:9:1240:A:H8	4:9:1267:C:O2'	2.00	0.45
9:E:144:ARG:NH2	9:E:194:GLN:O	2.50	0.45
80:13:25:U:H2'	80:13:26:G:H8	1.82	0.45
1:5:2326:G:OP2	34:e:101:HIS:ND1	2.36	0.44
1:5:3880:G:H2'	1:5:3881:G:C8	2.53	0.44
4:9:693:A:H61	4:9:733:C:N4	2.15	0.44
4:9:695:C:H2'	4:9:696:G:H8	1.83	0.44
4:9:1203:G:H2'	4:9:1204:A:C8	2.52	0.44
1:5:260:C:H2'	1:5:261:G:H8	1.80	0.44
1:5:465:G:H2'	1:5:466:A:H8	1.82	0.44
1:5:966:A:H1'	1:5:968:C:N4	2.33	0.44
1:5:1538:U:H2'	1:5:1539:G:H8	1.82	0.44
1:5:2065:G:H2'	1:5:2066:C:O4'	2.16	0.44
4:9:104:A:H62	4:9:356:C:H5	1.63	0.44
6:B:56:ILE:HG21	6:B:365:LEU:HD22	1.99	0.44
52:GG:20:ASP:OD2	52:GG:22:ARG:NH2	2.44	0.44
53:HH:10:LYS:HD2	53:HH:16:PRO:HA	1.99	0.44
58:MM:35:ILE:HG23	77:ff:102:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1516:G:OP2	30:a:32:ARG:NH1	2.45	0.44
1:5:2517:A:N3	1:5:2539:C:O2'	2.51	0.44
1:5:3827:G:O2'	1:5:3829:G:OP2	2.30	0.44
1:5:4637:G:H2'	1:5:4638:U:C6	2.52	0.44
4:9:1201:U:H2'	4:9:1202:U:C6	2.52	0.44
4:9:1253:A:OP2	4:9:1526:G:N2	2.44	0.44
4:9:1503:C:H2'	4:9:1504:U:C6	2.53	0.44
4:9:1864:U:OP2	72:aa:5:ARG:NH2	2.50	0.44
47:BB:35:ALA:HB3	47:BB:42:ARG:HA	1.98	0.44
58:MM:126:GLU:O	58:MM:130:CYS:N	2.48	0.44
1:5:1775:A:H2'	1:5:1776:A:C8	2.52	0.44
4:9:433:A:OP1	54:II:25:ARG:NH2	2.43	0.44
4:9:1412:C:H2'	4:9:1413:G:C8	2.53	0.44
4:9:1595:U:H2'	4:9:1596:U:C6	2.53	0.44
25:V:107:ASN:ND2	25:V:111:GLU:HB3	2.31	0.44
56:KK:83:LEU:HB2	56:KK:85:LEU:HG	1.99	0.44
62:QQ:41:MET:HA	62:QQ:41:MET:HE2	2.00	0.44
77:ff:122:PRO:HD2	77:ff:132:MET:HE3	2.00	0.44
1:5:966:A:H5''	1:5:967:C:C6	2.53	0.44
1:5:1460:C:H2'	1:5:1461:C:C6	2.53	0.44
1:5:3656:A:H2'	1:5:3657:U:C6	2.53	0.44
1:5:4042:G:H2'	1:5:4043:G:C8	2.53	0.44
12:I:188:LYS:NZ	12:I:212:LEU:O	2.40	0.44
20:Q:53:MET:HE1	20:Q:143:ARG:HH21	1.82	0.44
52:GG:52:ILE:HG23	52:GG:52:ILE:O	2.17	0.44
52:GG:157:VAL:HG21	52:GG:176:ILE:HD11	1.98	0.44
80:11:25:U:H2'	80:11:26:G:H8	1.81	0.44
1:5:1358:G:O2'	1:5:1359:G:O5'	2.34	0.44
1:5:2634:C:H2'	1:5:2635:U:H6	1.81	0.44
1:5:3934:G:H2'	1:5:3935:C:C6	2.53	0.44
1:5:4323:A:H4'	8:D:176:SER:HB3	1.98	0.44
1:5:4524:G:C2	6:B:252:ALA:HB1	2.52	0.44
4:9:842:C:H5	70:YY:11:LYS:HA	1.83	0.44
4:9:1863:A:H1'	72:aa:79:ILE:HD13	1.98	0.44
6:B:36:ASP:OD2	6:B:39:LYS:NZ	2.45	0.44
1:5:54:G:OP1	81:j:43:ARG:NH1	2.48	0.44
1:5:1502:G:H5''	1:5:1502:G:C8	2.53	0.44
4:9:201:C:O5'	4:9:201:C:H6	2.00	0.44
4:9:815:U:H2'	4:9:816:A:H8	1.83	0.44
4:9:1177:U:H2'	4:9:1178:U:C6	2.53	0.44
27:X:72:ASP:OD1	27:X:73:HIS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:13:63:A:H2'	80:13:64:U:H6	1.81	0.44
80:11:58:A:H1'	80:11:60:A:N7	2.32	0.44
80:11:71:C:H2'	80:11:72:U:C6	2.52	0.44
1:5:746:A:O2'	1:5:747:A:H5'	2.18	0.44
1:5:2664:G:H4'	1:5:2677:G:H4'	1.99	0.44
1:5:4578:G:H2'	1:5:4579:U:H6	1.82	0.44
4:9:220:U:H2'	4:9:221:A:H8	1.82	0.44
4:9:669:A:H5'	4:9:669:A:H8	1.82	0.44
4:9:1538:C:H2'	4:9:1539:U:C6	2.52	0.44
47:BB:27:LYS:HA	47:BB:51:ARG:HH21	1.83	0.44
48:CC:167:ARG:NH1	48:CC:218:GLY:O	2.51	0.44
66:UU:59:LYS:HB2	66:UU:84:ILE:HG12	1.99	0.44
1:5:195:C:O2'	28:Y:125:SER:OG	2.22	0.43
1:5:496:G:C6	1:5:659:G:C6	3.06	0.43
1:5:1444:G:H2'	1:5:1445:U:C6	2.53	0.43
1:5:1788:A:H2'	12:I:22:PHE:CZ	2.52	0.43
1:5:4134:C:H2'	1:5:4135:G:C8	2.52	0.43
1:5:4460:U:H6	1:5:4460:U:O5'	2.00	0.43
4:9:1784:G:C6	4:9:1785:C:C4	3.06	0.43
4:9:1823:A:H5''	4:9:1823:A:N3	2.33	0.43
10:G:237:LEU:HD23	10:G:243:LEU:HD11	2.00	0.43
80:13:53:G:H2'	80:13:54:A:H8	1.82	0.43
1:5:966:A:H4'	1:5:967:C:O5'	2.17	0.43
1:5:1176:C:H2'	1:5:1177:U:H6	1.82	0.43
1:5:2088:A:O3'	1:5:2089:G:H3'	2.19	0.43
1:5:3656:A:H2'	1:5:3657:U:H6	1.84	0.43
1:5:3969:G:H2'	1:5:3970:G:C8	2.53	0.43
1:5:4431:U:P	12:I:3:ARG:HH22	2.40	0.43
1:5:4586:G:C6	1:5:4717:A:C6	3.06	0.43
4:9:214:U:H5''	4:9:215:G:OP2	2.18	0.43
4:9:533:A:C6	4:9:552:G:C6	3.06	0.43
4:9:614:C:H2'	4:9:626:G:C8	2.53	0.43
7:C:155:GLU:HG3	7:C:157:LYS:H	1.82	0.43
11:H:69:THR:O	11:H:72:THR:HG22	2.19	0.43
52:GG:152:ASP:OD1	52:GG:154:ARG:NH1	2.49	0.43
73:bb:47:PHE:CE2	73:bb:49:HIS:HB2	2.53	0.43
1:5:699:C:H2'	1:5:700:G:C8	2.53	0.43
1:5:730:G:OP2	14:K:75:ARG:NH2	2.46	0.43
1:5:1198:G:H2'	1:5:1199:G:H8	1.82	0.43
1:5:2503:G:H5''	1:5:2503:G:C8	2.51	0.43
4:9:439:A:O2'	4:9:1799:G:H4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:604:A:N3	4:9:639:C:O2'	2.48	0.43
4:9:1236:G:H2'	4:9:1237:C:C6	2.53	0.43
4:9:1720:U:H5''	4:9:1721:U:OP2	2.18	0.43
4:9:1866:A:N1	72:aa:87:ARG:HD2	2.34	0.43
6:B:218:ASP:OD1	6:B:348:ARG:HB3	2.18	0.43
48:CC:166:ARG:HD3	48:CC:248:TYR:CE1	2.54	0.43
60:OO:65:ASP:HA	60:OO:68:GLU:HG3	1.99	0.43
78:gg:188:HIS:HB3	78:gg:219:TRP:CZ3	2.53	0.43
1:5:2787:A:H2	1:5:2801:U:H3	1.65	0.43
1:5:3959:U:O2'	1:5:3960:A:O5'	2.36	0.43
1:5:4037:C:H2'	1:5:4038:C:C6	2.53	0.43
1:5:4286:C:H2'	1:5:4287:G:C8	2.53	0.43
2:7:27:G:H21	2:7:55:A:N6	2.16	0.43
4:9:886:A:H2'	4:9:887:U:H4'	2.01	0.43
4:9:1310:U:H2'	4:9:1311:C:H6	1.83	0.43
4:9:1720:U:H3'	4:9:1721:U:H5''	2.01	0.43
80:11:47:U:H3'	80:11:48:C:H5'	2.01	0.43
80:11:71:C:H2'	80:11:72:U:H6	1.82	0.43
1:5:711:A:H2'	1:5:712:C:C6	2.54	0.43
1:5:1087:A:H2'	1:5:1088:C:C6	2.54	0.43
1:5:2021:G:C4	1:5:2022:C:C5	3.06	0.43
1:5:2622:G:OP2	24:U:84:LYS:NZ	2.39	0.43
1:5:2657:G:O6	32:c:32:LYS:NZ	2.50	0.43
1:5:2844:A:O2'	1:5:4631:G:H4'	2.19	0.43
1:5:3692:A:N6	1:5:3823:G:H21	2.00	0.43
1:5:4075:U:P	10:G:302:ARG:HH22	2.42	0.43
4:9:441:C:H2'	4:9:442:C:C6	2.54	0.43
58:MM:85:LEU:O	58:MM:89:VAL:HG23	2.18	0.43
59:NN:19:ARG:NH2	73:bb:84:HIS:O	2.47	0.43
73:bb:21:LYS:NZ	73:bb:26:GLN:OE1	2.46	0.43
1:5:300:A:H2'	1:5:301:G:H8	1.84	0.43
1:5:2409:U:H5	1:5:2783:A:N1	2.16	0.43
1:5:3893:C:H2'	1:5:3894:A:C8	2.54	0.43
3:8:71:A:P	28:Y:50:ARG:HD2	2.58	0.43
16:M:36:ALA:HB2	16:M:52:PHE:CZ	2.54	0.43
21:R:103:ARG:HD2	21:R:124:TYR:CE2	2.53	0.43
22:S:41:LYS:HG2	22:S:61:ILE:HD13	2.01	0.43
80:13:12:C:H2'	80:13:13:G:C8	2.53	0.43
1:5:759:G:OP1	11:H:50:LYS:N	2.51	0.43
1:5:1194:G:C2	1:5:1195:G:H1'	2.54	0.43
1:5:1396:G:N7	30:a:110:LYS:NZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2580:U:OP1	29:Z:36:ARG:NH1	2.48	0.43
1:5:4051:C:H2'	1:5:4052:C:C6	2.53	0.43
1:5:4124:G:H3'	5:A:69:PHE:CE1	2.54	0.43
4:9:85:A:H2'	4:9:86:C:H6	1.83	0.43
4:9:568:C:O2'	4:9:569:A:O5'	2.36	0.43
4:9:568:C:N4	4:9:583:A:C8	2.87	0.43
4:9:1181:A:H2'	4:9:1182:A:C8	2.54	0.43
4:9:1337:C:H2'	4:9:1338:G:H8	1.84	0.43
6:B:378:ARG:HG3	26:W:32:LEU:HD21	2.01	0.43
11:H:173:ARG:CD	41:m:101:VAL:HG13	2.49	0.43
36:g:41:ALA:O	36:g:52:ARG:NH1	2.46	0.43
49:DD:23:GLU:HG2	56:KK:64:TRP:HE1	1.84	0.43
53:HH:53:VAL:HG12	53:HH:54:GLY:N	2.34	0.43
1:5:910:G:H2'	1:5:911:U:C6	2.54	0.43
1:5:925:C:H3'	1:5:926:G:H5'	2.01	0.43
1:5:2326:G:H5''	34:e:127:ALA:CB	2.49	0.43
46:AA:200:ASP:OD1	46:AA:200:ASP:N	2.52	0.43
47:BB:30:TRP:CE2	47:BB:48:LEU:HD13	2.54	0.43
49:DD:57:ASN:O	49:DD:65:ARG:NH1	2.47	0.43
1:5:138:G:H2'	1:5:139:G:C8	2.53	0.43
1:5:1358:G:H4'	1:5:1359:G:OP1	2.19	0.43
4:9:1005:G:H2'	4:9:1006:C:C6	2.54	0.43
6:B:234:ARG:NH1	6:B:268:ARG:O	2.45	0.43
9:E:98:PRO:HA	9:E:107:THR:HG22	2.01	0.43
1:5:6:C:H2'	1:5:7:C:C6	2.54	0.43
1:5:425:U:H2'	1:5:426:A:H8	1.84	0.43
1:5:451:C:H2'	1:5:1294:A:C8	2.54	0.43
1:5:1074:G:H2'	1:5:1075:G:C8	2.54	0.43
1:5:1534:A:H8	81:j:15:THR:HG23	1.83	0.43
1:5:2422:C:OP1	19:P:127:ARG:NH2	2.27	0.43
1:5:4038:C:H2'	1:5:4039:G:C8	2.54	0.43
1:5:4413:C:H5	1:5:4429:C:N4	2.10	0.43
1:5:4585:U:H2'	1:5:4586:G:H8	1.83	0.43
1:5:5002:U:H2'	1:5:5003:U:C6	2.54	0.43
4:9:79:A:H3'	4:9:80:G:C8	2.51	0.43
4:9:151:C:H2'	4:9:152:U:C6	2.53	0.43
4:9:448:A:H61	54:II:29:LEU:HD13	1.83	0.43
4:9:688:U:H1'	4:9:689:U:C6	2.53	0.43
4:9:878:G:H22	4:9:908:A:H2	1.66	0.43
5:A:117:GLU:HG2	5:A:124:GLY:N	2.34	0.43
22:S:44:PHE:CZ	22:S:48:VAL:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:103:VAL:CG1	30:a:108:TYR:HB2	2.48	0.43
36:g:21:ARG:HG3	36:g:35:THR:CG2	2.49	0.43
69:XX:67:ARG:HE	69:XX:115:ILE:HD11	1.84	0.43
78:gg:260:ASP:CG	78:gg:263:GLY:H	2.26	0.43
1:5:64:A:H4'	1:5:65:A:O5'	2.19	0.42
1:5:164:G:H2'	1:5:165:A:C8	2.53	0.42
1:5:201:C:H5'	1:5:201:C:C6	2.54	0.42
1:5:1075:G:N2	1:5:1235:G:H22	2.17	0.42
1:5:1398:A:H61	1:5:1419:G:C2'	2.30	0.42
1:5:1558:A:H2'	1:5:1559:G:H8	1.84	0.42
1:5:2396:A:H4'	1:5:2397:G:OP2	2.18	0.42
4:9:126:G:O2'	4:9:127:C:OP1	2.33	0.42
4:9:569:A:H2'	4:9:570:C:O4'	2.19	0.42
4:9:606:G:H8	76:ee:131:ASN:HD21	1.67	0.42
4:9:734:C:H2'	4:9:735:C:C6	2.54	0.42
4:9:792:C:H2'	4:9:793:G:C8	2.54	0.42
7:C:70:GLY:C	7:C:72:ALA:H	2.27	0.42
9:E:180:GLY:O	9:E:181:PRO:C	2.62	0.42
10:G:153:HIS:CE1	10:G:156:ARG:HH11	2.37	0.42
33:d:19:GLU:OE1	33:d:92:ARG:NE	2.46	0.42
46:AA:123:VAL:HA	46:AA:145:ILE:O	2.19	0.42
46:AA:134:LEU:CD1	46:AA:144:THR:HG21	2.49	0.42
58:MM:53:ALA:HA	58:MM:79:VAL:O	2.19	0.42
65:TT:12:GLN:HA	65:TT:15:VAL:HG22	2.00	0.42
1:5:1173:G:H2'	1:5:1174:G:C8	2.54	0.42
1:5:1244:G:O5'	1:5:1244:G:H8	2.02	0.42
4:9:16:G:H2'	4:9:17:C:C6	2.54	0.42
4:9:895:G:H2'	4:9:896:U:C6	2.54	0.42
4:9:1102:G:OP1	47:BB:151:ARG:NH2	2.43	0.42
4:9:1292:C:H2'	4:9:1293:A:H5''	2.01	0.42
4:9:1801:A:H2'	4:9:1802:C:C6	2.54	0.42
42:n:2:ARG:HB3	42:n:5:TRP:CD1	2.54	0.42
51:FF:39:ILE:HG22	51:FF:41:VAL:HG23	2.01	0.42
58:MM:35:ILE:HD12	58:MM:61:TYR:CE2	2.54	0.42
62:QQ:89:SER:OG	62:QQ:112:LEU:HD13	2.20	0.42
1:5:1195:G:H2'	1:5:1196:G:H8	1.82	0.42
1:5:1564:A:OP1	59:NN:140:LYS:NZ	2.38	0.42
4:9:1115:U:H1'	4:9:1116:C:O2	2.19	0.42
4:9:1337:C:H2'	4:9:1338:G:C8	2.54	0.42
12:I:179:ASP:OD1	12:I:179:ASP:N	2.52	0.42
55:JJ:59:GLU:OE2	55:JJ:69:ARG:NH2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:666:G:P	45:r:67:ARG:HH21	2.41	0.42
1:5:1406(B):C:H2'	1:5:1406(C):G:H8	1.84	0.42
1:5:4039:G:H4'	1:5:4049:U:H2'	2.01	0.42
1:5:4460:U:H2'	1:5:4461:C:C6	2.54	0.42
1:5:4508:C:N3	1:5:4512:U:H5	2.17	0.42
1:5:5041:G:OP2	26:W:61:LYS:NZ	2.31	0.42
4:9:344:U:H2'	4:9:345:U:C6	2.55	0.42
50:EE:141:THR:OG1	50:EE:143:ASP:OD1	2.34	0.42
80:11:63:A:H2'	80:11:64:U:H6	1.84	0.42
1:5:1404:G:H2'	1:5:1405:C:C6	2.55	0.42
1:5:2411:C:H2'	1:5:2412:A:C8	2.55	0.42
1:5:2627:C:C2	1:5:2628:U:C5	3.06	0.42
4:9:382:C:H2'	4:9:383:G:H8	1.85	0.42
4:9:1643:U:H2'	4:9:1644:C:C6	2.54	0.42
4:9:1700:C:C2	4:9:1834:A:N6	2.88	0.42
22:S:78:PHE:CE1	22:S:102:THR:HG22	2.54	0.42
64:SS:26:ILE:HG13	64:SS:54:LYS:O	2.18	0.42
1:5:1765:A:C4	1:5:1766:A:C8	3.08	0.42
1:5:1982:G:N3	1:5:2009:A:O2'	2.49	0.42
4:9:62:G:H4'	4:9:172:U:C5	2.55	0.42
15:L:9:ILE:HG23	15:L:9:ILE:O	2.19	0.42
51:FF:80:GLY:HA2	51:FF:83:ASN:ND2	2.35	0.42
80:11:73:A:N6	84:11:101:ATP:N6	2.67	0.42
1:5:18:C:H4'	17:N:138:PHE:CD1	2.55	0.42
1:5:418:A:C2	3:8:17:A:H1'	2.55	0.42
1:5:738(A):C:O2'	1:5:740:G:OP2	2.26	0.42
1:5:1954:U:H2'	1:5:1955:G:C8	2.55	0.42
1:5:2477:A:H2'	1:5:2478:C:C5	2.54	0.42
1:5:3672:G:O5'	1:5:3672:G:C8	2.73	0.42
1:5:4066:U:H2'	1:5:4067:U:C6	2.54	0.42
1:5:4760:G:H2'	1:5:4761:G:O4'	2.19	0.42
5:A:142:GLU:CD	5:A:142:GLU:H	2.26	0.42
8:D:292:GLU:C	8:D:294:ALA:H	2.28	0.42
22:S:90:THR:HG23	23:T:156:TYR:CD2	2.55	0.42
22:S:112:ASP:OD1	22:S:116:ARG:NH1	2.47	0.42
45:r:90:LEU:HG	45:r:111:ILE:HG23	2.02	0.42
52:GG:73:VAL:HG12	52:GG:74:ARG:N	2.35	0.42
66:UU:50:VAL:HG23	66:UU:91:LEU:HD23	2.02	0.42
1:5:478:G:H2'	1:5:479:G:H8	1.84	0.42
1:5:1442:C:H2'	1:5:1443:A:H8	1.85	0.42
1:5:1494:U:H2'	1:5:1495:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1942:A:H2'	1:5:1943:A:C8	2.55	0.42
1:5:2580:U:OP1	29:Z:36:ARG:NH2	2.51	0.42
1:5:4500:U:H2'	1:5:4501:U:C6	2.55	0.42
1:5:4947:U:O2'	1:5:4948:C:OP1	2.34	0.42
27:X:88:LYS:HE2	27:X:88:LYS:HB2	1.84	0.42
78:gg:176:VAL:O	78:gg:185:LYS:N	2.48	0.42
80:11:13:G:H2'	80:11:14:C:O4'	2.20	0.42
1:5:116:G:H2'	1:5:117:C:C6	2.55	0.42
1:5:1890:G:N2	1:5:1939:A:H61	2.17	0.42
1:5:4507:A:H2'	1:5:4508:C:C6	2.54	0.42
1:5:5020:G:H2'	1:5:5021:C:C6	2.55	0.42
4:9:847:A:H61	50:EE:16:LYS:CE	2.33	0.42
4:9:1457:U:H2'	4:9:1458:G:C8	2.54	0.42
12:I:102:MET:HE1	12:I:114:GLY:O	2.20	0.42
19:P:40:HIS:CE1	19:P:42:ARG:HG2	2.55	0.42
35:f:63:LYS:HG2	35:f:64:PRO:HD2	2.01	0.42
63:RR:22:THR:O	78:gg:212:LYS:NZ	2.40	0.42
78:gg:78:ALA:O	78:gg:89:LEU:HD12	2.20	0.42
1:5:4978:G:H2'	1:5:4979:A:H5''	2.01	0.42
4:9:151:C:OP1	70:YY:120:THR:OG1	2.34	0.42
4:9:1240:A:H2'	4:9:1241:A:C8	2.54	0.42
15:L:7:GLY:O	30:a:49:HIS:NE2	2.45	0.42
35:f:7:CYS:HB2	35:f:103:VAL:CG2	2.50	0.42
44:p:42:CYS:CB	44:p:60:CYS:SG	2.95	0.42
53:HH:135:PHE:CG	53:HH:136:PRO:HA	2.55	0.42
59:NN:25:TRP:HE1	73:bb:83:GLN:C	2.28	0.42
78:gg:199:THR:HG23	78:gg:241:PHE:CE2	2.55	0.42
1:5:181:C:N3	1:5:256:G:C2	2.87	0.41
1:5:981:C:H4'	9:E:42:GLY:O	2.20	0.41
1:5:1314:C:C2	1:5:1315:C:C5	3.07	0.41
1:5:1990:A:H3'	1:5:1991:A:H5''	2.01	0.41
1:5:3723:A:H2'	1:5:3724:A:H8	1.84	0.41
4:9:1098:C:H2'	4:9:1099:G:C8	2.55	0.41
4:9:1415:C:C2	4:9:1416:C:C5	3.08	0.41
4:9:1476:A:H4'	4:9:1477:U:OP2	2.19	0.41
7:C:13:GLU:OE1	7:C:161:TYR:OH	2.19	0.41
11:H:92:MET:HE2	11:H:179:ILE:HG22	2.01	0.41
48:CC:254:ASP:OD1	48:CC:254:ASP:N	2.53	0.41
50:EE:188:ASN:HD22	50:EE:220:THR:HG22	1.85	0.41
64:SS:48:ALA:HB2	64:SS:70:ILE:HD12	2.02	0.41
65:TT:31:PRO:HG2	65:TT:33:TRP:CH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:ZZ:68:ILE:HB	71:ZZ:109:TYR:HB2	2.02	0.41
1:5:423:G:H5'	19:P:26:PHE:HZ	1.85	0.41
1:5:1098:G:C6	1:5:1198:G:N2	2.89	0.41
1:5:2021:G:C5	1:5:2022:C:C5	3.08	0.41
4:9:182:C:H4'	4:9:183:G:O5'	2.20	0.41
5:A:101:VAL:HG22	5:A:165:VAL:HG22	2.01	0.41
12:I:48:LEU:HD21	12:I:145:LYS:HA	2.02	0.41
12:I:84:GLY:O	12:I:140:THR:OG1	2.28	0.41
54:II:133:GLU:O	54:II:136:ILE:HG12	2.20	0.41
78:gg:5:MET:HA	78:gg:312:VAL:HA	2.01	0.41
1:5:288:G:H2'	1:5:289:C:C6	2.55	0.41
1:5:370:U:OP1	81:j:11:ARG:NH1	2.42	0.41
1:5:1234:G:O2'	1:5:1235:G:H8	2.02	0.41
1:5:3727:A:H2'	1:5:3728:A:C8	2.55	0.41
1:5:4481:U:H2'	1:5:4482:U:C6	2.55	0.41
1:5:4538:G:H2'	1:5:4539:U:C6	2.56	0.41
1:5:5003:U:H2'	1:5:5004:C:C6	2.56	0.41
45:r:46:ARG:HA	45:r:70:GLN:NE2	2.34	0.41
48:CC:69:LEU:HD11	48:CC:273:LEU:HD11	2.01	0.41
67:VV:20:SER:C	67:VV:22:ARG:H	2.28	0.41
69:XX:107:ARG:HB3	69:XX:110:HIS:HB3	2.01	0.41
1:5:3621:A:O2'	1:5:4658:G:O2'	2.38	0.41
2:7:23:A:N3	2:7:118:C:O2'	2.45	0.41
4:9:1679:A:C2	51:FF:60:ARG:HA	2.55	0.41
4:9:1690:U:H2'	4:9:1691:U:C6	2.56	0.41
25:V:35:LYS:HB2	25:V:67:LYS:HG3	2.01	0.41
43:o:24:THR:HG23	43:o:69:ARG:HB3	2.02	0.41
50:EE:87:MET:SD	50:EE:100:ARG:HD3	2.61	0.41
68:WW:121:THR:HG22	68:WW:122:GLY:O	2.20	0.41
