



Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 12:23 PM EST

PDB ID : 9YPO / pdb_00009ypo
EMDB ID : EMD-73302
Title : GTPBP1*GCP*Phe-tRNA*ribosome in the open state, Structure IIa
Authors : Susorov, D.; Korostelev, A.A.
Deposited on : 2025-10-14
Resolution : 3.00 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

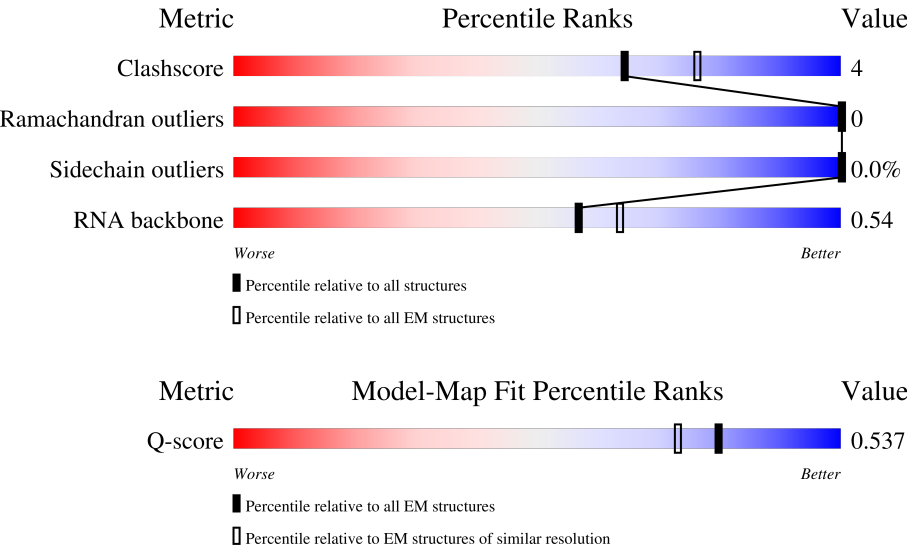
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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>68%</div> <div>27%</div> <div>5%</div> </div>
2	7	120	<div> <div>85%</div> <div>13%</div> <div>2%</div> </div>
3	8	156	<div> <div>72%</div> <div>23%</div> <div>5%</div> </div>


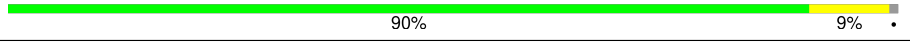
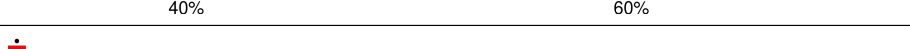
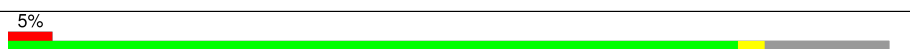

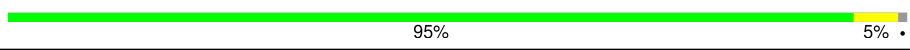
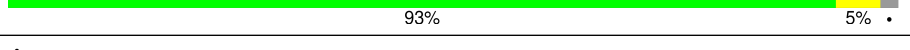
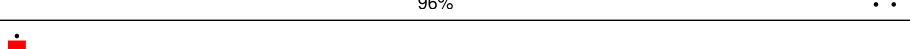


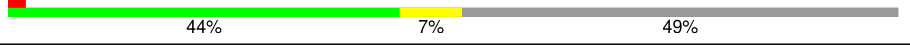
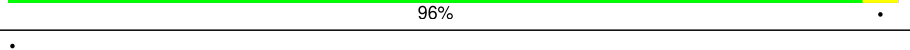

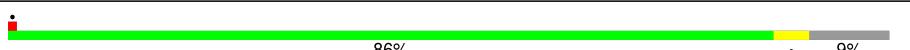


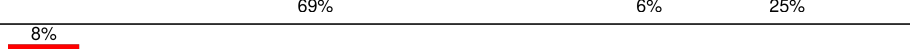







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Mol	Chain	Length	Quality of chain
4	9	1869	
5	A	257	
6	B	403	
7	C	425	
8	D	297	
9	E	291	
10	G	319	
11	H	192	
12	I	214	
13	J	178	
14	K	247	
15	L	211	
16	M	218	
17	N	204	
18	O	203	
19	P	184	
20	Q	188	
21	R	196	
22	S	176	
23	T	160	
24	U	128	
25	V	140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


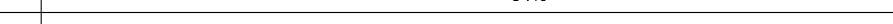




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Mol	Chain	Length	Quality of chain
54	II	208	
55	JJ	194	
56	KK	165	
57	LL	158	
58	MM	132	
59	NN	151	
60	OO	168	
61	PP	145	
62	QQ	146	
63	RR	135	
64	SS	152	
65	TT	145	
66	UU	119	
67	VV	83	
68	WW	130	
69	XX	143	
70	YY	130	
71	ZZ	125	
72	aa	115	
73	bb	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	
80	12	76	
81	11	75	
81	13	75	
82	j	97	
83	jj	703	

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 219555 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 is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	120	U	-	insertion	GB XR_011385821

- 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		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	1	C	-	insertion	GB XR_011385890
8	155	C	-	insertion	GB XR_011385890
8	156	U	-	insertion	GB XR_011385890

- 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
C	379	VAL	-	insertion	UNP G1SVW5
C	380	LYS	-	insertion	UNP G1SVW5
C	381	LYS	-	insertion	UNP G1SVW5

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Chain	Residue	Modelled	Actual	Comment	Reference
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-ribosomal protein eL40 fusion protein.

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	-	insertion	UNP P0DXC2
m	2	GLY	-	insertion	UNP P0DXC2
m	3	ASP	-	insertion	UNP P0DXC2
m	4	PRO	-	insertion	UNP P0DXC2
m	5	GLU	-	insertion	UNP P0DXC2
m	6	SER	-	insertion	UNP P0DXC2
m	7	GLY	-	insertion	UNP P0DXC2
m	8	GLY	-	insertion	UNP P0DXC2
m	9	CYS	-	insertion	UNP P0DXC2

- 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		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	101	GLY	-	insertion	UNP G1T040
o	102	GLN	-	insertion	UNP G1T040
o	103	VAL	-	insertion	UNP G1T040
o	104	ILE	-	insertion	UNP G1T040
o	105	GLN	-	insertion	UNP G1T040
o	106	PHE	-	insertion	UNP G1T040

- 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 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	13	ASP	GLY	conflict	UNP G1SWM1
CC	19	ILE	MET	conflict	UNP G1SWM1
CC	33	VAL	ILE	conflict	UNP G1SWM1
CC	97	PHE	CYS	conflict	UNP G1SWM1
CC	101	SER	ALA	conflict	UNP G1SWM1
CC	141	VAL	LEU	conflict	UNP G1SWM1
CC	181	PRO	LEU	conflict	UNP G1SWM1
CC	191	VAL	-	insertion	UNP G1SWM1
CC	215	MET	LEU	conflict	UNP G1SWM1
CC	271	ASP	ASN	conflict	UNP G1SWM1
CC	274	VAL	MET	conflict	UNP G1SWM1

- 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 Small ribosomal subunit protein eS10.

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	140	Total	C	N	O	S	0	0
			1157	728	231	197	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	57	Total	C	N	O	S	0	0
			457	282	101	73	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 Phe-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	12	75	Total	C	N	O	P	0	0
			1599	714	286	524	75		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
12	37	C	G	conflict	GB 176419

- Molecule 81 is a RNA chain called Met-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	13	74	Total	C	N	O	P	0	0
			1585	707	293	511	74		
81	11	74	Total	C	N	O	P	0	0
			1585	707	293	511	74		

- Molecule 82 is a protein called Ribosomal protein L37.

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

- Molecule 83 is a protein called GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	jj	513	Total	C	N	O	S	0	0
			3982	2508	702	748	24		

There are 34 discrepancies between the modelled and reference sequences:

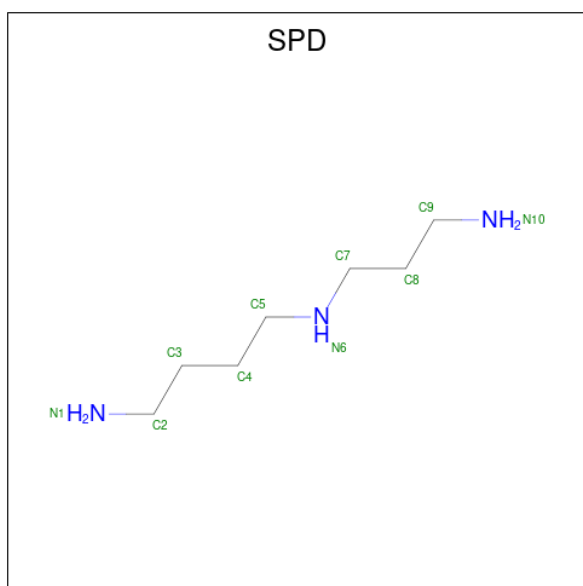
Chain	Residue	Modelled	Actual	Comment	Reference
jj	-33	MET	-	expression tag	UNP O00178
jj	-32	GLY	-	expression tag	UNP O00178
jj	-31	SER	-	expression tag	UNP O00178
jj	-30	SER	-	expression tag	UNP O00178
jj	-29	HIS	-	expression tag	UNP O00178
jj	-28	HIS	-	expression tag	UNP O00178
jj	-27	HIS	-	expression tag	UNP O00178
jj	-26	HIS	-	expression tag	UNP O00178
jj	-25	HIS	-	expression tag	UNP O00178
jj	-24	HIS	-	expression tag	UNP O00178
jj	-23	SER	-	expression tag	UNP O00178
jj	-22	SER	-	expression tag	UNP O00178
jj	-21	GLY	-	expression tag	UNP O00178
jj	-20	LEU	-	expression tag	UNP O00178
jj	-19	VAL	-	expression tag	UNP O00178
jj	-18	PRO	-	expression tag	UNP O00178
jj	-17	ARG	-	expression tag	UNP O00178
jj	-16	GLY	-	expression tag	UNP O00178
jj	-15	SER	-	expression tag	UNP O00178
jj	-14	HIS	-	expression tag	UNP O00178
jj	-13	MET	-	expression tag	UNP O00178
jj	-12	ALA	-	expression tag	UNP O00178
jj	-11	SER	-	expression tag	UNP O00178

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Chain	Residue	Modelled	Actual	Comment	Reference
jj	-10	MET	-	expression tag	UNP O00178
jj	-9	THR	-	expression tag	UNP O00178
jj	-8	GLY	-	expression tag	UNP O00178
jj	-7	GLY	-	expression tag	UNP O00178
jj	-6	GLN	-	expression tag	UNP O00178
jj	-5	GLN	-	expression tag	UNP O00178
jj	-4	MET	-	expression tag	UNP O00178
jj	-3	GLY	-	expression tag	UNP O00178
jj	-2	ARG	-	expression tag	UNP O00178
jj	-1	GLY	-	expression tag	UNP O00178
jj	0	SER	-	expression tag	UNP O00178

- Molecule 84 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
84	5	1	Total	C	N	0
			10	7	3	

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

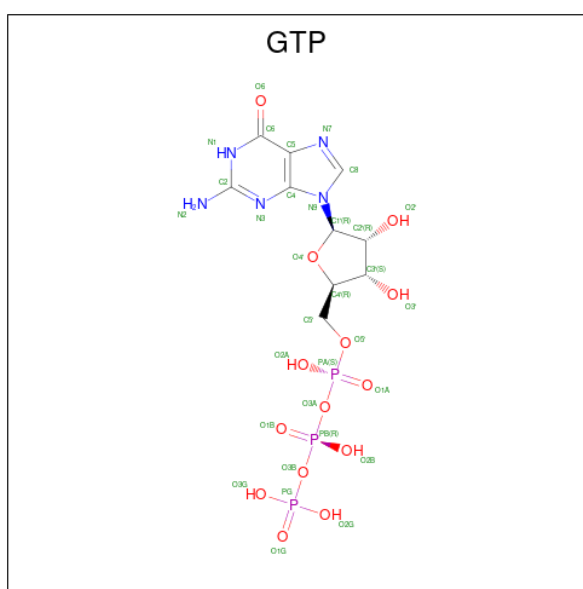
Mol	Chain	Residues	Atoms		AltConf
85	g	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	

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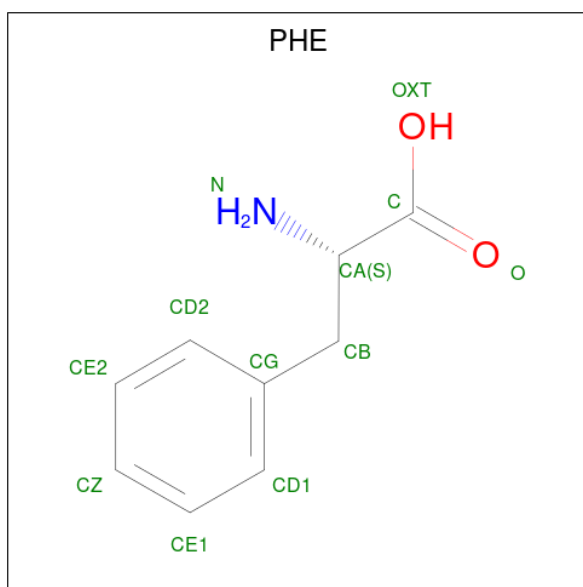
Mol	Chain	Residues	Atoms		AltConf
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	dd	1	Total	Zn	0
			1	1	
85	j	1	Total	Zn	0
			1	1	

- Molecule 86 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
86	12	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 87 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



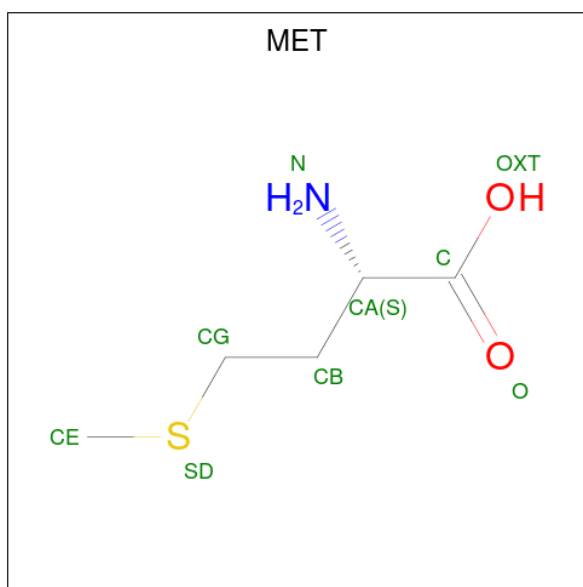
Mol	Chain	Residues	Atoms				AltConf
87	12	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 88 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



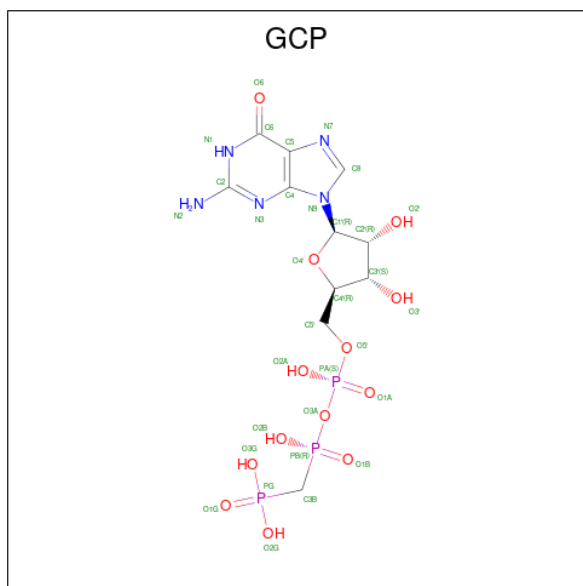
Mol	Chain	Residues	Atoms					AltConf
88	13	1	Total	C	N	O	P	0
			31	10	5	13	3	
88	11	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 89 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
89	13	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 91 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
91	jj	1	Total 1	Mg 1	0

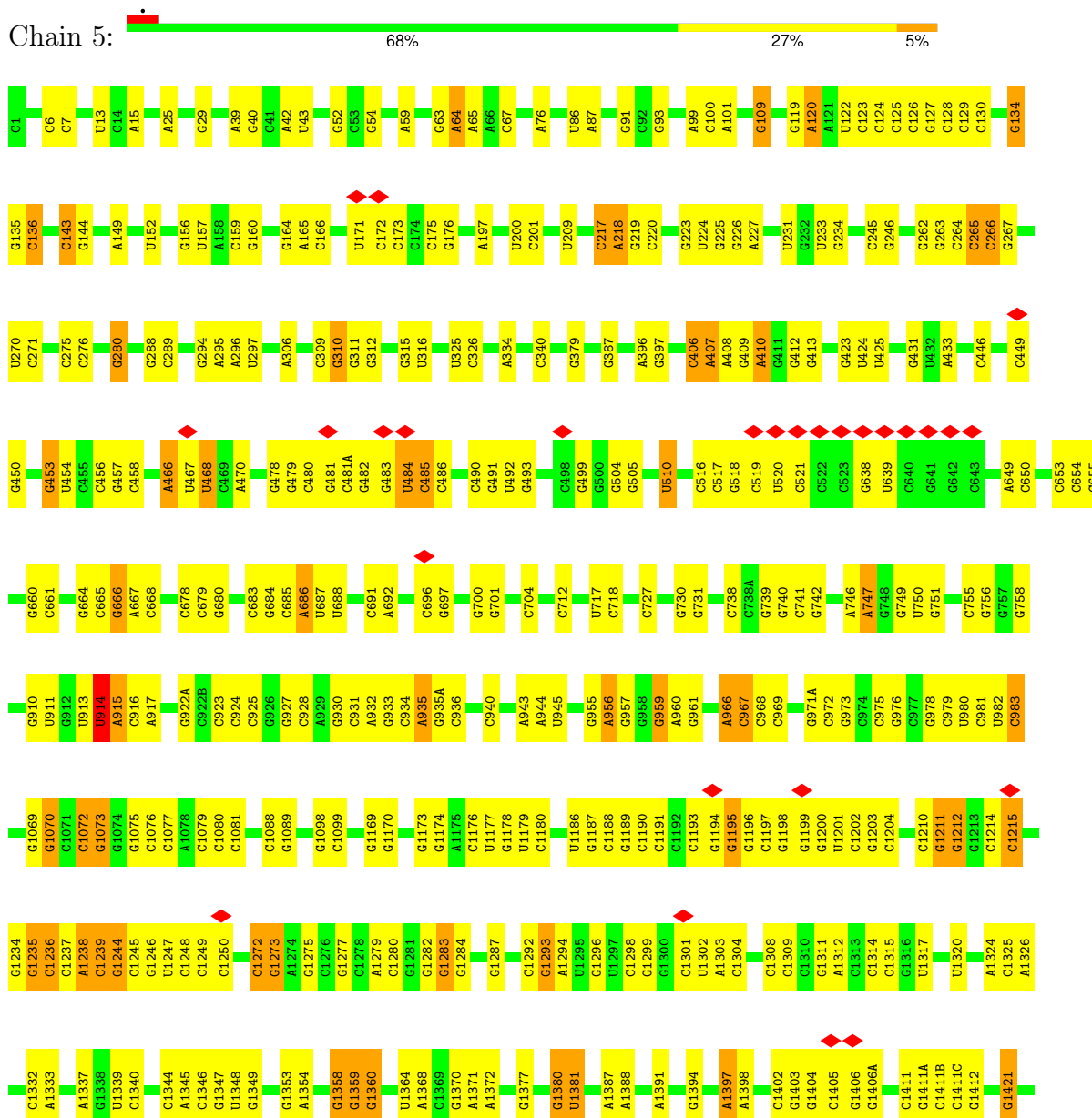
- Molecule 92 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
92	jj	1	Total 1	K 1	0