78:gg:216:ALA:HB3	78:gg:230:LEU:HB2	2.02	0.41
80:11:66:C:H2'	80:11:67:U:C6	2.54	0.41
1:5:1779:U:H2'	1:5:1780:A:C8	2.55	0.41
1:5:4504:C:H2'	1:5:4505:C:C6	2.56	0.41
1:5:4957:C:H3'	1:5:4958:C:H5''	2.03	0.41
3:8:71:A:H5''	28:Y:50:ARG:CZ	2.50	0.41
4:9:74:G:N2	4:9:77:A:OP1	2.53	0.41
4:9:398:A:H5'	4:9:398:A:C8	2.55	0.41
4:9:434:G:H2'	4:9:435:A:C8	2.54	0.41
4:9:847:A:H61	50:EE:16:LYS:HE2	1.85	0.41
4:9:1128:C:H2'	4:9:1129:G:C8	2.55	0.41
20:Q:50:ARG:HA	20:Q:53:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:7:LYS:HE2	30:a:11:LEU:HD11	2.01	0.41
36:g:15:THR:HG22	36:g:16:ALA:N	2.35	0.41
60:OO:84:ARG:NH1	60:OO:87:GLU:OE1	2.47	0.41
1:5:216:C:H2'	1:5:217:C:H2'	2.03	0.41
1:5:453:G:O2'	1:5:705:G:OP1	2.37	0.41
1:5:734:G:C2	1:5:735:G:C8	3.08	0.41
1:5:1884:C:H4'	1:5:2070:U:C4	2.55	0.41
1:5:2544:G:N2	3:8:126:C:H41	2.18	0.41
1:5:2732:G:H2'	1:5:2733:C:C6	2.56	0.41
1:5:3877:A:O2'	1:5:4400:G:N2	2.53	0.41
1:5:4759:C:H2'	1:5:4760:G:C8	2.56	0.41
4:9:164:A:H3'	4:9:165:G:N2	2.35	0.41
4:9:1088:U:H4'	4:9:1089:G:OP2	2.19	0.41
23:T:35:LYS:N	23:T:38:ASP:OD2	2.40	0.41
24:U:80:LYS:HE2	24:U:110:TYR:CZ	2.55	0.41
27:X:117:TYR:C	27:X:119:ILE:H	2.28	0.41
47:BB:153:THR:HB	47:BB:155:TYR:CD2	2.55	0.41
81:j:28:HIS:HE1	81:j:30:GLN:HB2	1.85	0.41
1:5:233:U:H3'	1:5:234:G:H5''	2.03	0.41
1:5:1484:G:N3	1:5:1484:G:H2'	2.35	0.41
1:5:1564:A:H2'	1:5:1565:A:C8	2.56	0.41
1:5:1693:U:OP1	20:Q:143:ARG:NH2	2.51	0.41
1:5:1954:U:H2'	1:5:1955:G:H8	1.86	0.41
1:5:1967:A:C2	1:5:2021:G:C4	3.08	0.41
1:5:2097:A:OP1	1:5:2107:A:N6	2.54	0.41
1:5:4291:G:H5''	1:5:4293:U:C5	2.55	0.41
1:5:4395:U:H5'	1:5:4395:U:C6	2.55	0.41
1:5:4697:U:H4'	41:m:78:HIS:CE1	2.56	0.41
4:9:71:G:O6	52:GG:170:ARG:NH1	2.50	0.41
11:H:177:ASP:OD1	11:H:177:ASP:N	2.53	0.41
62:QQ:129:SER:O	62:QQ:131:LYS:HE3	2.21	0.41
1:5:162:A:H2'	1:5:163:A:H8	1.86	0.41
1:5:963:G:H2'	1:5:964:A:C8	2.56	0.41
1:5:3751:G:N2	1:5:3775:A:H8	2.14	0.41
1:5:3907:G:H5'	1:5:4449:A:C2	2.56	0.41
3:8:1:C:N3	3:8:2:G:H1'	2.35	0.41
4:9:215:G:H2'	4:9:216:C:C6	2.56	0.41
4:9:751:G:C6	4:9:793:G:N1	2.89	0.41
4:9:795:A:H2'	4:9:796:G:C8	2.55	0.41
9:E:169:LYS:HE3	9:E:171:LEU:HD23	2.02	0.41
19:P:39:MET:O	19:P:114:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:o:66:ILE:HG21	43:o:91:PHE:CE1	2.55	0.41
80:11:26:G:H22	80:11:44:A:H2	1.69	0.41
1:5:272:U:H2'	1:5:273:U:C6	2.56	0.41
1:5:666:G:OP1	45:r:67:ARG:NH2	2.44	0.41
1:5:966:A:H5'	1:5:967:C:H2'	2.03	0.41
1:5:1186:U:H2'	1:5:1187:G:N3	2.35	0.41
1:5:1532:G:OP2	81:j:31:LYS:NZ	2.45	0.41
1:5:1670:G:N2	1:5:1854:G:H2'	2.36	0.41
1:5:1866:U:H2'	1:5:1867:A:O4'	2.20	0.41
1:5:1967:A:N1	1:5:2021:G:C5	2.88	0.41
1:5:2090:U:OP2	7:C:307:LYS:NZ	2.54	0.41
1:5:2465:C:H1'	1:5:3672:G:N2	2.33	0.41
1:5:2694:G:H5''	1:5:2696:A:N7	2.36	0.41
1:5:3635:A:N6	44:p:18:TYR:HA	2.36	0.41
1:5:4061:G:H2'	1:5:4062:A:H8	1.86	0.41
1:5:4922:C:C4	1:5:4923:U:C4	3.08	0.41
4:9:15:U:H2'	4:9:16:G:O4'	2.21	0.41
4:9:127:C:O2	50:EE:134:LYS:NZ	2.42	0.41
4:9:829:C:OP1	50:EE:21:ASP:HB2	2.20	0.41
4:9:1076:G:OP2	59:NN:107:LYS:HE3	2.21	0.41
4:9:1354:G:N2	4:9:1357:A:OP2	2.48	0.41
4:9:1556:A:N3	4:9:1556:A:H2'	2.36	0.41
4:9:1566:G:N7	65:TT:101:ARG:NH2	2.68	0.41
8:D:119:TYR:OH	8:D:139:PRO:O	2.37	0.41
35:f:7:CYS:HB2	35:f:103:VAL:HG22	2.02	0.41
40:l:51:LEU:O	81:j:14:LYS:NZ	2.42	0.41
51:FF:73:THR:HG22	51:FF:93:VAL:HG21	2.02	0.41
51:FF:102:LEU:HD22	71:ZZ:110:THR:HG21	2.02	0.41
68:WW:3:ARG:HD3	68:WW:6:VAL:HG12	2.03	0.41
69:XX:51:VAL:HG13	69:XX:70:VAL:CG2	2.49	0.41
69:XX:63:ASN:HD22	69:XX:114:ASP:CG	2.25	0.41
69:XX:68:LYS:HG3	76:ee:79:LEU:HD22	2.02	0.41
70:YY:74:MET:HE2	70:YY:74:MET:HB3	1.78	0.41
1:5:25:A:H4'	1:5:340:C:H2'	2.03	0.41
1:5:638:G:H2'	1:5:639:U:C6	2.56	0.41
1:5:3642:A:C4	81:j:3:LYS:HB3	2.56	0.41
1:5:4098:A:H2'	1:5:4099:G:C8	2.56	0.41
1:5:4657:U:H3'	1:5:4658:G:H5''	2.03	0.41
4:9:407:G:C2	69:XX:36:LEU:HD23	2.56	0.41
4:9:1670:C:H2'	4:9:1671:G:O4'	2.21	0.41
19:P:94:MET:HE3	19:P:94:MET:HB2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:83:LEU:O	24:U:87:THR:HG22	2.21	0.41
52:GG:3:LEU:N	52:GG:16:ILE:O	2.42	0.41
62:QQ:102:GLU:OE2	78:gg:58:ALA:N	2.52	0.41
80:11:3:G:OP2	84:11:101:ATP:O2'	2.31	0.41
80:11:18:G:H21	80:11:57:G:H2'	1.86	0.41
1:5:1200:G:H2'	1:5:1201:U:C6	2.55	0.40
1:5:4286:C:H2'	1:5:4287:G:H8	1.86	0.40
1:5:4584:A:H2'	1:5:4585:U:O4'	2.20	0.40
4:9:1424:G:H2'	4:9:1425:G:H8	1.85	0.40
4:9:1656:G:C2	4:9:1657:G:C8	3.09	0.40
4:9:1828:C:H2'	4:9:1829:G:O4'	2.21	0.40
4:9:1854:U:OP1	60:OO:150:ARG:NH1	2.39	0.40
31:b:101:HIS:HD2	31:b:104:LEU:H	1.69	0.40
58:MM:14:VAL:HG12	58:MM:17:ALA:H	1.85	0.40
58:MM:47:ALA:HB3	58:MM:74:ILE:HD13	2.03	0.40
59:NN:4:MET:HG2	59:NN:5:HIS:CD2	2.55	0.40
69:XX:115:ILE:HD12	69:XX:115:ILE:HG23	1.86	0.40
1:5:1968:G:H2'	1:5:1969:G:H8	1.86	0.40
1:5:2544:G:H21	3:8:126:C:N4	2.19	0.40
1:5:4305:G:N3	1:5:4305:G:H2'	2.36	0.40
1:5:4473:A:O3'	41:m:96:ARG:NH2	2.55	0.40
4:9:386:C:H2'	4:9:387:C:C6	2.56	0.40
4:9:692:G:H2'	4:9:693:A:C8	2.53	0.40
4:9:1292:C:C4	4:9:1293:A:C2	3.09	0.40
4:9:1845:A:H2'	4:9:1846:G:H8	1.86	0.40
22:S:76:LYS:NZ	22:S:100:LEU:O	2.53	0.40
61:PP:64:LYS:HB3	61:PP:64:LYS:HE3	1.97	0.40
70:YY:80:ASP:OD1	70:YY:80:ASP:N	2.54	0.40
80:11:25:U:C2	80:11:26:G:C8	3.09	0.40
1:5:2055:G:C4	18:O:130:LYS:HG2	2.56	0.40
1:5:4746:C:H2'	1:5:4747:C:H6	1.87	0.40
1:5:5001:U:OP1	6:B:385:LYS:NZ	2.47	0.40
4:9:85:A:H2'	4:9:86:C:C6	2.56	0.40
4:9:1457:U:H2'	4:9:1458:G:H8	1.86	0.40
5:A:137:ILE:HD11	5:A:149:LYS:HB2	2.03	0.40
6:B:380:GLN:HG2	26:W:14:TYR:CE2	2.56	0.40
8:D:33:ARG:O	8:D:37:VAL:HG22	2.22	0.40
19:P:54:LYS:HA	19:P:83:TRP:CD1	2.55	0.40
22:S:90:THR:HG23	23:T:156:TYR:CE2	2.56	0.40
34:e:113:GLU:OE2	34:e:117:GLN:NE2	2.33	0.40
47:BB:52:THR:HG23	47:BB:57:ILE:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:11:23:C:H2'	80:11:24:G:C8	2.56	0.40
1:5:1411(B):C:H2'	1:5:1411(C):C:C6	2.56	0.40
1:5:4361:U:H2'	1:5:4362:A:O4'	2.21	0.40
1:5:4572:U:H2'	1:5:4573:G:H8	1.86	0.40
1:5:4735:G:O2'	1:5:4736:C:O5'	2.39	0.40
1:5:4937:C:H2'	1:5:4939:C:C5	2.56	0.40
4:9:163:U:OP2	52:GG:87:ARG:NH2	2.53	0.40
4:9:641:A:H2'	4:9:642:U:O4'	2.22	0.40
4:9:643:A:OP1	55:JJ:41:ARG:NH2	2.54	0.40
4:9:743:U:H2'	4:9:744:G:C4	2.57	0.40
6:B:47:LEU:HD12	6:B:47:LEU:HA	1.88	0.40
6:B:115:LYS:HA	6:B:118:PHE:CD2	2.57	0.40
22:S:7:LEU:HA	22:S:7:LEU:HD23	1.88	0.40
46:AA:30:LEU:HD13	46:AA:38:ILE:HD11	2.04	0.40
46:AA:89:LYS:NZ	63:RR:82:ASP:OD2	2.53	0.40
49:DD:85:GLU:OE2	49:DD:87:TYR:OH	2.21	0.40
1:5:746:A:H2'	1:5:913:U:O4	2.22	0.40
1:5:1859:C:H2'	1:5:1860:U:C6	2.57	0.40
1:5:1982:G:H5'	1:5:1982:G:H8	1.87	0.40
1:5:2293:U:H2'	1:5:2294:G:H8	1.85	0.40
4:9:126:G:H1'	4:9:181:A:N3	2.36	0.40
4:9:1685:U:H2'	4:9:1686:G:O4'	2.21	0.40
11:H:92:MET:HB3	11:H:181:VAL:HA	2.04	0.40
20:Q:43:PHE:CD2	20:Q:133:GLY:HA3	2.56	0.40
55:JJ:45:ARG:O	55:JJ:49:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	A	246/257 (96%)	239 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B	392/403 (97%)	376 (96%)	16 (4%)	0	100	100
7	C	360/425 (85%)	353 (98%)	7 (2%)	0	100	100
8	D	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
9	E	208/291 (72%)	199 (96%)	9 (4%)	0	100	100
10	G	229/319 (72%)	222 (97%)	7 (3%)	0	100	100
11	H	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
12	I	201/214 (94%)	195 (97%)	6 (3%)	0	100	100
13	J	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
14	K	223/247 (90%)	216 (97%)	7 (3%)	0	100	100
15	L	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
16	M	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
17	N	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
18	O	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
19	P	151/184 (82%)	146 (97%)	5 (3%)	0	100	100
20	Q	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
21	R	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
22	S	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
23	T	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
24	U	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
25	V	127/140 (91%)	124 (98%)	3 (2%)	0	100	100
26	W	102/157 (65%)	101 (99%)	1 (1%)	0	100	100
27	X	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
28	Y	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
29	Z	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
30	a	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
31	b	94/245 (38%)	91 (97%)	3 (3%)	0	100	100
32	c	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
33	d	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
34	e	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
35	f	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
36	g	112/116 (97%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
38	i	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
39	k	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
40	l	48/51 (94%)	48 (100%)	0	0	100	100
41	m	50/102 (49%)	47 (94%)	3 (6%)	0	100	100
42	n	23/25 (92%)	23 (100%)	0	0	100	100
43	o	102/106 (96%)	97 (95%)	5 (5%)	0	100	100
44	p	89/92 (97%)	89 (100%)	0	0	100	100
45	r	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
46	AA	215/295 (73%)	205 (95%)	10 (5%)	0	100	100
47	BB	211/264 (80%)	206 (98%)	5 (2%)	0	100	100
48	CC	219/293 (75%)	213 (97%)	6 (3%)	0	100	100
49	DD	222/243 (91%)	219 (99%)	3 (1%)	0	100	100
50	EE	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
51	FF	180/204 (88%)	168 (93%)	12 (7%)	0	100	100
52	GG	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
53	HH	181/194 (93%)	177 (98%)	4 (2%)	0	100	100
54	II	194/208 (93%)	190 (98%)	4 (2%)	0	100	100
55	JJ	179/194 (92%)	177 (99%)	2 (1%)	0	100	100
56	KK	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
57	LL	139/158 (88%)	136 (98%)	3 (2%)	0	100	100
58	MM	108/132 (82%)	104 (96%)	4 (4%)	0	100	100
59	NN	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
60	OO	134/168 (80%)	133 (99%)	1 (1%)	0	100	100
61	PP	127/145 (88%)	123 (97%)	4 (3%)	0	100	100
62	QQ	140/146 (96%)	135 (96%)	5 (4%)	0	100	100
63	RR	130/135 (96%)	128 (98%)	2 (2%)	0	100	100
64	SS	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
65	TT	139/145 (96%)	134 (96%)	5 (4%)	0	100	100
66	UU	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
67	VV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	WW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
69	XX	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
70	YY	122/130 (94%)	118 (97%)	4 (3%)	0	100	100
71	ZZ	73/125 (58%)	72 (99%)	1 (1%)	0	100	100
72	aa	99/115 (86%)	96 (97%)	3 (3%)	0	100	100
73	bb	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
74	cc	60/69 (87%)	60 (100%)	0	0	100	100
75	dd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
76	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
77	ff	66/156 (42%)	61 (92%)	5 (8%)	0	100	100
78	gg	311/317 (98%)	289 (93%)	22 (7%)	0	100	100
81	j	84/97 (87%)	81 (96%)	3 (4%)	0	100	100
All	All	11148/12891 (86%)	10834 (97%)	314 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
5	A	190/199 (96%)	190 (100%)	0	100	100
6	B	342/348 (98%)	342 (100%)	0	100	100
7	C	302/347 (87%)	302 (100%)	0	100	100
8	D	247/250 (99%)	247 (100%)	0	100	100
9	E	190/251 (76%)	190 (100%)	0	100	100
10	G	200/272 (74%)	199 (100%)	1 (0%)	86	96
11	H	169/171 (99%)	169 (100%)	0	100	100
12	I	175/181 (97%)	175 (100%)	0	100	100
13	J	143/149 (96%)	143 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	K	196/215 (91%)	196 (100%)	0	100	100
15	L	175/176 (99%)	174 (99%)	1 (1%)	84	95
16	M	117/161 (73%)	117 (100%)	0	100	100
17	N	171/172 (99%)	171 (100%)	0	100	100
18	O	171/173 (99%)	170 (99%)	1 (1%)	84	95
19	P	134/163 (82%)	134 (100%)	0	100	100
20	Q	164/165 (99%)	164 (100%)	0	100	100
21	R	159/175 (91%)	159 (100%)	0	100	100
22	S	157/157 (100%)	156 (99%)	1 (1%)	84	95
23	T	139/140 (99%)	139 (100%)	0	100	100
24	U	89/114 (78%)	89 (100%)	0	100	100
25	V	100/107 (94%)	100 (100%)	0	100	100
26	W	86/126 (68%)	86 (100%)	0	100	100
27	X	106/134 (79%)	106 (100%)	0	100	100
28	Y	124/135 (92%)	124 (100%)	0	100	100
29	Z	117/118 (99%)	117 (100%)	0	100	100
30	a	119/120 (99%)	119 (100%)	0	100	100
31	b	80/184 (44%)	80 (100%)	0	100	100
32	c	84/98 (86%)	84 (100%)	0	100	100
33	d	98/110 (89%)	98 (100%)	0	100	100
34	e	114/121 (94%)	114 (100%)	0	100	100
35	f	88/89 (99%)	88 (100%)	0	100	100
36	g	98/99 (99%)	98 (100%)	0	100	100
37	h	109/110 (99%)	109 (100%)	0	100	100
38	i	86/89 (97%)	86 (100%)	0	100	100
39	k	64/65 (98%)	64 (100%)	0	100	100
40	l	47/48 (98%)	47 (100%)	0	100	100
41	m	48/90 (53%)	48 (100%)	0	100	100
42	n	24/24 (100%)	24 (100%)	0	100	100
43	o	92/94 (98%)	92 (100%)	0	100	100
44	p	74/75 (99%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	r	108/121 (89%)	108 (100%)	0	100	100
46	AA	180/245 (74%)	180 (100%)	0	100	100
47	BB	194/231 (84%)	194 (100%)	0	100	100
48	CC	187/225 (83%)	186 (100%)	1 (0%)	86	96
49	DD	187/202 (93%)	187 (100%)	0	100	100
50	EE	224/225 (100%)	224 (100%)	0	100	100
51	FF	157/170 (92%)	157 (100%)	0	100	100
52	GG	207/218 (95%)	207 (100%)	0	100	100
53	HH	165/174 (95%)	165 (100%)	0	100	100
54	II	172/180 (96%)	172 (100%)	0	100	100
55	JJ	161/168 (96%)	161 (100%)	0	100	100
56	KK	87/136 (64%)	87 (100%)	0	100	100
57	LL	130/142 (92%)	130 (100%)	0	100	100
58	MM	94/108 (87%)	94 (100%)	0	100	100
59	NN	130/131 (99%)	130 (100%)	0	100	100
60	OO	106/130 (82%)	105 (99%)	1 (1%)	75	92
61	PP	115/130 (88%)	115 (100%)	0	100	100
62	QQ	117/121 (97%)	117 (100%)	0	100	100
63	RR	119/121 (98%)	119 (100%)	0	100	100
64	SS	125/132 (95%)	124 (99%)	1 (1%)	79	93
65	TT	111/115 (96%)	110 (99%)	1 (1%)	75	92
66	UU	92/107 (86%)	92 (100%)	0	100	100
67	VV	67/67 (100%)	67 (100%)	0	100	100
68	WW	112/113 (99%)	112 (100%)	0	100	100
69	XX	112/115 (97%)	112 (100%)	0	100	100
70	YY	107/112 (96%)	107 (100%)	0	100	100
71	ZZ	66/103 (64%)	66 (100%)	0	100	100
72	aa	88/98 (90%)	88 (100%)	0	100	100
73	bb	75/76 (99%)	75 (100%)	0	100	100
74	cc	55/62 (89%)	55 (100%)	0	100	100
75	dd	48/49 (98%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	ee	46/106 (43%)	46 (100%)	0	100	100
77	ff	61/140 (44%)	60 (98%)	1 (2%)	58	84
78	gg	272/275 (99%)	270 (99%)	2 (1%)	81	94
81	j	73/80 (91%)	73 (100%)	0	100	100
All	All	9738/10943 (89%)	9727 (100%)	11 (0%)	92	98