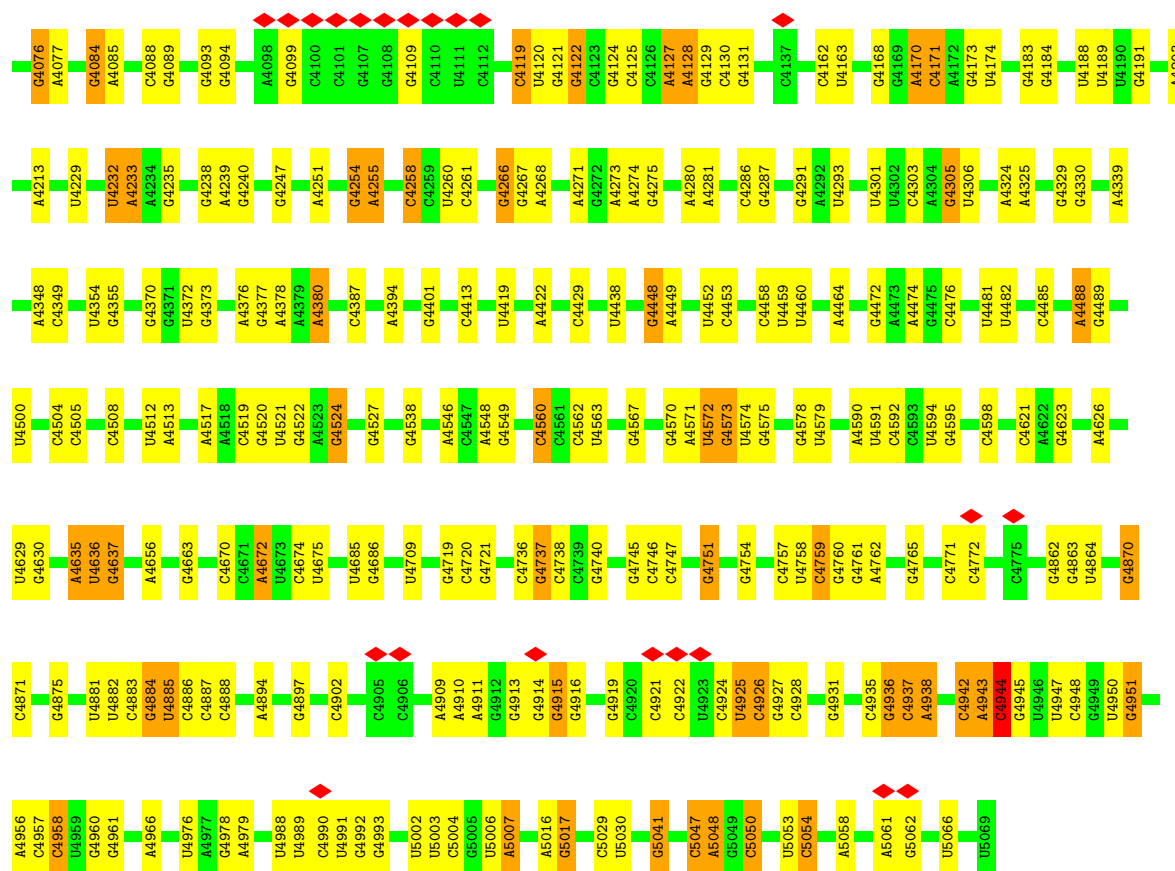
3 Residue-property plots

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



G3953	G3954	G3955	G3956	G3957	G3958	G3959	G3960	G3961	G3962	G3963	G3964	G3965	G3966	G3967	G3968	G3969	G3970	G3971	G3972	G3973	G3974	G3975	G3976	G4035	G4036	G4037	G4038	G4039	G4040	G4041	G4042	G4043	G4044	G4045	A4046	A4047	A4048	A4049	A4050	C4051	C4052	A4053	C4054	A4055	A4056	C4057	U4058	U4059	U4060	A4061	A4062	U4063	C4064	G4065	U4066	U4067	U4068	U4069	U4070																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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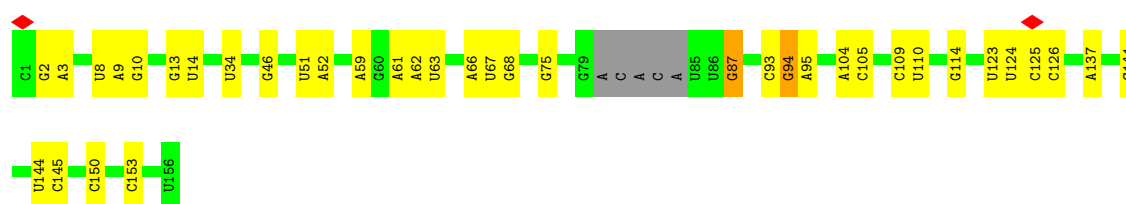
• Molecule 2: 5S ribosomal RNA

Chain 7: 85% 13% ..



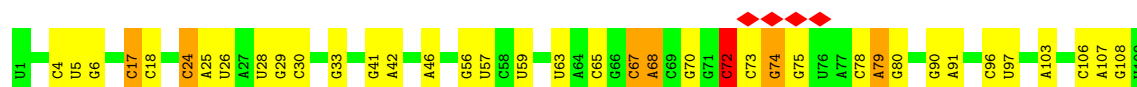
• Molecule 3: 5.8S ribosomal RNA

Chain 8: 72% 23% ..

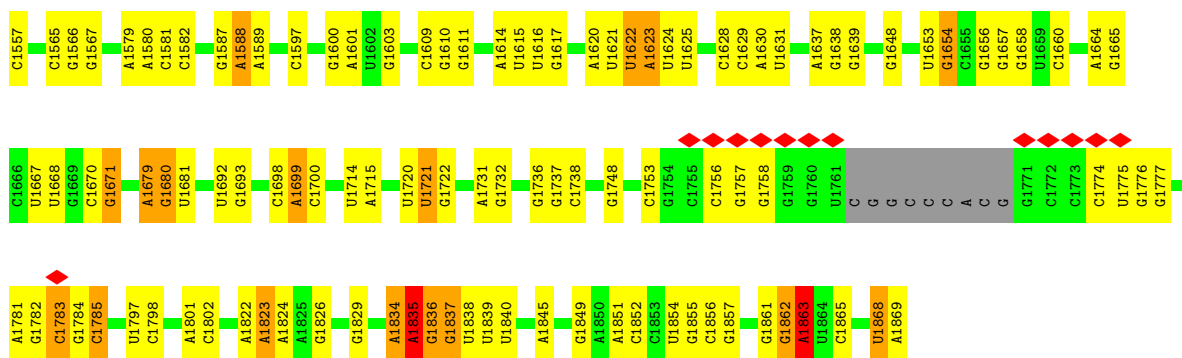


• Molecule 4: 18S ribosomal RNA

Chain 9: 5% 60% 26% 9%







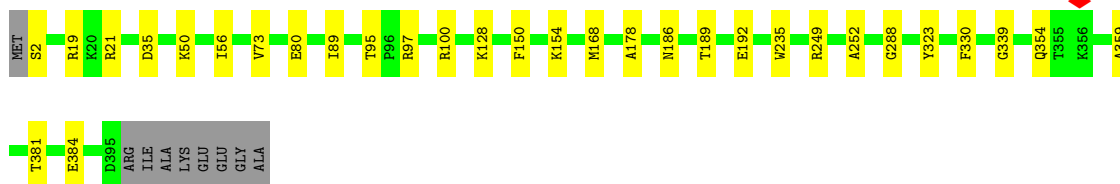
• Molecule 5: Ribosomal protein L8

Chain A: 88% 9% .



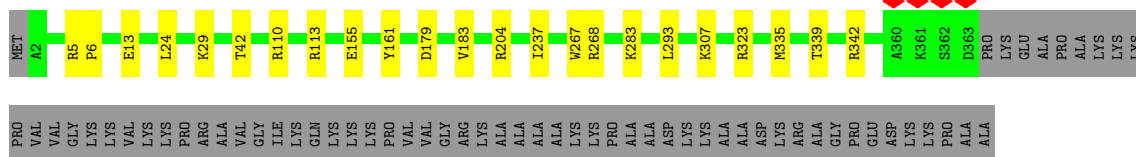
• Molecule 6: Ribosomal protein L3

Chain B: 90% 8% .



• Molecule 7: 60S ribosomal protein L4

Chain C: 80% 5% 15%



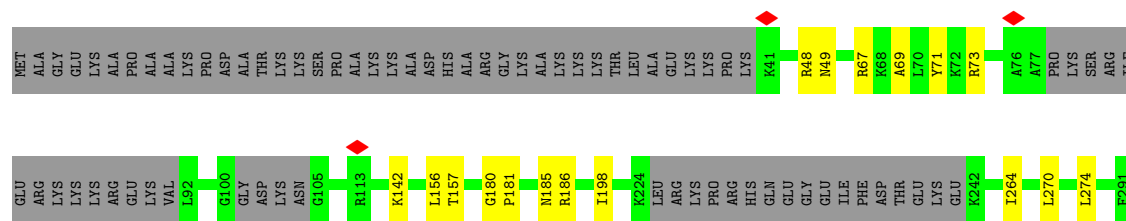
• Molecule 8: Large ribosomal subunit protein uL18

Chain D: 93% 5% ..

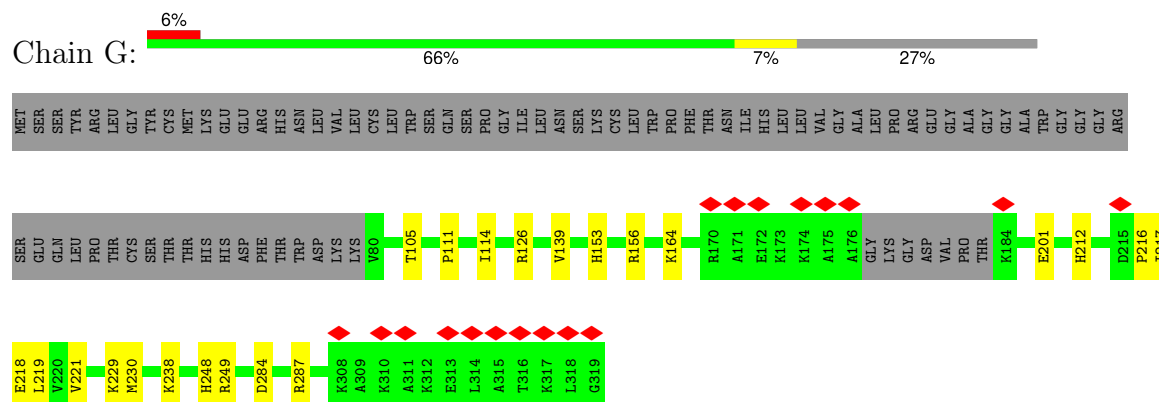


• Molecule 9: 60S ribosomal protein L6

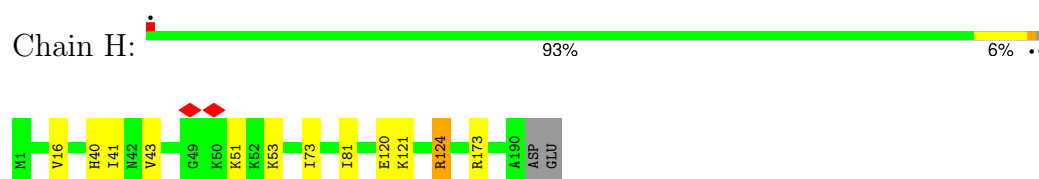
Chain E: 68% 6% 26%



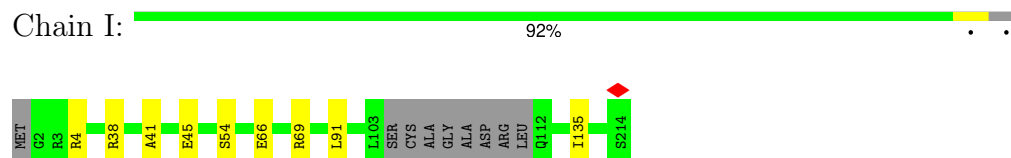
• Molecule 10: 60S ribosomal protein L7a