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	G	212	HIS
15	L	67	HIS
18	O	106	ASP
22	S	84	TYR
48	CC	248	TYR
60	OO	65	ASP
64	SS	83	PHE
65	TT	33	TRP
77	ff	140	TYR
78	gg	90	TRP
78	gg	107	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	38	HIS
5	A	216	HIS
6	B	55	HIS
6	B	109	HIS
6	B	167	GLN
6	B	204	GLN
6	B	289	GLN
6	B	376	HIS
7	C	38	ASN
8	D	45	ASN
8	D	244	HIS
9	E	170	GLN
9	E	185	ASN
9	E	194	GLN
9	E	253	GLN
10	G	91	ASN

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Mol	Chain	Res	Type
10	G	134	ASN
10	G	153	HIS
10	G	202	ASN
11	H	8	GLN
11	H	42	ASN
11	H	78	GLN
11	H	108	ASN
11	H	188	GLN
12	I	59	GLN
12	I	73	ASN
12	I	144	ASN
12	I	213	HIS
13	J	71	HIS
13	J	104	ASN
14	K	79	ASN
14	K	199	HIS
16	M	20	HIS
16	M	131	GLN
17	N	8	GLN
17	N	87	HIS
17	N	156	HIS
18	O	50	ASN
19	P	116	HIS
20	Q	7	HIS
21	R	141	HIS
21	R	143	HIS
21	R	158	GLN
24	U	94	ASN
25	V	77	HIS
25	V	135	ASN
26	W	17	HIS
26	W	59	HIS
26	W	63	GLN
27	X	93	ASN
27	X	107	HIS
28	Y	20	ASN
28	Y	56	GLN
31	b	101	HIS
33	d	100	ASN
35	f	20	ASN
37	h	65	GLN
38	i	36	HIS

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Mol	Chain	Res	Type
40	l	4	HIS
40	l	33	ASN
43	o	105	GLN
44	p	72	ASN
45	r	30	ASN
45	r	45	HIS
45	r	70	GLN
46	AA	132	GLN
47	BB	53	GLN
47	BB	158	HIS
47	BB	163	GLN
47	BB	179	ASN
48	CC	272	HIS
49	DD	145	GLN
50	EE	157	ASN
50	EE	188	ASN
50	EE	260	GLN
51	FF	83	ASN
51	FF	179	ASN
52	GG	110	ASN
52	GG	155	GLN
53	HH	44	ASN
53	HH	73	GLN
54	II	181	GLN
55	JJ	113	GLN
55	JJ	124	HIS
56	KK	28	HIS
57	LL	18	GLN
57	LL	106	HIS
57	LL	112	HIS
58	MM	19	GLN
59	NN	105	ASN
60	OO	32	HIS
62	QQ	24	HIS
62	QQ	80	GLN
64	SS	11	HIS
64	SS	76	GLN
65	TT	51	ASN
68	WW	113	HIS
69	XX	46	HIS
69	XX	92	ASN
70	YY	29	HIS

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Mol	Chain	Res	Type
70	YY	63	HIS
71	ZZ	46	ASN
71	ZZ	89	GLN
72	aa	17	HIS
73	bb	84	HIS
78	gg	56	GLN
78	gg	117	ASN
78	gg	187	ASN
78	gg	191	HIS
81	j	66	HIS
81	j	76	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3579/3601 (99%)	552 (15%)	172 (4%)
2	7	118/120 (98%)	6 (5%)	0
3	8	149/156 (95%)	19 (12%)	3 (2%)
4	9	1686/1869 (90%)	232 (13%)	64 (3%)
79	10	10/185 (5%)	2 (20%)	0
80	11	73/75 (97%)	13 (17%)	5 (6%)
80	13	73/75 (97%)	11 (15%)	5 (6%)
All	All	5688/6081 (93%)	835 (14%)	249 (4%)

All (835) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	13	U
1	5	15	A
1	5	25	A
1	5	39	A
1	5	42	A
1	5	43	U
1	5	59	A
1	5	65	A
1	5	91	G
1	5	109	G
1	5	119	G
1	5	120	A
1	5	122	U
1	5	126	C

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Mol	Chain	Res	Type
1	5	134	G
1	5	135	G
1	5	136	C
1	5	143	C
1	5	144	G
1	5	159	C
1	5	160	G
1	5	171	U
1	5	172	C
1	5	200	U
1	5	201	C
1	5	202	C
1	5	209	U
1	5	217	C
1	5	218	A
1	5	219	G
1	5	220	C
1	5	224	U
1	5	226	G
1	5	227	A
1	5	233	U
1	5	234	G
1	5	246	G
1	5	265	C
1	5	266	C
1	5	267	G
1	5	275	C
1	5	276	C
1	5	280	G
1	5	297	U
1	5	306	A
1	5	309	C
1	5	315	G
1	5	316	U
1	5	334	A
1	5	340	C
1	5	362	A
1	5	386	A
1	5	387	G
1	5	408	A
1	5	409	G
1	5	410	A

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Mol	Chain	Res	Type
1	5	412	G
1	5	413	G
1	5	431	G
1	5	432	U
1	5	449	C
1	5	450	G
1	5	452	A
1	5	453	G
1	5	454	U
1	5	467	U
1	5	468	U
1	5	481	G
1	5	481(A)	C
1	5	482	G
1	5	483	G
1	5	484	U
1	5	485	C
1	5	486	C
1	5	492	U
1	5	493	G
1	5	498	C
1	5	499	G
1	5	505	G
1	5	666	G
1	5	667	A
1	5	668	C
1	5	683	C
1	5	686	A
1	5	696	C
1	5	697	G
1	5	704	C
1	5	705	G
1	5	730	G
1	5	731	G
1	5	738	C
1	5	739	G
1	5	747	A
1	5	748	G
1	5	749	G
1	5	758	G
1	5	913	U
1	5	914	U

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Mol	Chain	Res	Type
1	5	915	A
1	5	916	C
1	5	917	A
1	5	923	C
1	5	924	C
1	5	925	C
1	5	926	G
1	5	929	A
1	5	930	G
1	5	931	C
1	5	932	A
1	5	934	C
1	5	935	A
1	5	935(A)	G
1	5	936	C
1	5	937	U
1	5	941	C
1	5	944	A
1	5	945	U
1	5	959	G
1	5	960	A
1	5	961	G
1	5	967	C
1	5	969	C
1	5	971(A)	G
1	5	972	C
1	5	973	G
1	5	979	C
1	5	983	C
1	5	1065	G
1	5	1070	G
1	5	1072	C
1	5	1073	G
1	5	1076	C
1	5	1079	C
1	5	1180	C
1	5	1195	G
1	5	1211	G
1	5	1212	G
1	5	1214	C
1	5	1215	C
1	5	1234	G

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Mol	Chain	Res	Type
1	5	1235	G
1	5	1236	C
1	5	1237	C
1	5	1238	A
1	5	1239	C
1	5	1244	G
1	5	1248	C
1	5	1249	C
1	5	1250	C
1	5	1272	C
1	5	1273	G
1	5	1283	G
1	5	1284	G
1	5	1287	G
1	5	1292	C
1	5	1293	G
1	5	1296	G
1	5	1297	U
1	5	1301	C
1	5	1304	C
1	5	1326	A
1	5	1337	A
1	5	1339	U
1	5	1354	A
1	5	1359	G
1	5	1370	G
1	5	1371	A
1	5	1377	G
1	5	1378	C
1	5	1380	G
1	5	1381	U
1	5	1387	A
1	5	1388	A
1	5	1394	G
1	5	1397	A
1	5	1398	A
1	5	1421	G
1	5	1437	C
1	5	1438	U
1	5	1441	C
1	5	1445	U
1	5	1446	C

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Mol	Chain	Res	Type
1	5	1456	C
1	5	1458	C
1	5	1478	C
1	5	1482	G
1	5	1483	C
1	5	1484	G
1	5	1485	C
1	5	1486	C
1	5	1498	G
1	5	1502	G
1	5	1523	A
1	5	1534	A
1	5	1566	C
1	5	1578	U
1	5	1591	U
1	5	1596	U
1	5	1602	U
1	5	1612	G
1	5	1613	A
1	5	1614	C
1	5	1624	G
1	5	1625	G
1	5	1631	A
1	5	1633	G
1	5	1634	A
1	5	1641	G
1	5	1654	G
1	5	1661	C
1	5	1676	C
1	5	1677	U
1	5	1691	G
1	5	1724	G
1	5	1733	G
1	5	1734	G
1	5	1741	G
1	5	1742	A
1	5	1750	G
1	5	1755	C
1	5	1756	U
1	5	1761	G
1	5	1764	G
1	5	1766	A

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Mol	Chain	Res	Type
1	5	1768	C
1	5	1769	G
1	5	1773	U
1	5	1787	A
1	5	1805	A
1	5	1819	G
1	5	1821	G
1	5	1834	U
1	5	1836	G
1	5	1837	A
1	5	1842	G
1	5	1855	G
1	5	1869	G
1	5	1897	A
1	5	1899	G
1	5	1918	U
1	5	1921	C
1	5	1922	G
1	5	1930	U
1	5	1931	C
1	5	1940	G
1	5	1948	G
1	5	1958	A
1	5	1962	A
1	5	1964	A
1	5	1978	C
1	5	1980	U
1	5	1981	G
1	5	1982	G
1	5	1983	A
1	5	1984	A
1	5	1987	C
1	5	1991	A
1	5	1992	U
1	5	1993	C
1	5	2004	U
1	5	2005	G
1	5	2007	G
1	5	2008	U
1	5	2011	C
1	5	2017	A
1	5	2026	A

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Mol	Chain	Res	Type
1	5	2044	U
1	5	2048	U
1	5	2052	G
1	5	2055	G
1	5	2056	G
1	5	2068	C
1	5	2069	A
1	5	2084	U
1	5	2089	G
1	5	2090	U
1	5	2092	G
1	5	2093	G
1	5	2094	C
1	5	2097	A
1	5	2098	G
1	5	2100	G
1	5	2102	G
1	5	2104	A
1	5	2106	G
1	5	2107	A
1	5	2108	G
1	5	2259	G
1	5	2260	C
1	5	2266	C
1	5	2267	U
1	5	2268	A
1	5	2269	C
1	5	2289	C
1	5	2300	A
1	5	2301	G
1	5	2313	A
1	5	2314	G
1	5	2332	A
1	5	2333	G
1	5	2348	G
1	5	2351	C
1	5	2395	A
1	5	2396	A
1	5	2397	G
1	5	2422	C
1	5	2441	C
1	5	2475	G

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Mol	Chain	Res	Type
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2503	G
1	5	2504	C
1	5	2505	C
1	5	2506	G
1	5	2507	A
1	5	2511	A
1	5	2513	A
1	5	2520	C
1	5	2546	G
1	5	2547	G
1	5	2553	A
1	5	2554	U
1	5	2555	G
1	5	2587	A
1	5	2601	A
1	5	2602	G
1	5	2669	C
1	5	2686	G
1	5	2687	U
1	5	2695	A
1	5	2696	A
1	5	2705	G
1	5	2708	U
1	5	2709	C
1	5	2712	G
1	5	2719	C
1	5	2724	G
1	5	2725	A
1	5	2726	G
1	5	2740	U
1	5	2743	A
1	5	2760	G
1	5	2761	U
1	5	2763	U
1	5	2764	A
1	5	2772	C
1	5	2787	A
1	5	2788	U

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Mol	Chain	Res	Type
1	5	2790	U
1	5	2794	C
1	5	2795	A
1	5	2796	G
1	5	2814	C
1	5	2826	U
1	5	2827	G
1	5	2828	U
1	5	2855	G
1	5	3598	C
1	5	3604	A
1	5	3605	C
1	5	3614	G
1	5	3615	G
1	5	3625	G
1	5	3626	G
1	5	3635	A
1	5	3644	U
1	5	3662	A
1	5	3672	G
1	5	3673	C
1	5	3674	G
1	5	3696	C
1	5	3711	A
1	5	3712	A
1	5	3714	G
1	5	3748	A
1	5	3750	G
1	5	3753	G
1	5	3759	A
1	5	3760	A
1	5	3761	C
1	5	3777	G
1	5	3783	A
1	5	3784	A
1	5	3785	A
1	5	3811	G
1	5	3817	A
1	5	3819	G
1	5	3838	U
1	5	3839	G
1	5	3840	U

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Mol	Chain	Res	Type
1	5	3877	A
1	5	3878	C
1	5	3879	G
1	5	3888	G
1	5	3889	G
1	5	3897	G
1	5	3901	A
1	5	3905	A
1	5	3906	A
1	5	3907	G
1	5	3908	A
1	5	3915	U
1	5	3939	G
1	5	3949	A
1	5	3950	U
1	5	3952	A
1	5	3960	A
1	5	3963	A
1	5	3964	U
1	5	3966	A
1	5	3967	G
1	5	3969	G
1	5	3971	G
1	5	3972	A
1	5	3973	G
1	5	3976	C
1	5	4041	C
1	5	4042	G
1	5	4046	A
1	5	4047	A
1	5	4048	A
1	5	4049	U
1	5	4069	U
1	5	4070	U
1	5	4076	G
1	5	4077	A
1	5	4085	A
1	5	4119	C
1	5	4120	U
1	5	4121	G
1	5	4122	G
1	5	4125	C

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Mol	Chain	Res	Type
1	5	4127	A
1	5	4128	A
1	5	4162	C
1	5	4163	U
1	5	4170	A
1	5	4183	G
1	5	4184	G
1	5	4191	G
1	5	4203	A
1	5	4229	U
1	5	4233	A
1	5	4251	A
1	5	4255	A
1	5	4258	C
1	5	4266	G
1	5	4268	A
1	5	4271	A
1	5	4273	A
1	5	4281	A
1	5	4291	G
1	5	4292	A
1	5	4305	G
1	5	4306	U
1	5	4330	G
1	5	4339	A
1	5	4349	C
1	5	4350	C
1	5	4354	U
1	5	4355	G
1	5	4373	G
1	5	4376	A
1	5	4377	G
1	5	4378	A
1	5	4380	A
1	5	4387	C
1	5	4394	A
1	5	4395	U
1	5	4396	A
1	5	4422	A
1	5	4438	U
1	5	4448	G
1	5	4449	A

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Mol	Chain	Res	Type
1	5	4452	U
1	5	4464	A
1	5	4476	C
1	5	4500	U
1	5	4512	U
1	5	4513	A
1	5	4519	C
1	5	4522	G
1	5	4524	G
1	5	4527	G
1	5	4528	G
1	5	4548	A
1	5	4549	G
1	5	4567	G
1	5	4575	G
1	5	4590	A
1	5	4626	A
1	5	4627	U
1	5	4635	A
1	5	4636	U
1	5	4637	G
1	5	4656	A
1	5	4670	C
1	5	4672	A
1	5	4700	A
1	5	4709	U
1	5	4719	G
1	5	4720	C
1	5	4721	G
1	5	4736	C
1	5	4737	G
1	5	4745	G
1	5	4751	G
1	5	4754	G
1	5	4757	C
1	5	4759	C
1	5	4765	G
1	5	4771	C
1	5	4870	G
1	5	4871	C
1	5	4874	A
1	5	4876	A

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Mol	Chain	Res	Type
1	5	4877	G
1	5	4882	U
1	5	4883	C
1	5	4885	U
1	5	4895	C
1	5	4909	A
1	5	4910	A
1	5	4913	G
1	5	4914	G
1	5	4915	G
1	5	4926	C
1	5	4927	G
1	5	4934	A
1	5	4937	C
1	5	4943	A
1	5	4944	C
1	5	4945	G
1	5	4948	C
1	5	4951	G
1	5	4956	A
1	5	4958	C
1	5	4976	U
1	5	4988	U
1	5	4989	U
1	5	4990	C
1	5	4991	U
1	5	4993	G
1	5	5017	G
1	5	5041	G
1	5	5047	C
1	5	5050	C
1	5	5054	C
1	5	5058	A
1	5	5062	G
2	7	7	G
2	7	42	A
2	7	53	U
2	7	64	G
2	7	100	A
2	7	110	G
3	8	2	G
3	8	3	A

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Mol	Chain	Res	Type
3	8	34	U
3	8	35	C
3	8	59	A
3	8	62	A
3	8	63	U
3	8	87	G
3	8	94	G
3	8	104	A
3	8	105	C
3	8	110	U
3	8	111	U
3	8	114	G
3	8	123	U
3	8	125	C
3	8	126	C
3	8	127	U
3	8	137	A
4	9	4	C
4	9	17	C
4	9	25	A
4	9	33	G
4	9	41	G
4	9	46	A
4	9	56	G
4	9	58	C
4	9	59	U
4	9	67	C
4	9	68	A
4	9	73	C
4	9	74	G
4	9	75	G
4	9	79	A
4	9	103	A
4	9	111	A
4	9	113	G
4	9	115	U
4	9	126	G
4	9	127	C
4	9	143	U
4	9	147	A
4	9	155	G
4	9	161	U