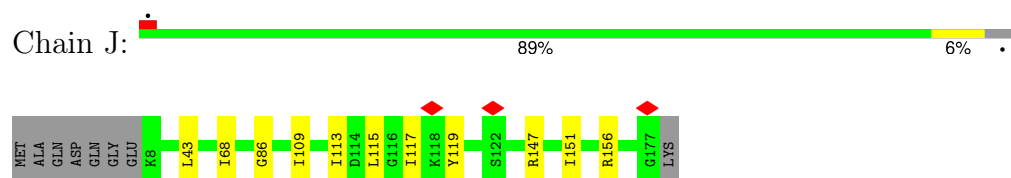
• Molecule 11: 60S ribosomal protein L9



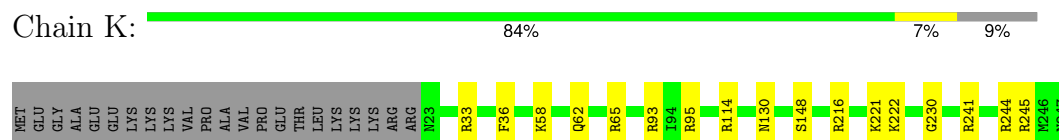
• Molecule 12: 60S ribosomal protein L10



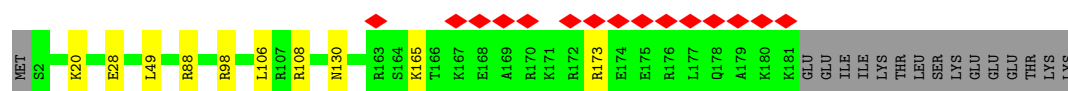
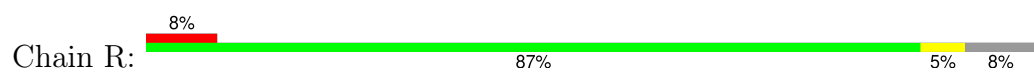
• Molecule 13: Ribosomal protein L11



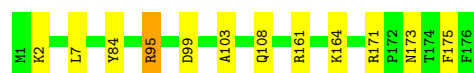
• Molecule 14: 60S ribosomal protein L7



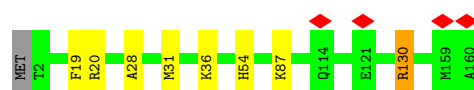
- Molecule 21: Ribosomal protein L19



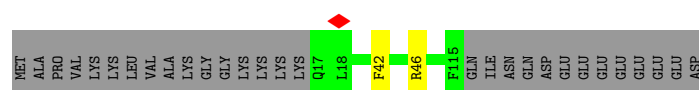
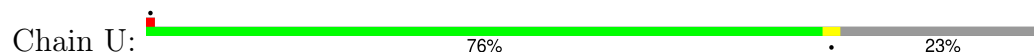
- Molecule 22: 60S ribosomal protein L18a



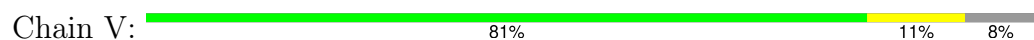
- Molecule 23: eL21



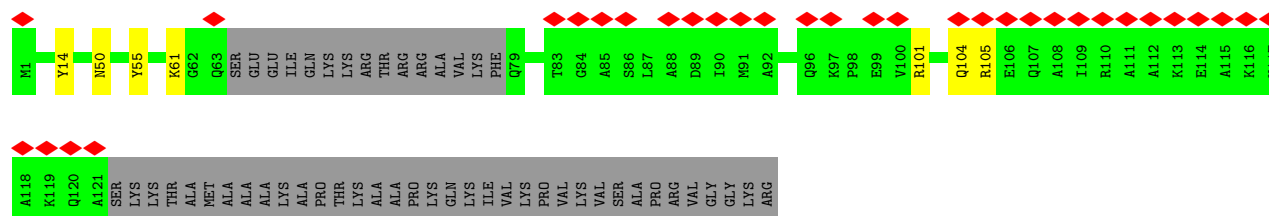
- Molecule 24: eL22



- Molecule 25: Ribosomal protein L23

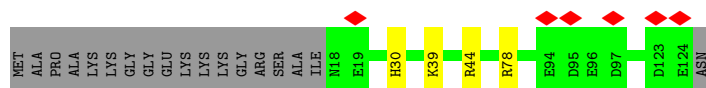


- Molecule 26: eL24



- Molecule 27: eL23





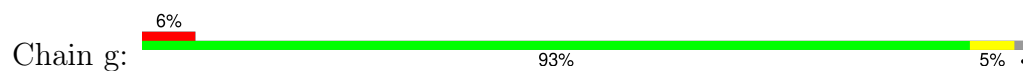
- Molecule 34: Ribosomal protein L32



- Molecule 35: eL33



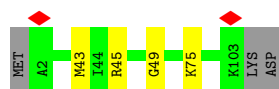
- Molecule 36: Large ribosomal subunit protein eL34



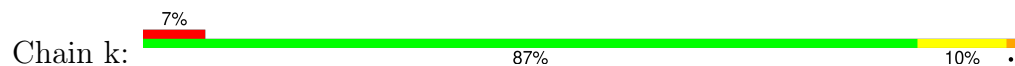
- Molecule 37: eL35




- Molecule 38: 60S ribosomal protein L36



- Molecule 39: eL38



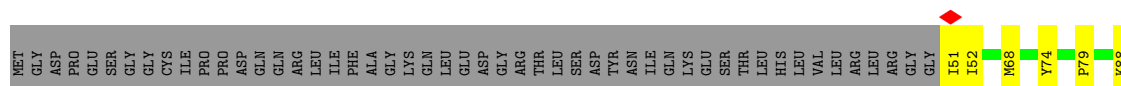
- Molecule 40: eL39

Chain l:  92% 6%



- Molecule 41: Ubiquitin-ribosomal protein eL40 fusion protein

Chain m:  44% 7% 49%




- Molecule 42: eL41

Chain n:  96%




- Molecule 43: Large ribosomal subunit protein eL42

Chain o:  88% 10%




- Molecule 44: eL43

Chain p:  89% 10%



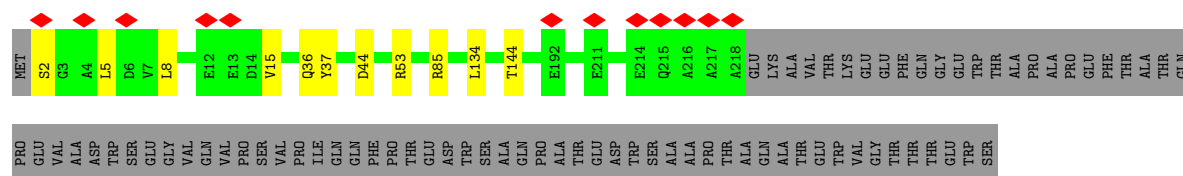
- Molecule 45: eL28

Chain r:  86% 9%



- Molecule 46: uS2 (SA)

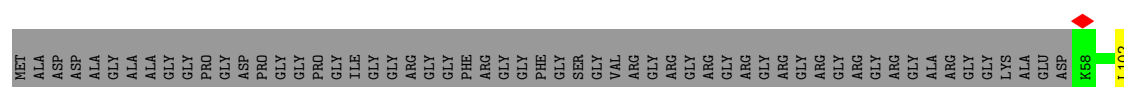
Chain AA:  70% 26%



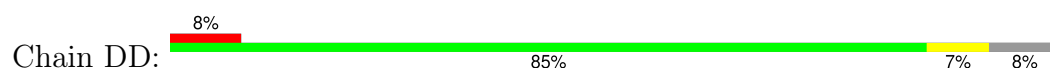
- Molecule 47: 40S ribosomal protein S3a



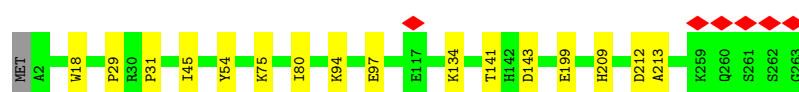
- Molecule 48: Small ribosomal subunit protein uS5



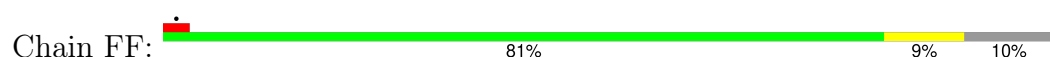
- Molecule 49: Ribosomal protein S3

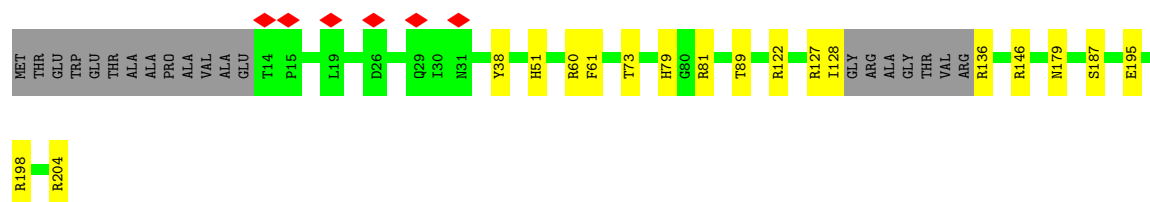


- Molecule 50: eS4 (S4 X isoform)

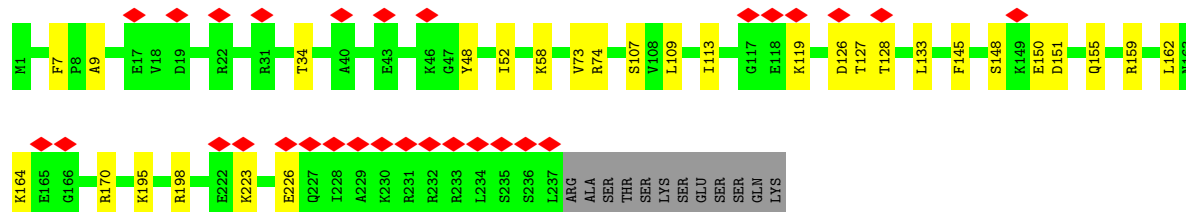
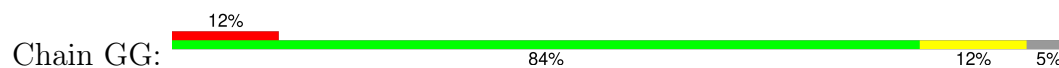


- Molecule 51: Ribosomal protein S5

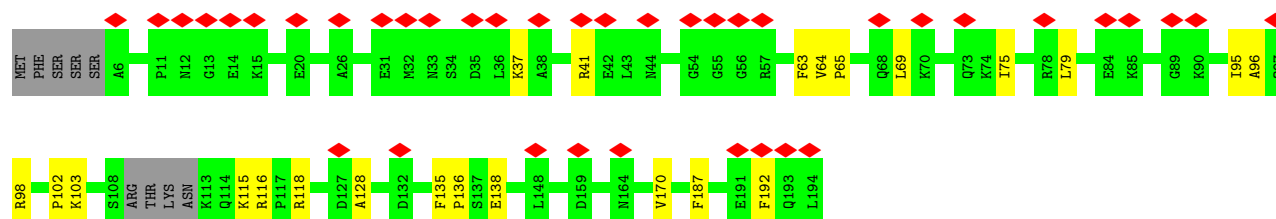
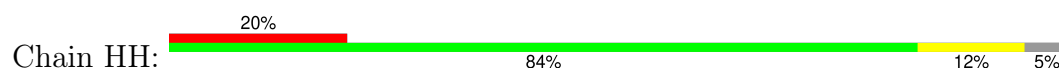




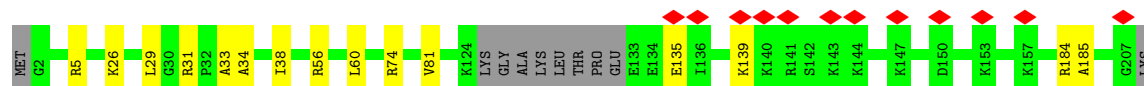
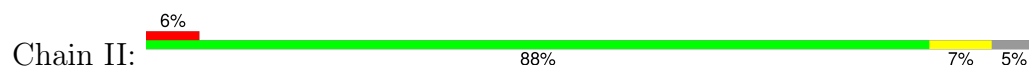
- Molecule 52: 40S ribosomal protein S6



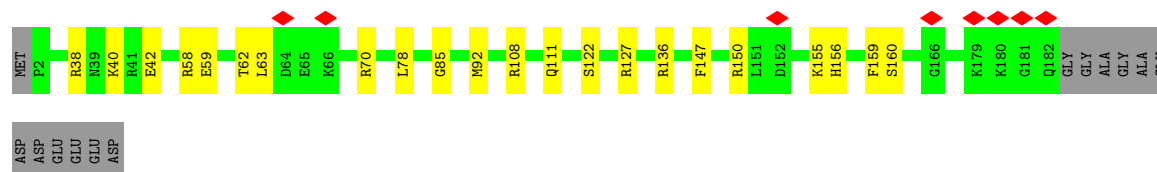
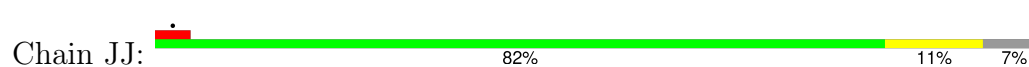
- Molecule 53: 40S ribosomal protein S7



- Molecule 54: 40S ribosomal protein S8

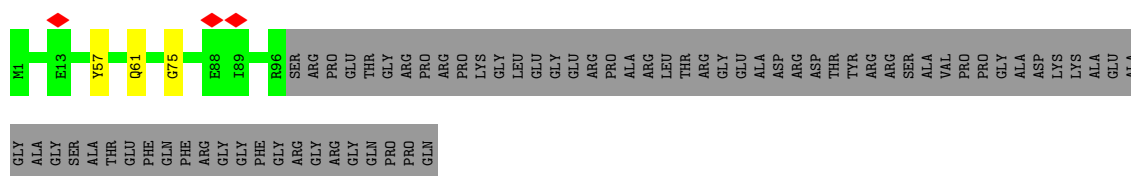


- Molecule 55: Ribosomal protein S9 (Predicted)

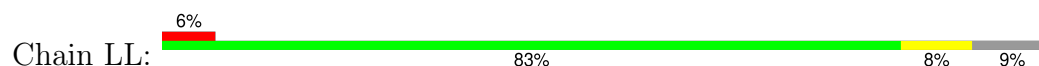


- Molecule 56: Small ribosomal subunit protein eS10

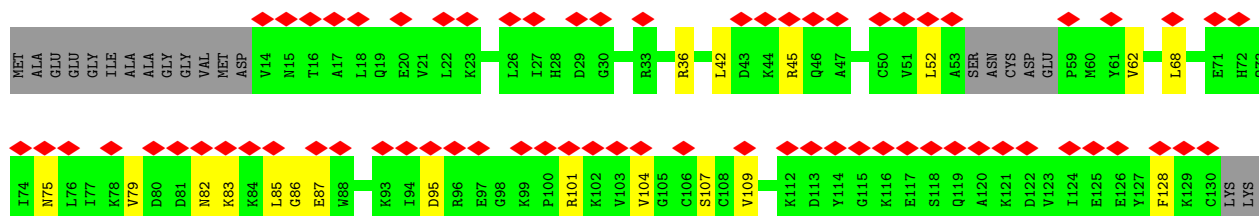
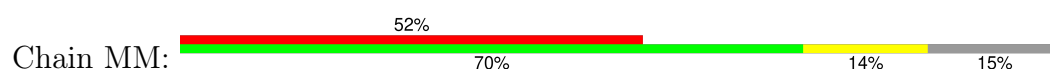




• Molecule 57: Ribosomal protein S11



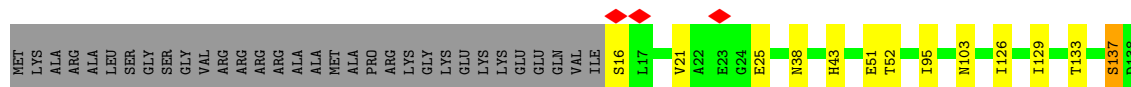
• Molecule 58: 40S ribosomal protein S12



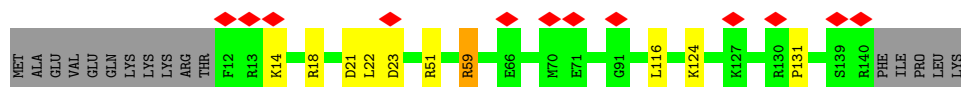
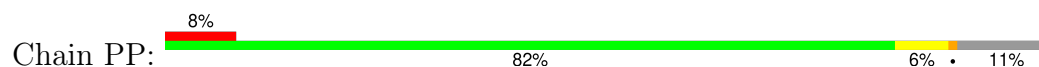
• Molecule 59: Ribosomal protein S13



• Molecule 60: Small ribosomal subunit protein uS11

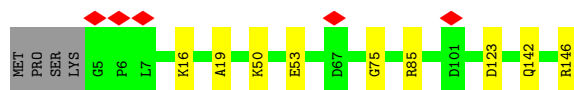


• Molecule 61: uS19




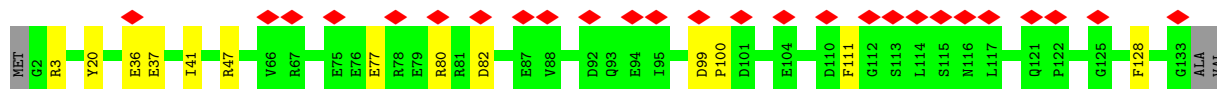
- Molecule 62: uS9

Chain QQ:  91% 6%




- Molecule 63: eS17

Chain RR:  19% 88% 10%




- Molecule 64: uS13

Chain SS:  5% 82% 11% 8%




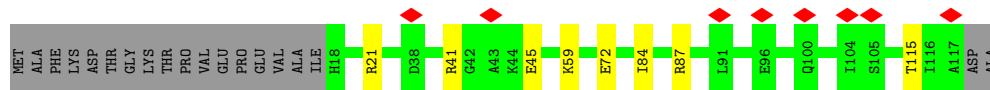
- Molecule 65: eS19

Chain TT:  85% 12%



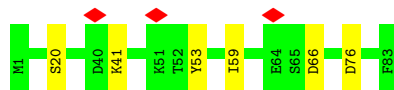
- Molecule 66: uS10

Chain UU:  7% 77% 7% 16%



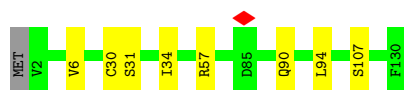
- Molecule 67: eS21

Chain VV:  93% 7%



- Molecule 68: Ribosomal protein S15a

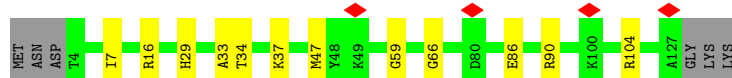
Chain WW:  93% 6%



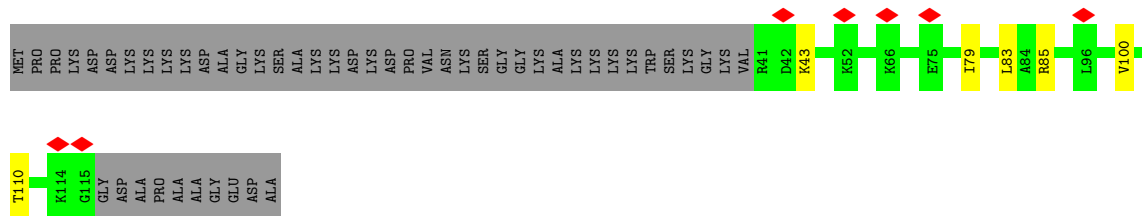
- Molecule 69: uS12



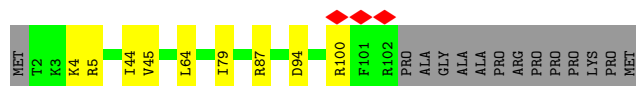
- Molecule 70: 40S ribosomal protein S24



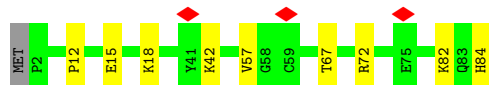
- Molecule 71: eS25



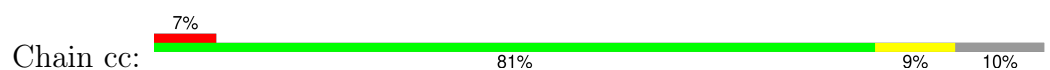
- Molecule 72: 40S ribosomal protein S26