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Mol	Chain	Res	Type
4	9	162	C
4	9	182	C
4	9	183	G
4	9	184	G
4	9	188	C
4	9	192	C
4	9	215	G
4	9	294	U
4	9	309	G
4	9	312	G
4	9	319	C
4	9	323	C
4	9	347	G
4	9	362	C
4	9	364	A
4	9	369	C
4	9	370	G
4	9	383	G
4	9	385	G
4	9	386	C
4	9	400	C
4	9	401	A
4	9	407	G
4	9	408	A
4	9	409	C
4	9	418	A
4	9	448	A
4	9	449	A
4	9	450	C
4	9	452	G
4	9	465	A
4	9	466	G
4	9	472	C
4	9	474	G
4	9	482	G
4	9	487	U
4	9	492	C
4	9	516	A
4	9	517	C
4	9	532	C
4	9	533	A
4	9	544	G

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Mol	Chain	Res	Type
4	9	550	C
4	9	551	U
4	9	554	A
4	9	555	A
4	9	556	U
4	9	559	G
4	9	564	A
4	9	568	C
4	9	569	A
4	9	587	A
4	9	588	G
4	9	590	A
4	9	591	U
4	9	606	G
4	9	607	U
4	9	608	C
4	9	614	C
4	9	620	G
4	9	621	C
4	9	628	A
4	9	643	A
4	9	644	G
4	9	668	A
4	9	669	A
4	9	671	A
4	9	672	A
4	9	673	G
4	9	690	G
4	9	744	G
4	9	745	C
4	9	752	G
4	9	753	C
4	9	754	G
4	9	798	G
4	9	799	U
4	9	811	A
4	9	821	G
4	9	822	U
4	9	830	A
4	9	842	C
4	9	847	A
4	9	859	G

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Mol	Chain	Res	Type
4	9	869	A
4	9	870	A
4	9	872	A
4	9	873	G
4	9	874	G
4	9	875	A
4	9	876	C
4	9	887	U
4	9	888	U
4	9	889	U
4	9	909	G
4	9	913	A
4	9	914	U
4	9	920	A
4	9	922	A
4	9	933	G
4	9	943	U
4	9	971	G
4	9	990	A
4	9	992	A
4	9	1017	U
4	9	1023	A
4	9	1062	A
4	9	1083	A
4	9	1085	C
4	9	1115	U
4	9	1118	C
4	9	1119	A
4	9	1133	A
4	9	1138	C
4	9	1139	C
4	9	1150	A
4	9	1153	C
4	9	1154	U
4	9	1195	A
4	9	1207	G
4	9	1208	A
4	9	1215	C
4	9	1216	C
4	9	1242	U
4	9	1251	A
4	9	1253	A

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Mol	Chain	Res	Type
4	9	1254	C
4	9	1256	G
4	9	1257	G
4	9	1259	A
4	9	1274	G
4	9	1275	G
4	9	1285	G
4	9	1286	G
4	9	1293	A
4	9	1300	U
4	9	1301	A
4	9	1302	G
4	9	1309	C
4	9	1371	U
4	9	1372	U
4	9	1378	A
4	9	1396	A
4	9	1397	U
4	9	1401	A
4	9	1404	U
4	9	1428	G
4	9	1429	G
4	9	1454	A
4	9	1455	A
4	9	1462	U
4	9	1463	U
4	9	1466	G
4	9	1477	U
4	9	1490	G
4	9	1497	G
4	9	1498	A
4	9	1509	U
4	9	1521	C
4	9	1522	A
4	9	1533	A
4	9	1548	G
4	9	1552	G
4	9	1553	C
4	9	1554	C
4	9	1556	A
4	9	1557	C
4	9	1567	G

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Mol	Chain	Res	Type
4	9	1574	C
4	9	1579	A
4	9	1580	A
4	9	1587	G
4	9	1588	A
4	9	1601	A
4	9	1621	U
4	9	1623	A
4	9	1637	A
4	9	1638	G
4	9	1639	G
4	9	1648	G
4	9	1654	G
4	9	1665	G
4	9	1671	G
4	9	1680	G
4	9	1699	A
4	9	1721	U
4	9	1722	G
4	9	1748	G
4	9	1753	C
4	9	1756	C
4	9	1757	G
4	9	1783	C
4	9	1785	C
4	9	1823	A
4	9	1824	A
4	9	1829	G
4	9	1834	A
4	9	1835	A
4	9	1836	G
4	9	1837	G
4	9	1838	U
4	9	1849	G
4	9	1852	C
4	9	1861	G
4	9	1863	A
4	9	1865	C
4	9	1869	A
79	10	19	U
79	10	20	U
80	13	17	C

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Mol	Chain	Res	Type
80	13	18	G
80	13	20	A
80	13	22	G
80	13	47	U
80	13	48	C
80	13	58	A
80	13	59	A
80	13	74	C
80	13	75	C
80	13	76	A
80	11	10	G
80	11	11	G
80	11	17	C
80	11	18	G
80	11	20	A
80	11	22	G
80	11	47	U
80	11	48	C
80	11	58	A
80	11	59	A
80	11	74	C
80	11	75	C
80	11	76	A

All (249) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	42	A
1	5	64	A
1	5	125	C
1	5	134	G
1	5	201	C
1	5	217	C
1	5	218	A
1	5	224	U
1	5	226	G
1	5	245	C
1	5	262	G
1	5	265	C
1	5	266	C
1	5	275	C
1	5	294	G

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Mol	Chain	Res	Type
1	5	309	C
1	5	315	G
1	5	385	A
1	5	408	A
1	5	432	U
1	5	449	C
1	5	467	U
1	5	480	C
1	5	481(A)	C
1	5	484	U
1	5	485	C
1	5	492	U
1	5	504	G
1	5	667	A
1	5	685	C
1	5	696	C
1	5	747	A
1	5	913	U
1	5	915	A
1	5	916	C
1	5	924	C
1	5	929	A
1	5	930	G
1	5	933	G
1	5	935(A)	G
1	5	936	C
1	5	955	G
1	5	959	G
1	5	960	A
1	5	966	A
1	5	971(A)	G
1	5	972	C
1	5	1072	C
1	5	1211	G
1	5	1214	C
1	5	1236	C
1	5	1237	C
1	5	1238	A
1	5	1249	C
1	5	1283	G
1	5	1292	C
1	5	1294	A

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Mol	Chain	Res	Type
1	5	1324	A
1	5	1358	G
1	5	1359	G
1	5	1370	G
1	5	1377	G
1	5	1380	G
1	5	1387	A
1	5	1440	U
1	5	1445	U
1	5	1455	G
1	5	1477	C
1	5	1483	C
1	5	1484	G
1	5	1485	C
1	5	1534	A
1	5	1590	C
1	5	1613	A
1	5	1625	G
1	5	1633	G
1	5	1654	G
1	5	1733	G
1	5	1741	G
1	5	1804	A
1	5	1818	G
1	5	1835	G
1	5	1898	C
1	5	1921	C
1	5	1929	A
1	5	1977	C
1	5	1982	G
1	5	1992	U
1	5	2001	G
1	5	2002	A
1	5	2007	G
1	5	2010	A
1	5	2016	C
1	5	2068	C
1	5	2089	G
1	5	2093	G
1	5	2106	G
1	5	2110	G
1	5	2266	C

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Mol	Chain	Res	Type
1	5	2267	U
1	5	2268	A
1	5	2313	A
1	5	2396	A
1	5	2421	G
1	5	2428	A
1	5	2474	G
1	5	2502	A
1	5	2505	C
1	5	2506	G
1	5	2513	A
1	5	2529	A
1	5	2546	G
1	5	2553	A
1	5	2587	A
1	5	2696	A
1	5	2711	G
1	5	2724	G
1	5	2725	A
1	5	2761	U
1	5	2763	U
1	5	2787	A
1	5	2794	C
1	5	3603	G
1	5	3614	G
1	5	3625	G
1	5	3672	G
1	5	3673	C
1	5	3710	G
1	5	3784	A
1	5	3810	C
1	5	3876	A
1	5	3888	G
1	5	3904	G
1	5	3949	A
1	5	3951	G
1	5	3956	G
1	5	3959	U
1	5	3966	A
1	5	3968	U
1	5	3972	A
1	5	4041	C

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Mol	Chain	Res	Type
1	5	4046	A
1	5	4047	A
1	5	4069	U
1	5	4084	G
1	5	4119	C
1	5	4121	G
1	5	4124	G
1	5	4127	A
1	5	4232	U
1	5	4254	G
1	5	4291	G
1	5	4305	G
1	5	4395	U
1	5	4448	G
1	5	4464	A
1	5	4527	G
1	5	4572	U
1	5	4626	A
1	5	4635	A
1	5	4699	U
1	5	4884	G
1	5	4909	A
1	5	4921	C
1	5	4925	U
1	5	4926	C
1	5	4931	G
1	5	4936	G
1	5	4942	C
1	5	4947	U
1	5	4975	G
1	5	5061	A
3	8	2	G
3	8	51	U
3	8	124	U
4	9	24	C
4	9	58	C
4	9	72	C
4	9	74	G
4	9	110	U
4	9	126	G
4	9	141	A
4	9	142	C

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Mol	Chain	Res	Type
4	9	160	U
4	9	182	C
4	9	369	C
4	9	400	C
4	9	448	A
4	9	465	A
4	9	516	A
4	9	532	C
4	9	553	U
4	9	555	A
4	9	568	C
4	9	587	A
4	9	591	U
4	9	606	G
4	9	620	G
4	9	752	G
4	9	821	G
4	9	869	A
4	9	870	A
4	9	872	A
4	9	873	G
4	9	875	A
4	9	919	A
4	9	1016	U
4	9	1061	U
4	9	1087	A
4	9	1115	U
4	9	1118	C
4	9	1137	U
4	9	1138	C
4	9	1153	C
4	9	1165	G
4	9	1215	C
4	9	1253	A
4	9	1274	G
4	9	1285	G
4	9	1300	U
4	9	1308	U
4	9	1395	C
4	9	1396	A
4	9	1428	G
4	9	1454	A

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Mol	Chain	Res	Type
4	9	1463	U
4	9	1488	C
4	9	1489	A
4	9	1497	G
4	9	1553	C
4	9	1556	A
4	9	1636	G
4	9	1637	A
4	9	1638	G
4	9	1679	A
4	9	1757	G
4	9	1837	G
4	9	1863	A
4	9	1868	U
80	13	16	G
80	13	19	G
80	13	20	A
80	13	58	A
80	13	74	C
80	11	10	G
80	11	16	G
80	11	19	G
80	11	58	A
80	11	74	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\# Z > 2$
85	MET	13	102	80	6,7,8	0.45	0	2,7,9	0.38	0
84	ATP	13	101	80	28,33,33	0.66	0	34,52,52	0.85	1 (2%)
82	SPD	5	5101	-	9,9,9	0.29	0	8,8,8	0.51	0
84	ATP	11	101	80	28,33,33	0.72	0	34,52,52	1.03	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	MET	13	102	80	-	0/5/6/8	-
84	ATP	13	101	80	-	1/18/38/38	0/3/3/3
82	SPD	5	5101	-	-	0/7/7/7	-
84	ATP	11	101	80	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	11	101	ATP	O4'-C1'-N9	3.36	113.20	108.75
84	13	101	ATP	C5-C6-N6	2.27	123.77	120.31
84	11	101	ATP	C5-C6-N6	2.22	123.70	120.31

There are no chirality outliers.

All (3) torsion outliers are listed below:

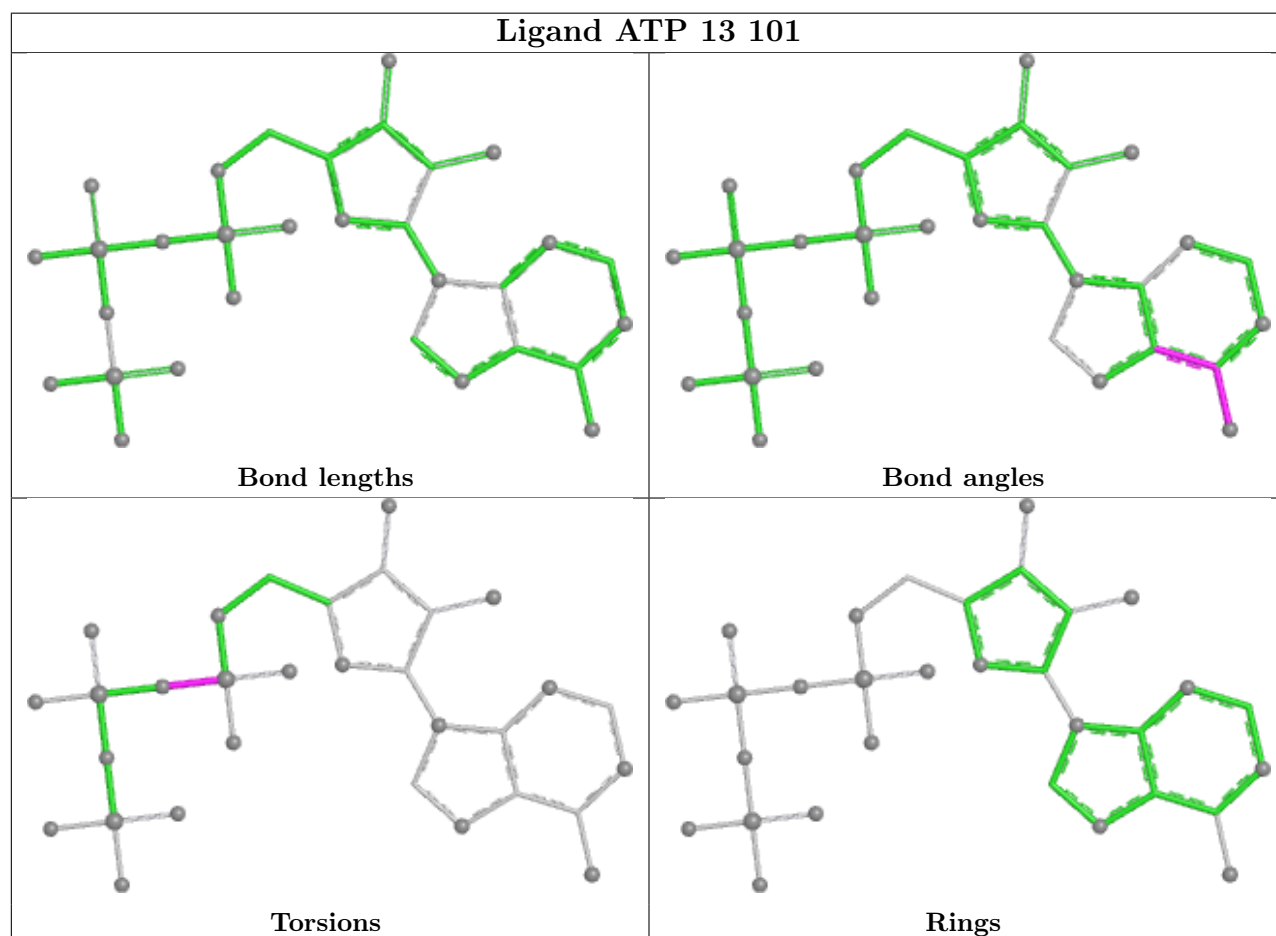
Mol	Chain	Res	Type	Atoms
84	11	101	ATP	O4'-C4'-C5'-O5'
84	13	101	ATP	PB-O3A-PA-O5'
84	11	101	ATP	C3'-C4'-C5'-O5'