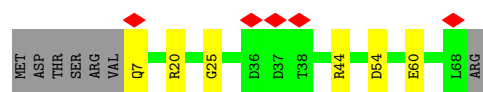


- Molecule 73: 40S ribosomal protein S27



- Molecule 74: Ribosomal protein S28

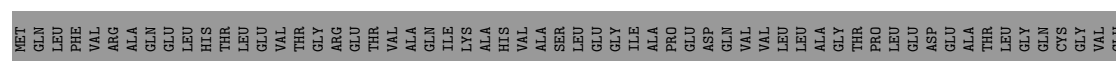




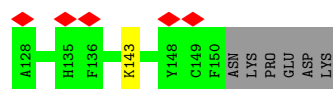
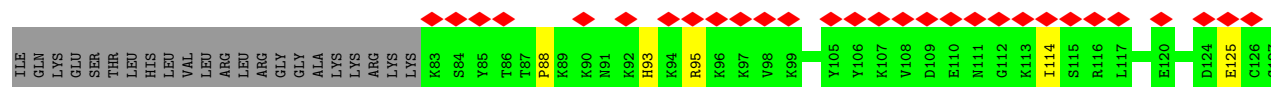
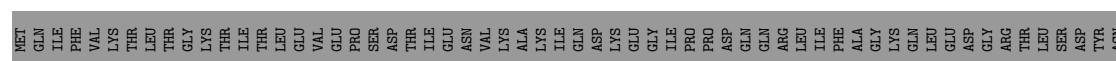
- Molecule 75: eS29



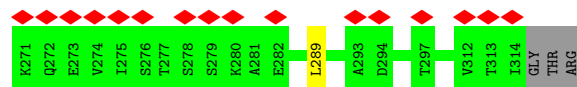
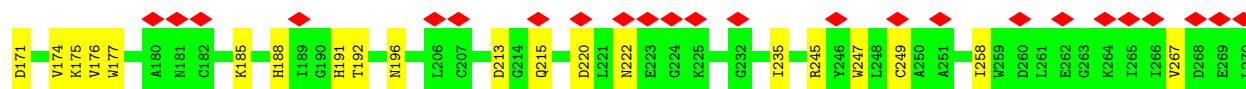
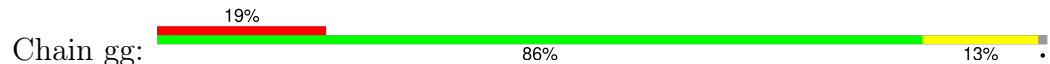
- Molecule 76: 40S ribosomal protein S30



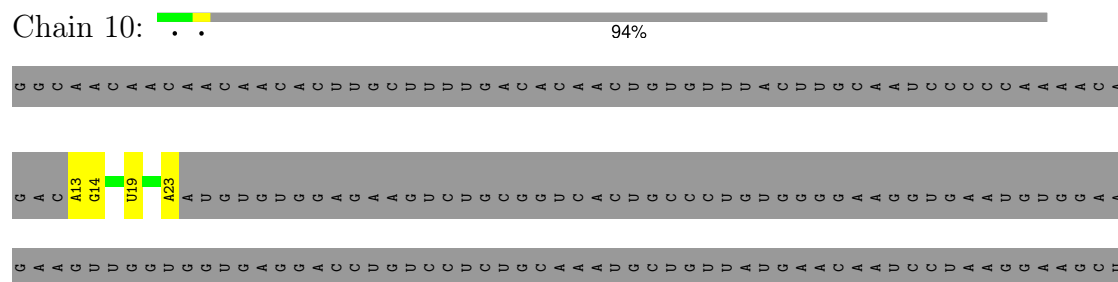
- Molecule 77: Ribosomal protein S27a



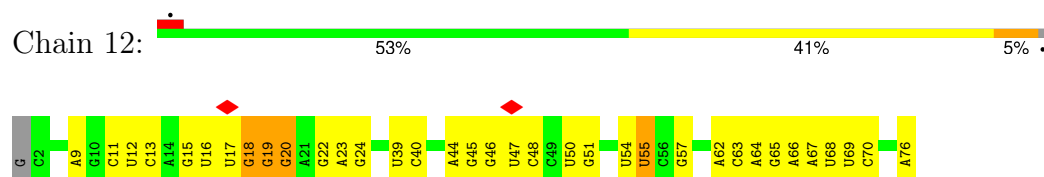
- Molecule 78: RACK1



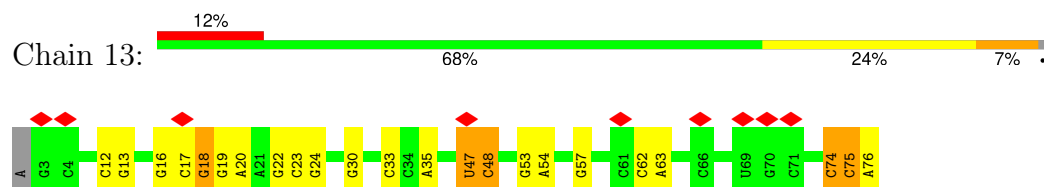
- Molecule 79: MF mRNA



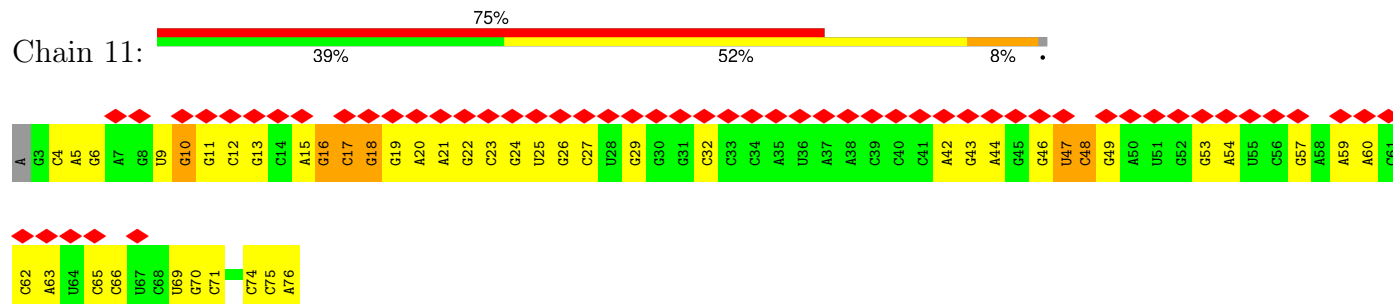
- Molecule 80: Phe-tRNA



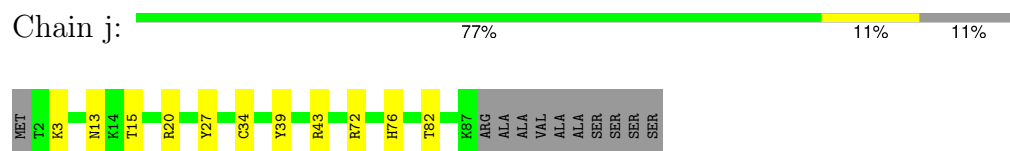
- Molecule 81: Met-tRNA



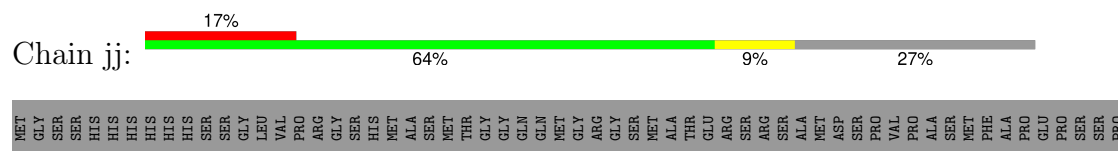
- Molecule 81: Met-tRNA

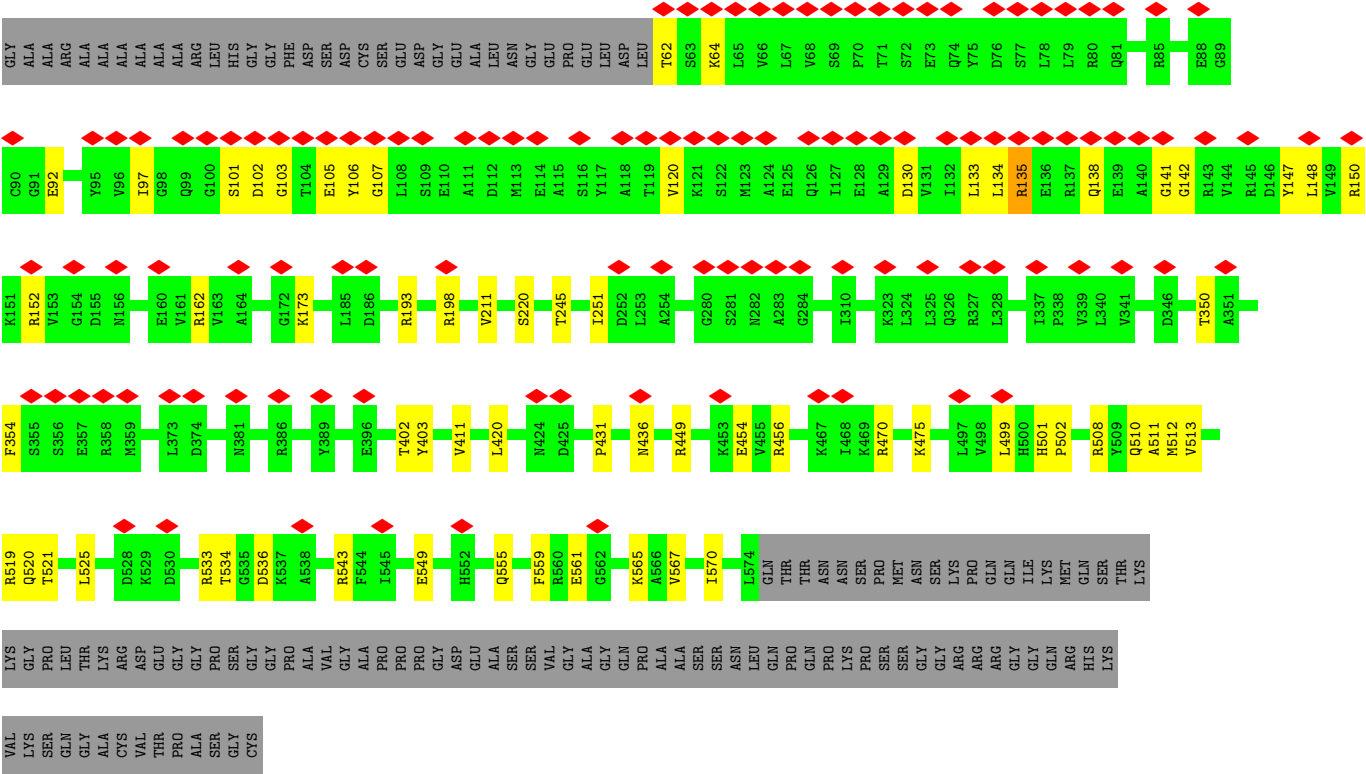


- Molecule 82: Ribosomal protein L37



- Molecule 83: GTP-binding protein 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8005	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 ($e^-/\text{\AA}^2$)	29.7955	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	0.100	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 [i](#)

5.1 Standard geometry [i](#)

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

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	14/134721 (0.0%)
2	7	0.45	0/2836	0.61	0/4421
3	8	0.46	0/3581	0.65	0/5577
4	9	0.41	0/40509	0.66	8/63128 (0.0%)
5	A	0.37	0/1936	0.53	0/2596
6	B	0.34	0/3240	0.53	0/4339
7	C	0.36	0/2937	0.54	0/3946
8	D	0.32	0/2437	0.49	0/3264
9	E	0.30	0/1762	0.54	0/2362
10	G	0.31	0/1910	0.52	0/2569
11	H	0.32	0/1535	0.48	0/2063
12	I	0.33	0/1702	0.48	0/2272
13	J	0.28	0/1385	0.48	0/1852
14	K	0.37	0/1911	0.52	0/2549
15	L	0.33	0/1733	0.50	0/2316
16	M	0.32	0/1158	0.51	0/1547
17	N	0.40	0/1746	0.55	0/2338
18	O	0.37	0/1662	0.55	1/2222 (0.0%)
19	P	0.36	0/1268	0.55	0/1700
20	Q	0.38	0/1539	0.53	0/2054
21	R	0.33	0/1524	0.53	0/2013
22	S	0.36	0/1501	0.49	0/2012
23	T	0.34	0/1326	0.50	0/1770
24	U	0.29	0/823	0.51	0/1104
25	V	0.35	0/983	0.53	0/1319
26	W	0.31	0/873	0.52	0/1158
27	X	0.31	0/984	0.48	0/1323
28	Y	0.33	0/1132	0.49	0/1504
29	Z	0.34	0/1130	0.49	0/1507
30	a	0.38	0/1191	0.56	0/1590
31	b	0.31	0/819	0.54	0/1081
32	c	0.36	0/771	0.53	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.37	0/903	0.54	0/1216
34	e	0.39	0/1071	0.58	0/1429
35	f	0.39	0/895	0.49	0/1198
36	g	0.34	0/916	0.52	0/1220
37	h	0.34	0/1021	0.53	0/1348
38	i	0.30	0/841	0.60	0/1112
39	k	0.30	0/575	0.47	0/761
40	l	0.39	0/459	0.57	0/608
41	m	0.34	0/435	0.48	0/575
42	n	0.37	0/241	0.56	0/305
43	o	0.34	0/864	0.49	0/1140
44	p	0.36	0/718	0.59	0/953
45	r	0.35	0/1010	0.56	0/1354
46	AA	0.28	0/1747	0.50	0/2374
47	BB	0.30	0/1756	0.51	0/2350
48	CC	0.31	0/1753	0.52	0/2369
49	DD	0.27	0/1767	0.49	0/2378
50	EE	0.26	0/2118	0.50	0/2849
51	FF	0.27	0/1481	0.50	0/1991
52	GG	0.24	0/1946	0.52	0/2590
53	HH	0.23	0/1511	0.48	0/2022
54	II	0.28	0/1655	0.51	0/2205
55	JJ	0.26	0/1533	0.51	0/2047
56	KK	0.26	0/834	0.46	0/1125
57	LL	0.30	0/1195	0.53	0/1597
58	MM	0.20	0/880	0.57	0/1179
59	NN	0.29	0/1226	0.52	0/1649
60	OO	0.32	0/1029	0.56	0/1380
61	PP	0.24	0/1079	0.55	0/1441
62	QQ	0.27	0/1146	0.51	0/1534
63	RR	0.25	0/1082	0.54	0/1452
64	SS	0.26	0/1175	0.52	0/1575
65	TT	0.25	0/1115	0.53	0/1493
66	UU	0.25	0/805	0.45	0/1081
67	VV	0.27	0/644	0.43	0/860
68	WW	0.34	0/1051	0.50	0/1406
69	XX	0.31	0/1105	0.51	0/1476
70	YY	0.23	0/1028	0.47	0/1366
71	ZZ	0.23	0/604	0.46	0/810
72	aa	0.32	0/828	0.50	0/1109
73	bb	0.25	0/665	0.45	0/891
74	cc	0.25	0/490	0.42	0/656
75	dd	0.32	0/470	0.57	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
76	ee	0.24	0/462	0.56	0/607
77	ff	0.16	0/567	0.56	0/753
78	gg	0.22	0/2493	0.48	0/3394
79	10	0.38	0/261	0.53	0/404
80	12	0.31	0/1787	0.66	0/2783
81	11	0.26	0/1773	0.67	0/2763
81	13	0.31	0/1773	0.66	0/2763
82	j	0.38	0/720	0.53	0/952
83	jj	0.21	0/4047	0.49	0/5462
All	All	0.40	0/235774	0.62	23/346229 (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	1
5	A	0	1
6	B	0	1
7	C	0	1
8	D	0	3
9	E	0	1
11	H	0	2
15	L	0	1
18	O	0	1
20	Q	0	3
22	S	0	1
23	T	0	1
27	X	0	2
29	Z	0	2
31	b	0	1
34	e	0	1
35	f	0	1
36	g	0	1
39	k	0	1
44	p	0	1
51	FF	0	1
54	II	0	2
60	OO	0	1
61	PP	0	1
77	ff	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
83	jj	0	2
All	All	0	35

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9	1835	A	C2'-C3'-O3'	7.03	120.04	109.50
1	5	2544	G	C8-N9-C1'	-6.55	107.34	127.00
1	5	1440	U	C2'-C3'-O3'	6.47	119.20	109.50
1	5	914	U	C2'-C3'-O3'	6.09	118.64	109.50
1	5	4119	C	C2'-C3'-O3'	5.97	118.46	109.50
1	5	2544	G	C4-N9-C1'	5.79	143.87	126.50
1	5	4064	C	P-O3'-C3'	5.70	128.75	120.20
1	5	4170	A	C4'-C3'-O3'	5.54	117.71	109.40
1	5	4944	C	C1'-O4'-C4'	-5.53	104.17	109.70
4	9	1863	A	C1'-O4'-C4'	-5.37	104.33	109.70
4	9	532	C	C2'-C3'-O3'	5.35	121.72	113.70
1	5	3888	G	C2'-C3'-O3'	5.32	121.67	113.70
4	9	72	C	P-O3'-C3'	5.26	128.10	120.20
18	O	110	PRO	N-CA-C	5.25	117.10	110.70
4	9	24	C	C2'-C3'-O3'	5.13	121.40	113.70
1	5	1485	C	C2'-C3'-O3'	5.08	117.11	109.50
4	9	1060	A	C3'-C2'-C1'	-5.08	96.42	101.50
1	5	406	C	C2'-C3'-O3'	5.05	121.28	113.70
4	9	918	U	N1-C1'-C2'	5.04	119.57	112.00
1	5	4448	G	C4'-C3'-O3'	5.04	120.55	113.00
1	5	4065	G	N9-C1'-C2'	5.02	119.53	112.00
4	9	532	C	C5'-C4'-O4'	5.01	117.32	109.80
1	5	2089	G	C4'-C3'-O3'	5.01	116.92	109.40

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	5	2544	G	Sidechain
5	A	123	ARG	Sidechain
6	B	21	ARG	Sidechain
7	C	204	ARG	Sidechain
8	D	24	ARG	Sidechain
8	D	33	ARG	Sidechain

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Mol	Chain	Res	Type	Group
8	D	68	ARG	Sidechain
9	E	67	ARG	Sidechain
51	FF	204	ARG	Sidechain
11	H	124	ARG	Sidechain
11	H	173	ARG	Sidechain
54	II	5	ARG	Sidechain
54	II	74	ARG	Sidechain
15	L	71	ARG	Sidechain
18	O	49	ARG	Sidechain
60	OO	137	SER	Peptide
61	PP	59	ARG	Sidechain
20	Q	108	ARG	Sidechain
20	Q	143	ARG	Sidechain
20	Q	91	ARG	Sidechain
22	S	95	ARG	Sidechain
23	T	130	ARG	Sidechain
27	X	47	ARG	Sidechain
27	X	67	ARG	Sidechain
29	Z	21	ARG	Sidechain
29	Z	65	ARG	Sidechain
31	b	44	ARG	Sidechain
34	e	27	ARG	Sidechain
35	f	100	ARG	Sidechain
77	ff	114	ILE	Peptide
36	g	8	ARG	Sidechain
83	jj	135	ARG	Sidechain
83	jj	519	ARG	Sidechain
39	k	17	ARG	Sidechain
44	p	49	ARG	Sidechain