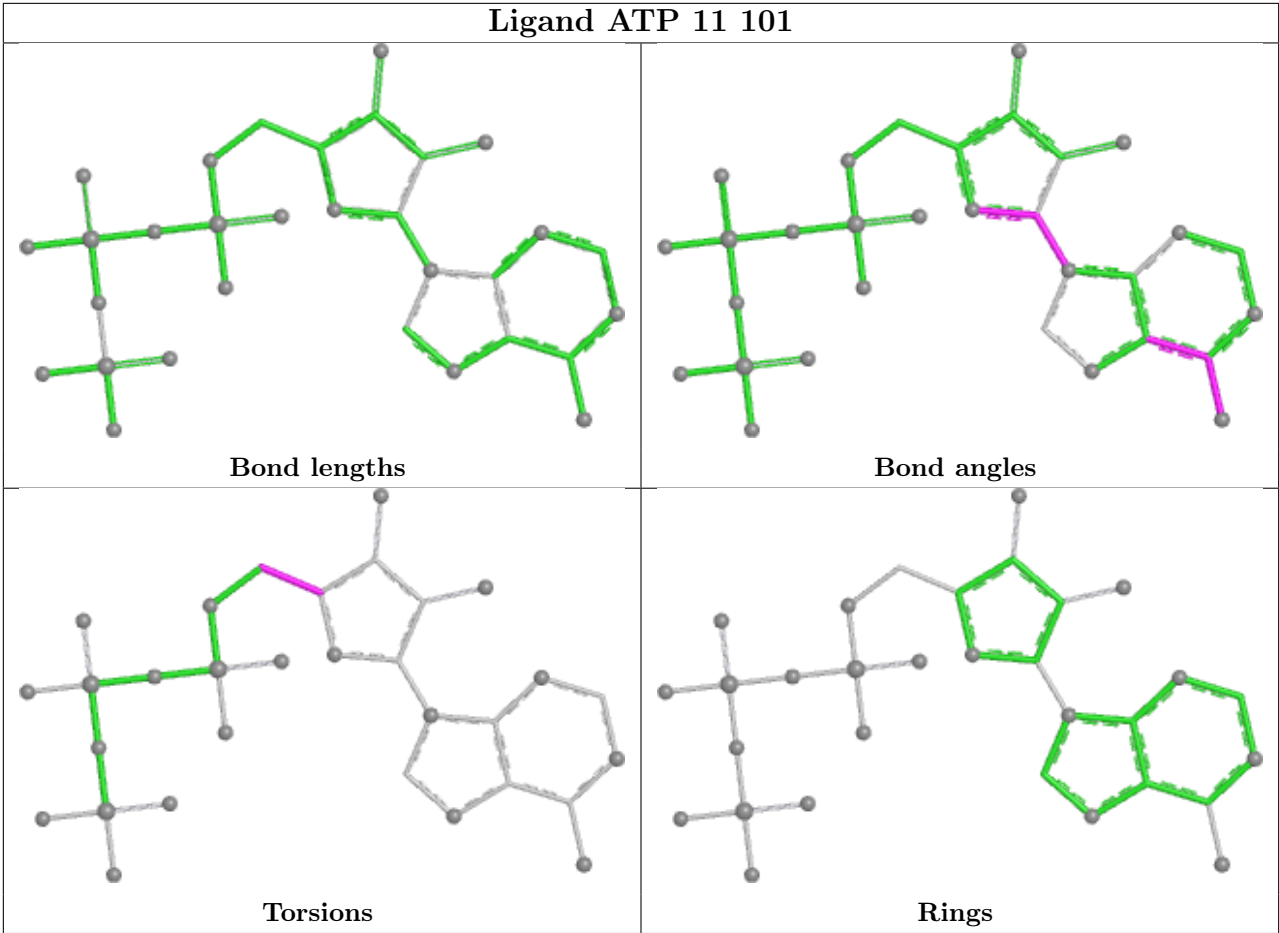
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	11	101	ATP	2	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	23

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.67
1	5	1252:C	O3'	1271:G	P	35.00
1	5	1219:G	O3'	1233:G	P	21.32
1	5	523:C	O3'	638:G	P	18.06
1	5	1406(C):G	O3'	1411:C	P	17.72

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	4101:C	O3'	4107:G	P	17.29
1	5	990:C	O3'	1064:G	P	17.19
1	5	3976:C	O3'	4035:G	P	17.13
1	5	4777:C	O3'	4859:C	P	16.96
1	5	4138:C	O3'	4146:G	P	16.64
1	5	1696:C	O3'	1720:C	P	15.27
1	5	5022:U	O3'	5028:G	P	14.79
1	5	1364:U	O3'	1368:A	P	14.58
1	5	760:G	O3'	904:C	P	14.27
1	5	2901:G	O3'	3597:G	P	12.93
1	5	182:G	O3'	189:G	P	11.15
1	5	1180:C	O3'	1183:C	P	9.90
1	5	4729:A	O3'	4735:G	P	9.87
1	5	512:U	O3'	515:C	P	8.17
1	5	500:G	O3'	504:G	P	6.21
1	5	4740:G	O3'	4743:G	P	6.01
1	5	1100:U	O3'	1168:G	P	5.43
1	5	4899:G	O3'	4902:C	P	3.02

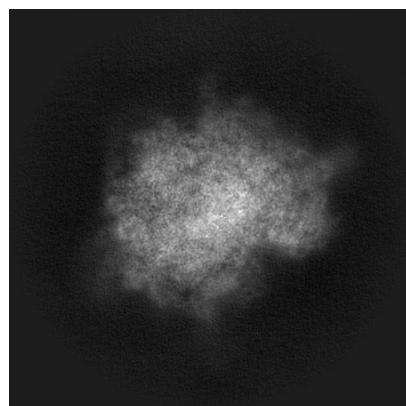
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73316. These allow visual inspection of the internal detail of the map and identification of artifacts.

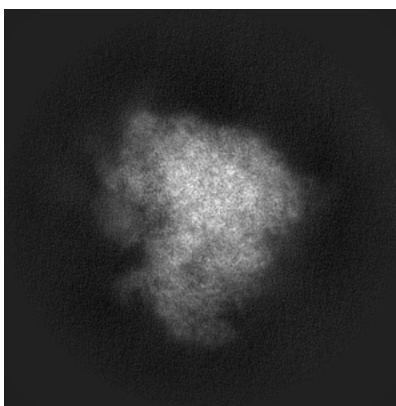
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

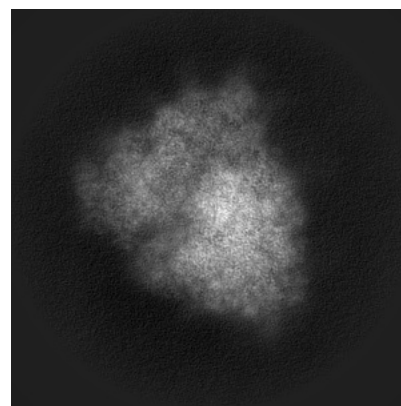
6.1.1 Primary map



X

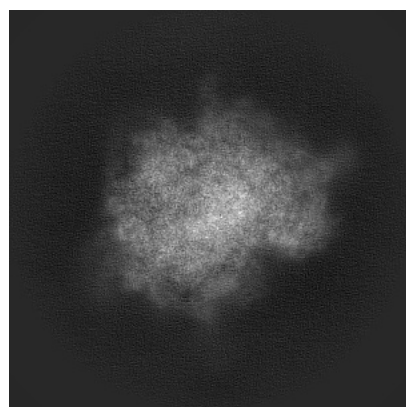


Y

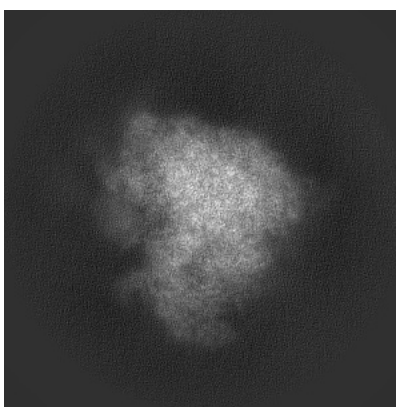


Z

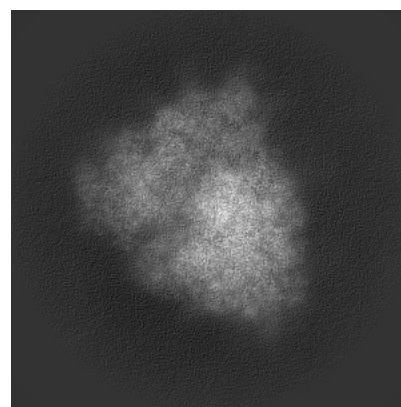
6.1.2 Raw map



X



Y

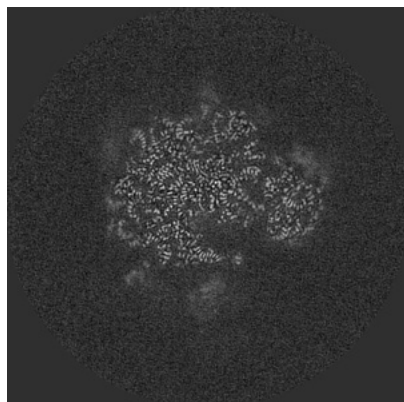


Z

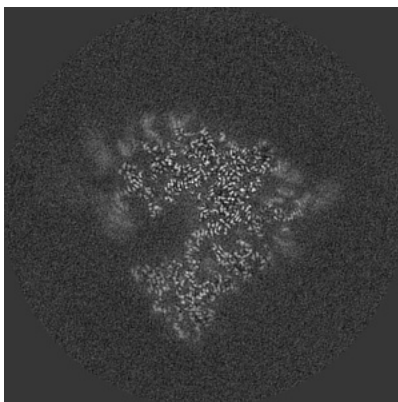
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

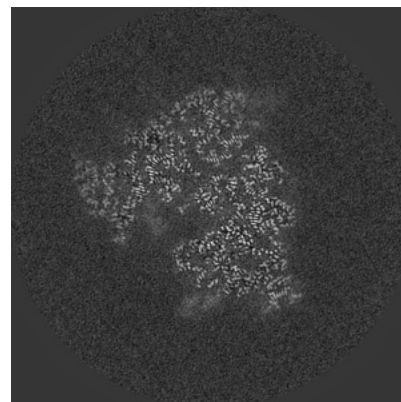
6.2.1 Primary map



X Index: 200

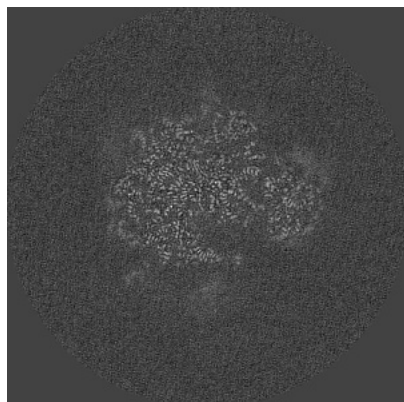


Y Index: 200

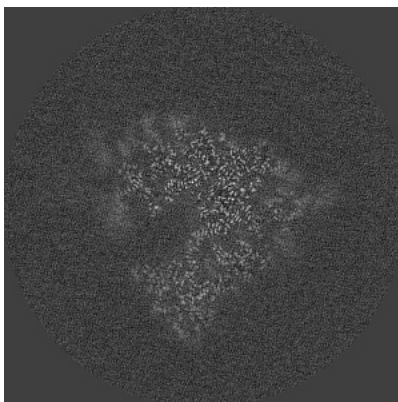


Z Index: 200

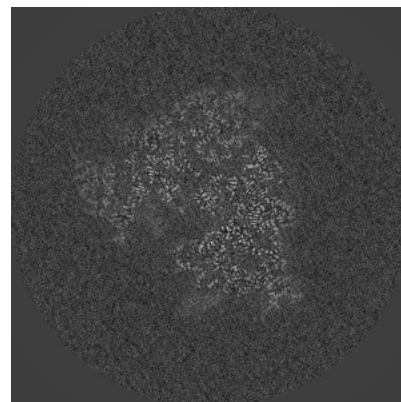
6.2.2 Raw map



X Index: 200



Y Index: 200

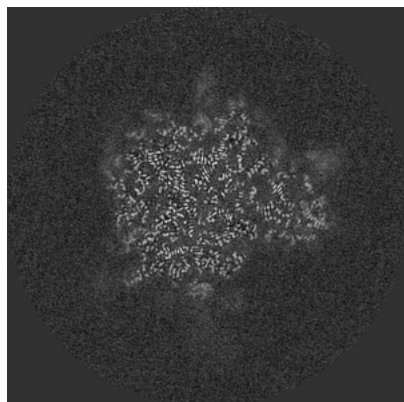


Z Index: 200

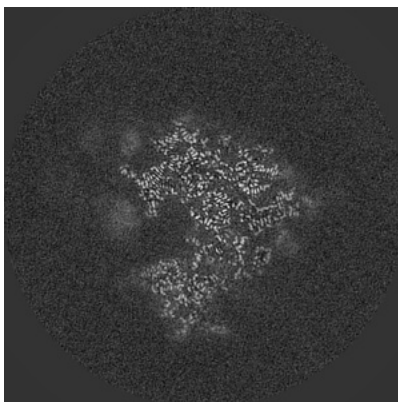
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

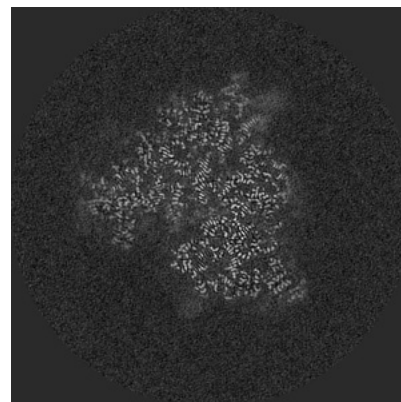
6.3.1 Primary map



X Index: 214

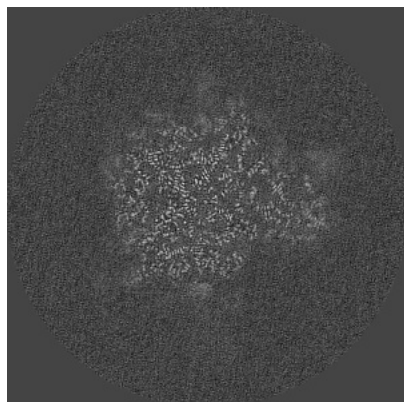


Y Index: 209

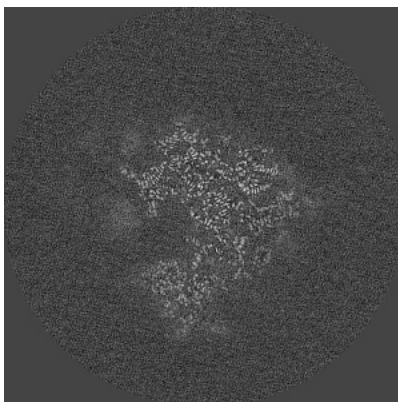


Z Index: 192

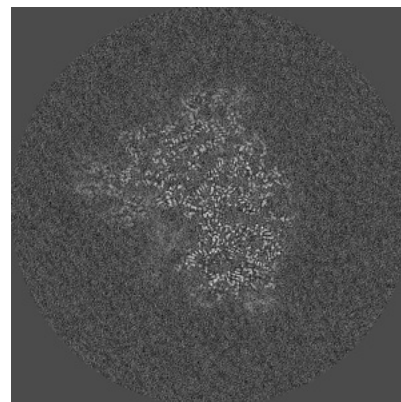
6.3.2 Raw map



X Index: 214



Y Index: 209

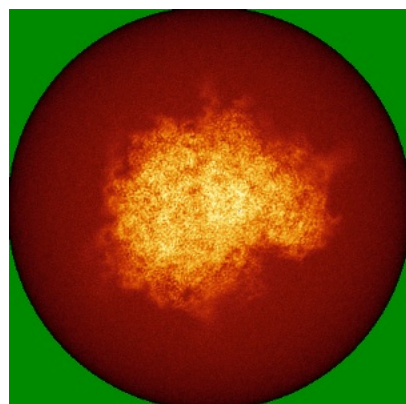


Z Index: 212

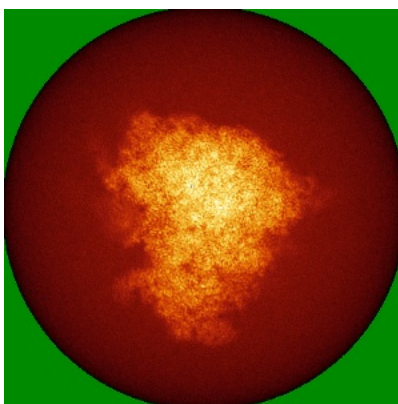
The images above show the largest variance slices of the map in three orthogonal directions.

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

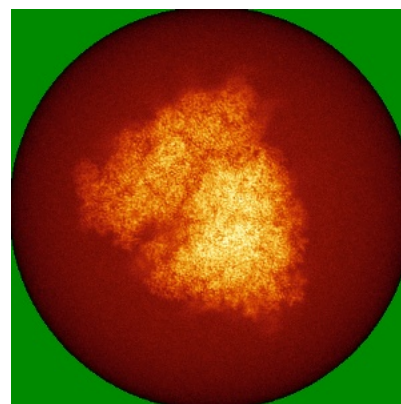
6.4.1 Primary map



X

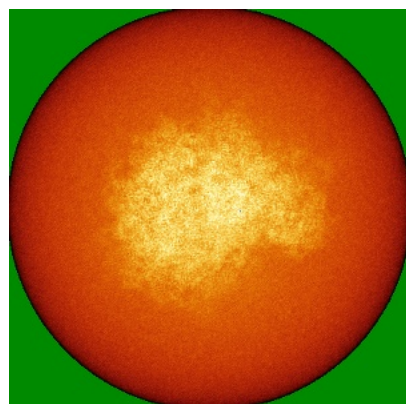


Y

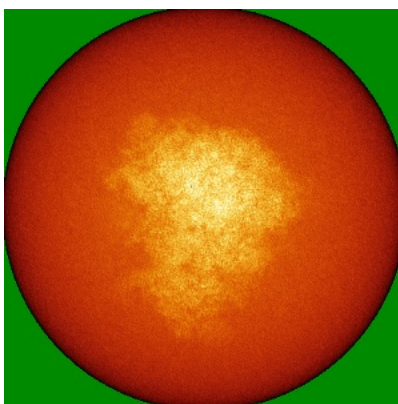


Z

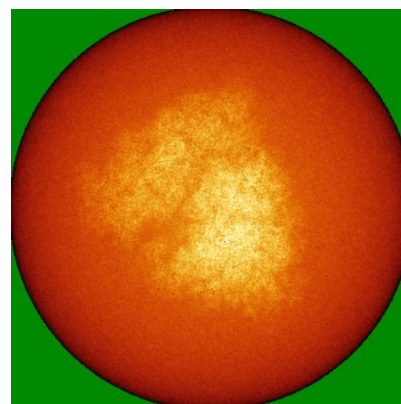
6.4.2 Raw map



X



Y

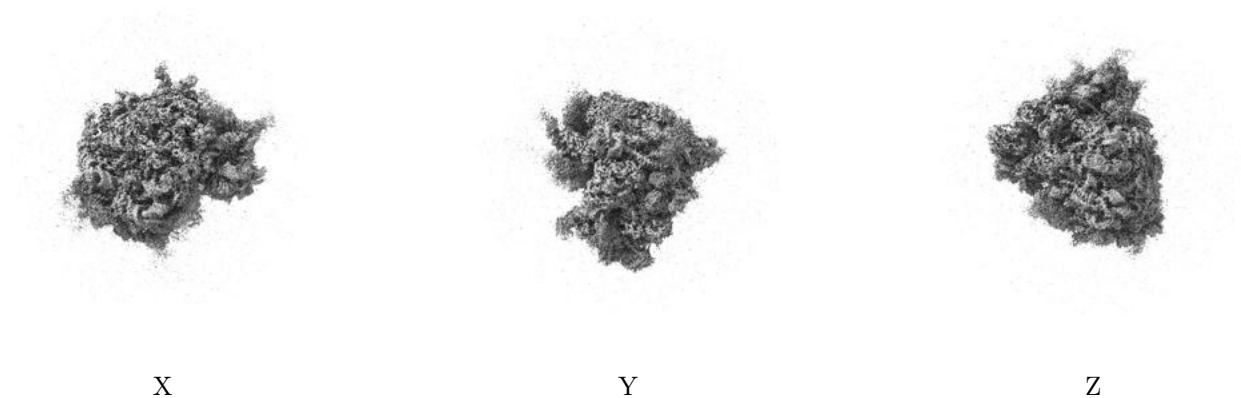


Z

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.

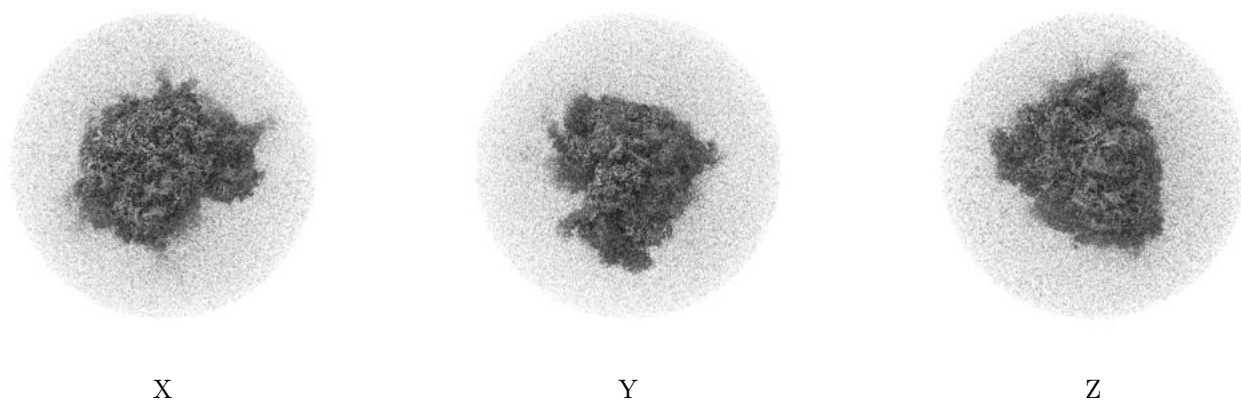
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

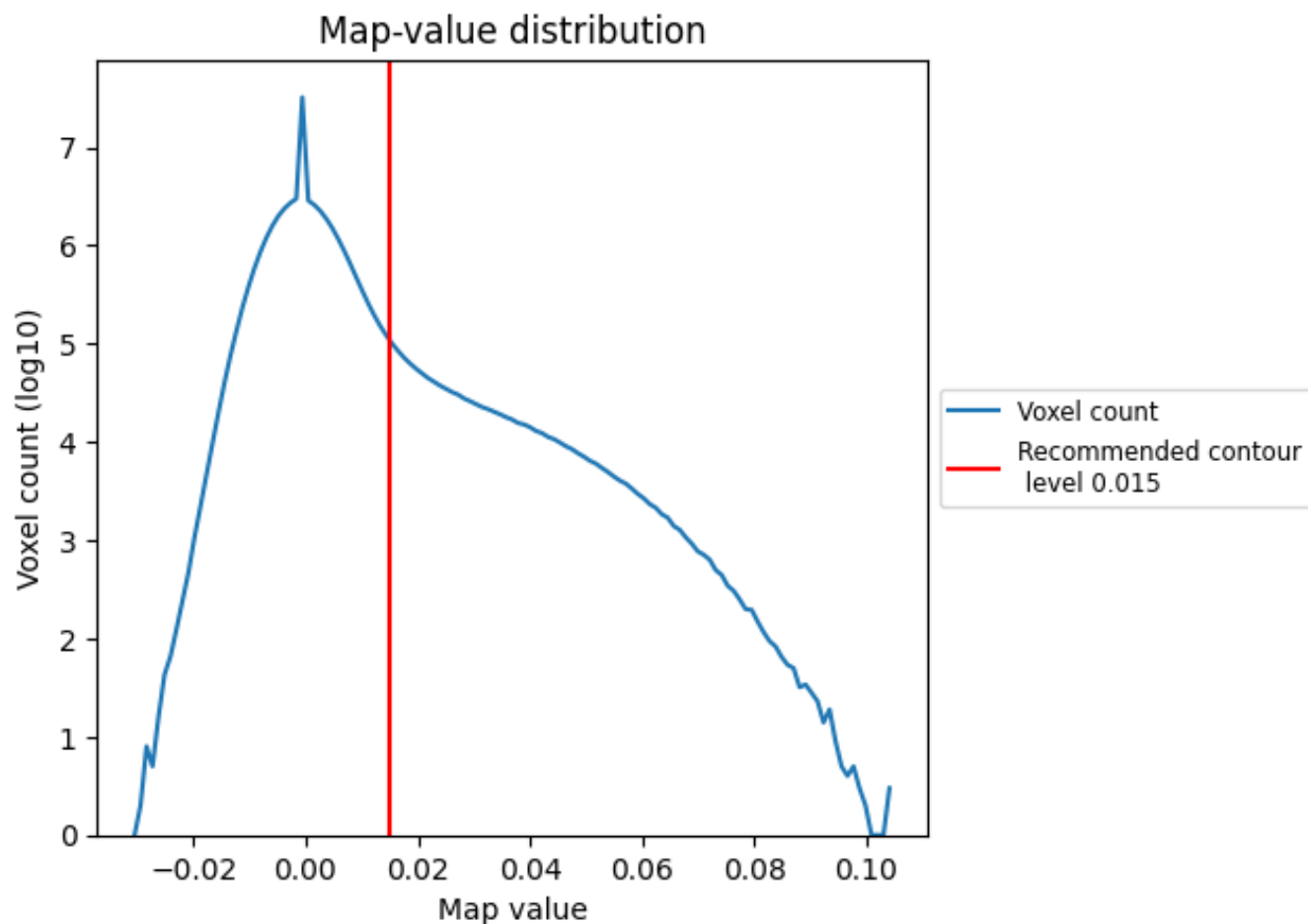
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

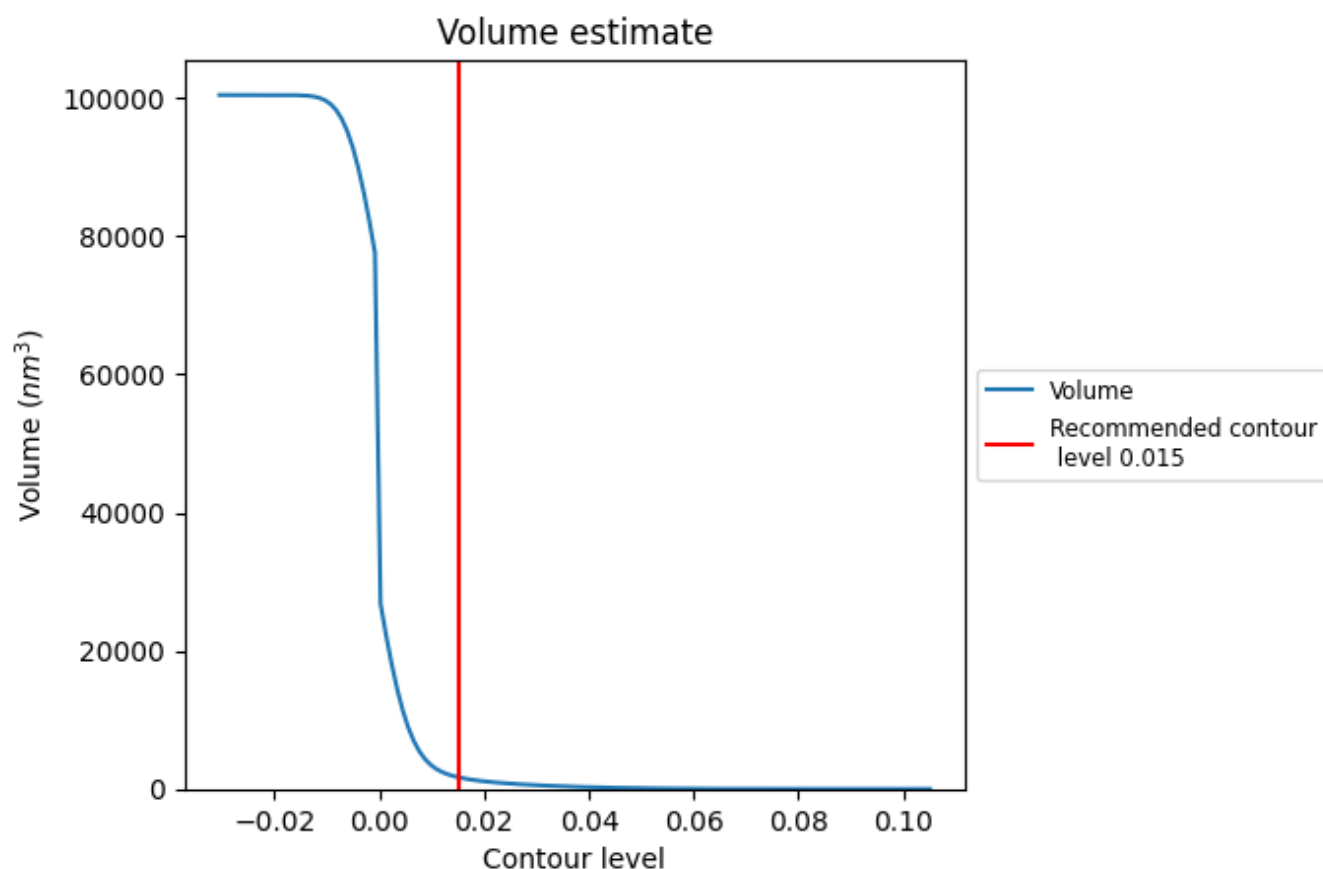
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

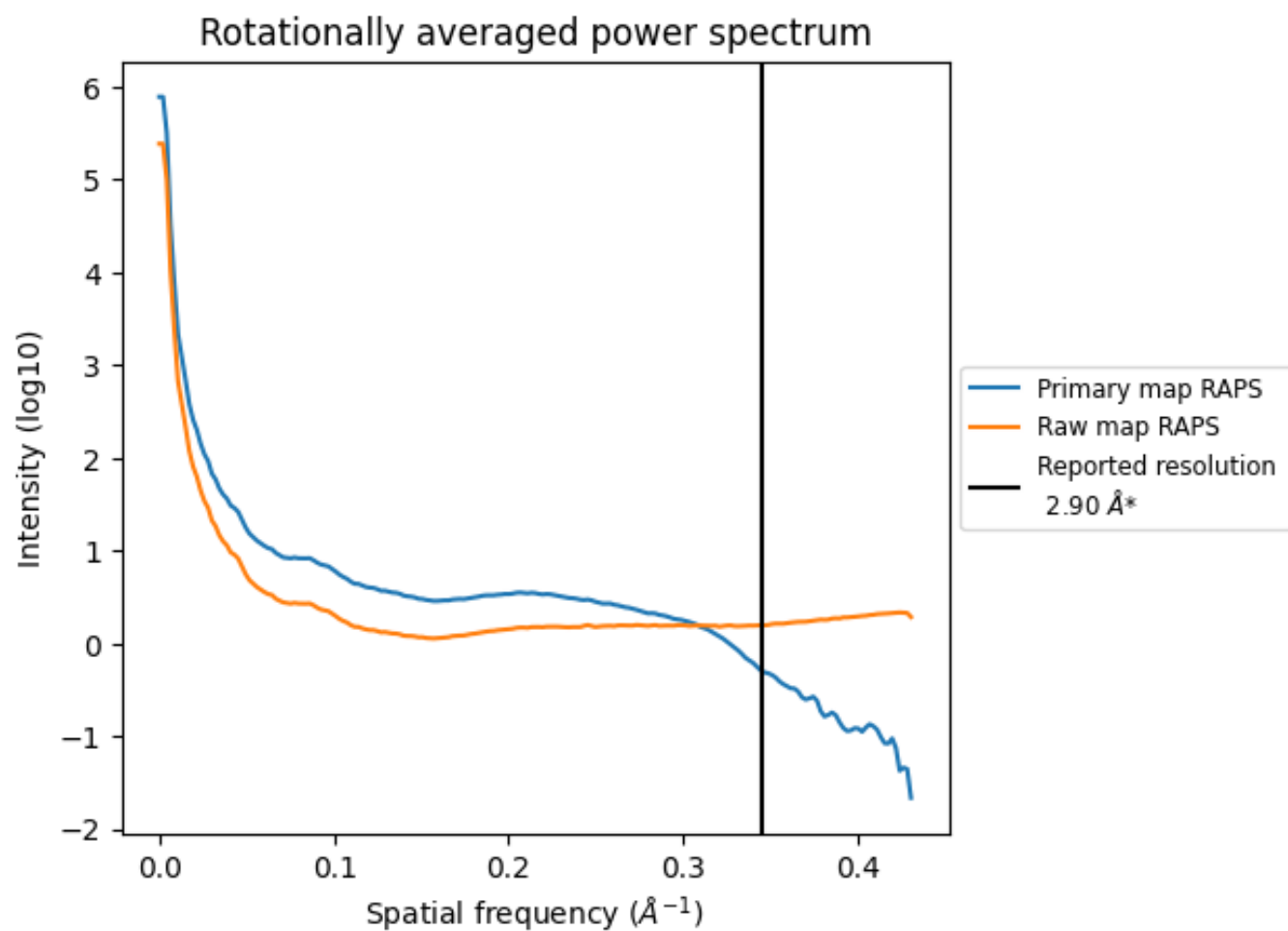
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1708 nm^3 ; this corresponds to an approximate mass of 1543 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 ⓘ

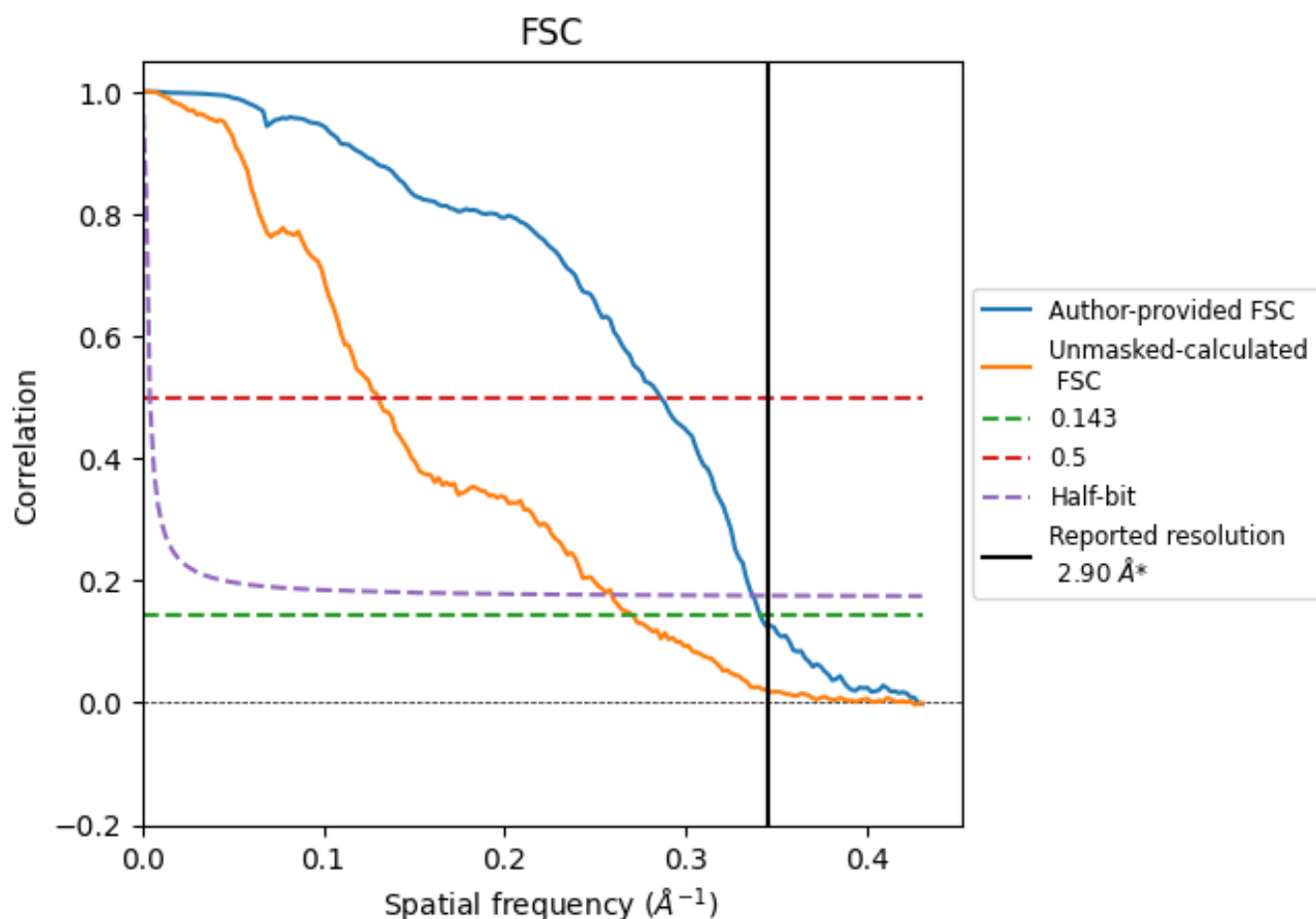


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

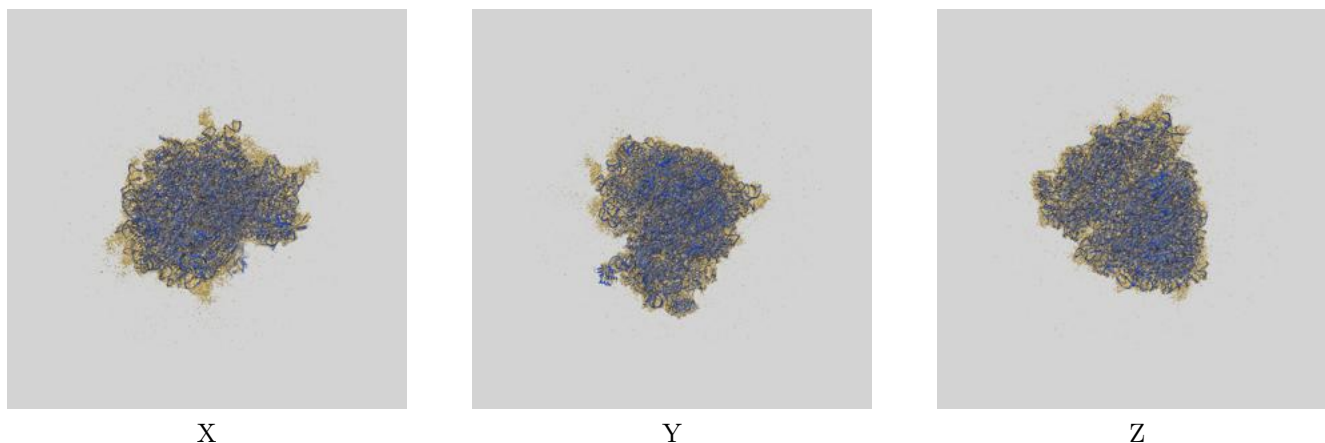
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.93	3.50	2.97
Unmasked-calculated*	3.70	7.69	3.86

*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 3.70 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

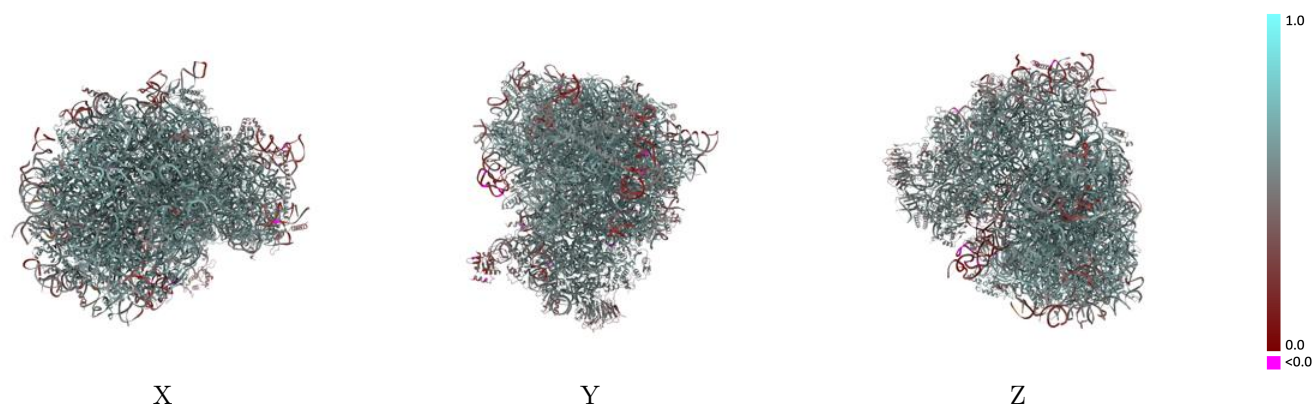
This section contains information regarding the fit between EMDB map EMD-73316 and PDB model 9YQ0. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



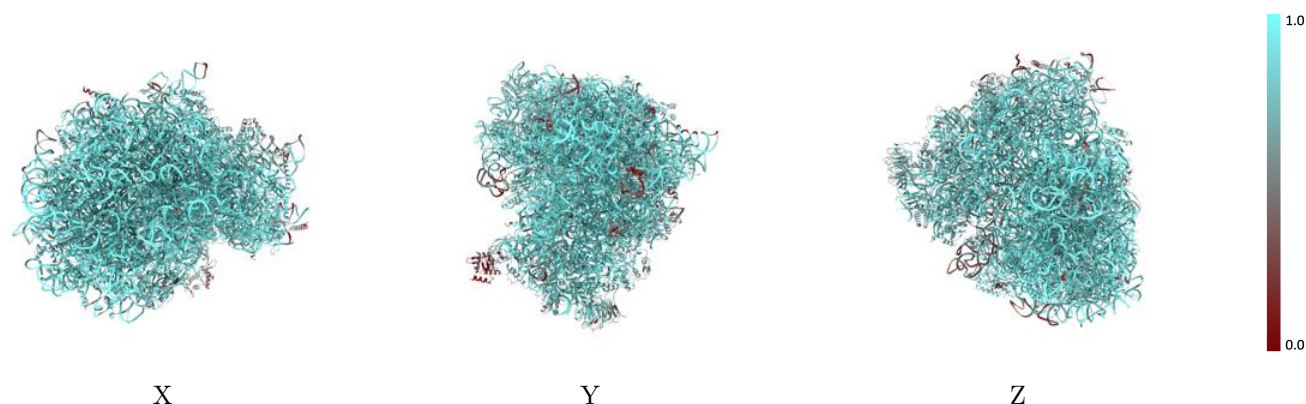
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



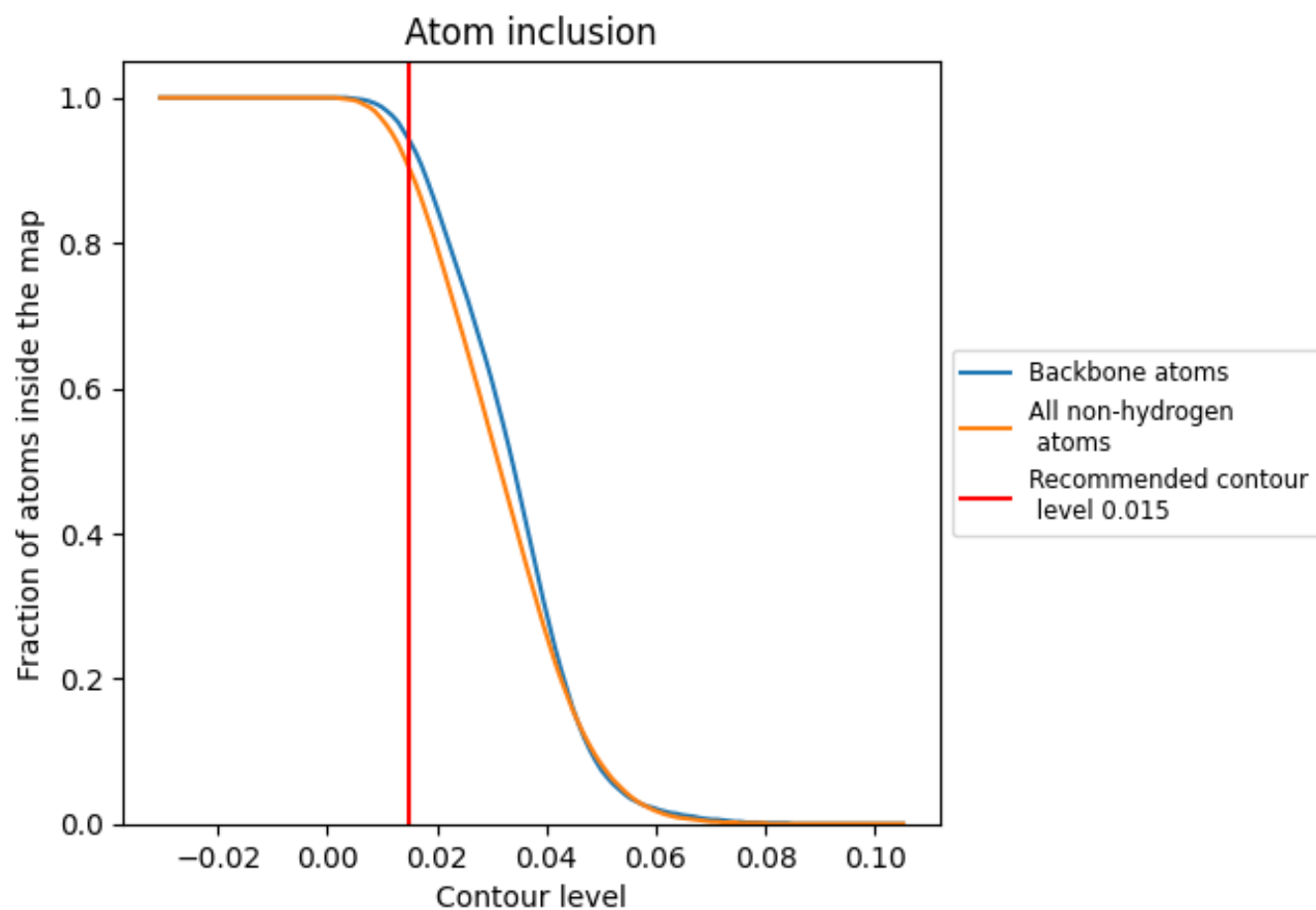
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.5540
10	 0.8500	 0.5010
11	 0.6150	 0.2550
13	 0.9090	 0.4840
5	 0.9380	 0.5560
7	 0.9940	 0.6080
8	 0.9730	 0.5810
9	 0.9390	 0.5510
A	 0.9560	 0.6150
AA	 0.8320	 0.5490
B	 0.9210	 0.5970
BB	 0.8520	 0.5590
C	 0.9250	 0.5970
CC	 0.8820	 0.5680
D	 0.8800	 0.5710
DD	 0.7730	 0.5090
E	 0.8770	 0.5570
EE	 0.8760	 0.5630
FF	 0.8330	 0.5330
G	 0.8160	 0.5440
GG	 0.7740	 0.4960
H	 0.8730	 0.5750
HH	 0.6870	 0.4880
I	 0.9040	 0.5860
II	 0.8700	 0.5600
J	 0.8400	 0.5470
JJ	 0.8410	 0.5460
K	 0.9360	 0.6040
KK	 0.7710	 0.4860
L	 0.8690	 0.5770
LL	 0.9040	 0.5820
M	 0.8910	 0.5740
MM	 0.2360	 0.2760
N	 0.9750	 0.6180
NN	 0.8820	 0.5670















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Chain	Atom inclusion	Q-score
O	 0.9390	 0.6010
OO	 0.8860	 0.5740
P	 0.9310	 0.6010
PP	 0.7470	 0.4890
Q	 0.9330	 0.6100
QQ	 0.8470	 0.5530
R	 0.8820	 0.5660
RR	 0.7590	 0.5190
S	 0.9330	 0.6020
SS	 0.8070	 0.5160
T	 0.8890	 0.5780
TT	 0.8240	 0.5260
U	 0.8030	 0.5100
UU	 0.7180	 0.4770
V	 0.9230	 0.5970
VV	 0.8120	 0.5360
W	 0.7760	 0.5130
WW	 0.9100	 0.5850
X	 0.8990	 0.5850
XX	 0.9090	 0.5820
Y	 0.8780	 0.5740
YY	 0.8260	 0.5300
Z	 0.8700	 0.5710
ZZ	 0.7480	 0.5140
a	 0.9400	 0.6050
aa	 0.8940	 0.5580
b	 0.8770	 0.5540
bb	 0.7890	 0.5130
c	 0.8740	 0.5740
cc	 0.8130	 0.5300
d	 0.8910	 0.5780
dd	 0.9000	 0.5520
e	 0.9370	 0.6030
ee	 0.7180	 0.4790
f	 0.9600	 0.6150
ff	 0.3220	 0.3200
g	 0.8950	 0.5870
gg	 0.6690	 0.4410
h	 0.8810	 0.5690
i	 0.8710	 0.5530
j	 0.9630	 0.6140
k	 0.7860	 0.5300

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Chain	Atom inclusion	Q-score
l	 0.9370	 0.5990
m	 0.8970	 0.5830
n	 0.9360	 0.5940
o	 0.9210	 0.6040
p	 0.9130	 0.5980
r	 0.9280	 0.5930