5.2 Too-close contacts

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	600	0
2	7	2538	0	1286	8	0
3	8	3208	0	1629	18	0
4	9	36229	0	18300	326	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1898	0	1993	15	0
6	B	3172	0	3310	22	0
7	C	2883	0	3053	17	0
8	D	2391	0	2424	11	0
9	E	1729	0	1887	13	0
10	G	1879	0	2027	19	0
11	H	1516	0	1597	8	0
12	I	1664	0	1712	6	0
13	J	1362	0	1399	8	0
14	K	1875	0	1995	14	0
15	L	1702	0	1820	9	0
16	M	1137	0	1211	6	0
17	N	1701	0	1749	22	0
18	O	1630	0	1778	9	0
19	P	1242	0	1274	13	0
20	Q	1515	0	1634	12	0
21	R	1508	0	1664	9	0
22	S	1462	0	1508	7	0
23	T	1298	0	1366	6	0
24	U	809	0	833	1	0
25	V	969	0	1031	13	0
26	W	860	0	903	6	0
27	X	967	0	1040	5	0
28	Y	1115	0	1205	3	0
29	Z	1107	0	1182	16	0
30	a	1162	0	1209	12	0
31	b	806	0	866	0	0
32	c	761	0	794	6	0
33	d	888	0	930	4	0
34	e	1053	0	1147	4	0
35	f	876	0	912	2	0
36	g	906	0	998	5	0
37	h	1013	0	1147	4	0
38	i	830	0	916	3	0
39	k	569	0	637	5	0
40	l	447	0	480	3	0
41	m	429	0	465	8	0
42	n	240	0	289	1	0
43	o	851	0	920	7	0
44	p	708	0	756	8	0
45	r	994	0	1051	5	0
46	AA	1710	0	1708	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BB	1729	0	1803	17	0
48	CC	1716	0	1806	11	0
49	DD	1739	0	1832	11	0
50	EE	2076	0	2177	10	0
51	FF	1460	0	1509	13	0
52	GG	1923	0	2089	23	0
53	HH	1489	0	1582	15	0
54	II	1628	0	1706	10	0
55	JJ	1508	0	1626	16	0
56	KK	810	0	836	2	0
57	LL	1175	0	1249	9	0
58	MM	871	0	913	14	0
59	NN	1202	0	1289	6	0
60	OO	1016	0	1039	12	0
61	PP	1058	0	1104	9	0
62	QQ	1128	0	1195	7	0
63	RR	1068	0	1121	10	0
64	SS	1157	0	1213	13	0
65	TT	1097	0	1132	11	0
66	UU	795	0	862	6	0
67	VV	637	0	637	4	0
68	WW	1034	0	1080	5	0
69	XX	1087	0	1154	12	0
70	YY	1011	0	1083	12	0
71	ZZ	598	0	656	4	0
72	aa	814	0	867	7	0
73	bb	651	0	672	6	0
74	cc	488	0	514	4	0
75	dd	459	0	448	3	0
76	ee	457	0	502	6	0
77	ff	555	0	567	4	0
78	gg	2436	0	2393	22	0
79	10	234	0	118	1	0
80	12	1599	0	808	20	0
81	11	1585	0	804	32	0
81	13	1585	0	803	14	0
82	j	705	0	737	9	0
83	jj	3982	0	4069	42	0
84	5	10	0	19	0	0
85	dd	1	0	0	0	0
85	g	1	0	0	0	0
85	j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	m	1	0	0	0	0
85	o	1	0	0	0	0
85	p	1	0	0	0	0
86	12	32	0	11	1	0
87	12	11	0	8	0	0
88	11	31	0	11	1	0
88	13	31	0	11	0	0
89	13	8	0	8	0	0
90	jj	32	0	14	2	0
91	jj	1	0	0	0	0
92	jj	1	0	0	0	0
All	All	219555	0	163125	1457	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 4.

All (1457) 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	2.09	0.99
1:5:2395:A:O2'	1:5:2806:A:H1'	1.72	0.89
44:p:42:CYS:HB3	44:p:60:CYS:SG	2.15	0.87
1:5:982:U:H3	1:5:1273:G:H1	1.23	0.86
4:9:1272:C:O2'	4:9:1274:G:N2	2.10	0.85
1:5:980:U:H3	1:5:1275:G:H1	1.23	0.83
1:5:978:G:H22	1:5:1277:G:H1	1.26	0.83
1:5:978:G:N2	1:5:1277:G:H1	1.78	0.82
83:jj:198:ARG:NH1	83:jj:211:VAL:O	2.14	0.81
4:9:1299:A:OP1	61:PP:59:ARG:NH1	2.14	0.80
4:9:919:A:OP2	59:NN:64:ARG:NH2	2.14	0.80
1:5:2262:G:OP2	45:r:98:ARG:NH2	2.12	0.80
1:5:29:G:N7	17:N:189:ARG:NH2	2.27	0.80
1:5:4039:G:N7	1:5:4041:C:N4	2.29	0.80
1:5:173:C:OP1	15:L:129:ARG:NH1	2.15	0.79
41:m:51:ILE:HG23	41:m:52:ILE:H	1.49	0.78
1:5:1073:G:H22	1:5:1238:A:H2	1.32	0.78
1:5:1976:G:O6	1:5:1991:A:N6	2.17	0.78
4:9:1600:G:H4'	71:ZZ:43:LYS:HE3	1.66	0.77
1:5:453:G:N2	1:5:1293:G:O6	2.17	0.77
1:5:2457:G:H21	1:5:3672:G:H21	1.33	0.77
44:p:42:CYS:CB	44:p:60:CYS:SG	2.71	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:107:ARG:NH2	8:D:116:ASP:OD1	2.19	0.76
51:FF:195:GLU:OE1	51:FF:198:ARG:NH1	2.19	0.76
55:JJ:63:LEU:O	55:JJ:70:ARG:NH1	2.19	0.75
78:gg:83:TRP:HA	78:gg:107:ASP:HB2	1.68	0.75
1:5:1555:G:O6	44:p:4:ARG:NH2	2.21	0.74
4:9:908:A:OP2	21:R:165:LYS:NZ	2.20	0.74
1:5:3717:A:H2'	1:5:3718:A:C8	2.22	0.73
1:5:4635:A:H2	1:5:4663:G:H21	1.35	0.73
4:9:1228:A:H2'	4:9:1229:G:C8	2.24	0.73
7:C:110:ARG:O	7:C:113:ARG:NH1	2.22	0.73
1:5:2457:G:H21	1:5:3672:G:N2	1.86	0.72
1:5:29:G:OP2	17:N:189:ARG:NH1	2.21	0.72
1:5:2313:A:O2'	1:5:2314:G:OP1	2.07	0.72
1:5:2407:G:O6	40:l:2:SER:N	2.23	0.72
4:9:959:G:OP2	60:OO:38:ASN:ND2	2.17	0.72
4:9:536:A:H61	4:9:547:G:H22	1.37	0.72
1:5:1802:A:N3	23:T:130:ARG:NH2	2.38	0.71
26:W:104:GLN:NE2	52:GG:155:GLN:OE1	2.23	0.71
1:5:87:A:OP2	20:Q:173:LYS:NZ	2.24	0.71
4:9:1834:A:H2	4:9:1837:G:H1	1.38	0.71
83:jj:134:LEU:O	83:jj:135:ARG:NH1	2.22	0.71
1:5:1444:G:H21	1:5:2110:G:H1	1.39	0.71
53:HH:138:GLU:OE2	59:NN:19:ARG:NH1	2.24	0.70
81:11:16:G:OP2	81:11:17:C:N4	2.24	0.70
1:5:4099:G:H1	1:5:4109:G:H22	1.37	0.70
4:9:1293:A:H62	4:9:1306:U:H3	1.38	0.70
1:5:1771:U:H2'	1:5:1772:C:C6	2.27	0.70
1:5:4635:A:H8	1:5:5048:A:H61	1.40	0.69
1:5:1577:G:OP1	44:p:17:ARG:NH1	2.25	0.69
3:8:94:G:OP2	82:j:72:ARG:NH1	2.26	0.69
82:j:20:ARG:NH2	82:j:39:TYR:OH	2.25	0.69
65:TT:108:GLU:OE2	65:TT:121:ARG:NH1	2.25	0.69
4:9:1565:C:OP2	65:TT:101:ARG:NH1	2.25	0.69
1:5:3932:U:H2'	1:5:3933:G:H8	1.57	0.68
4:9:1488:C:O2'	4:9:1490:G:OP2	2.08	0.68
1:5:1188:C:H2'	1:5:1189:G:H8	1.58	0.68
21:R:98:ARG:NH2	21:R:130:ASN:OD1	2.25	0.68
62:QQ:146:ARG:NH2	81:13:33:C:OP2	2.25	0.68
74:cc:44:ARG:NH2	74:cc:60:GLU:O	2.26	0.68
78:gg:73:SER:OG	78:gg:117:ASN:ND2	2.23	0.68
4:9:127:C:O2	50:EE:134:LYS:NZ	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:JJ:136:ARG:NH1	55:JJ:159:PHE:O	2.27	0.68
4:9:190:G:O2'	4:9:209:A:N6	2.26	0.68
4:9:367:U:H4'	4:9:371:A:C8	2.29	0.68
4:9:686:U:O2	53:HH:118:ARG:NH2	2.23	0.68
1:5:983:C:C5	9:E:73:ARG:HD3	2.28	0.68
69:XX:67:ARG:NH2	69:XX:114:ASP:OD2	2.27	0.67
25:V:13:LYS:HD3	25:V:128:LEU:HD11	1.75	0.67
1:5:2758:G:O2'	1:5:2765:A:N3	2.24	0.67
4:9:1144:A:H2'	4:9:1145:A:C8	2.30	0.67
49:DD:106:ARG:NH1	49:DD:174:HIS:O	2.27	0.67
1:5:1075:G:H1	1:5:1235:G:N2	1.93	0.67
1:5:1317:U:OP1	30:a:21:ARG:NH2	2.28	0.67
1:5:3974:G:OP2	1:5:3975:C:N4	2.26	0.67
1:5:1075:G:H1	1:5:1235:G:H22	1.42	0.67
1:5:1976:G:N1	1:5:1991:A:N7	2.43	0.66
4:9:448:A:N6	54:II:29:LEU:HD13	2.10	0.66
1:5:143:C:OP2	10:G:164:LYS:NZ	2.29	0.66
1:5:1364:U:OP2	15:L:36:ARG:NH2	2.23	0.66
3:8:87:G:OP2	37:h:7:ARG:NH2	2.25	0.66
65:TT:25:SER:HB3	65:TT:27:LYS:HE2	1.78	0.66
47:BB:37:ALA:HA	47:BB:42:ARG:HD3	1.78	0.66
1:5:3599:A:H2'	1:5:3600:G:C8	2.30	0.66
1:5:4076:G:OP1	10:G:126:ARG:NH1	2.27	0.66
15:L:79:GLU:OE1	15:L:82:ARG:NH1	2.28	0.66
1:5:1197:C:H2'	1:5:1198:G:C8	2.31	0.66
1:5:3710:G:H1'	1:5:3712:A:N6	2.10	0.66
1:5:517:C:H2'	1:5:518:G:H8	1.61	0.66
81:11:69:U:H2'	81:11:70:G:H8	1.60	0.65
1:5:4925:U:H4'	1:5:4926:C:H5'	1.78	0.65
4:9:903:A:H2'	4:9:904:A:H8	1.62	0.65
4:9:546:G:H2'	4:9:547:G:C8	2.31	0.65
4:9:928:G:H2'	4:9:929:G:C8	2.32	0.65
17:N:155:VAL:O	17:N:162:ARG:NH2	2.30	0.65
1:5:456:C:H2'	1:5:457:G:H8	1.61	0.65
1:5:910:G:H2'	1:5:911:U:C6	2.31	0.65
10:G:139:VAL:HG12	10:G:212:HIS:NE2	2.12	0.65
11:H:41:ILE:HG21	11:H:73:ILE:HD11	1.79	0.65
4:9:303:C:O2	54:II:184:ARG:NH2	2.28	0.65
15:L:28:GLN:OE1	17:N:202:ARG:NH1	2.29	0.65
22:S:99:ASP:OD2	22:S:108:GLN:NE2	2.29	0.65
54:II:135:GLU:OE2	54:II:139:LYS:NZ	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:11:53:G:H2'	81:11:54:A:H8	1.62	0.64
13:J:151:ILE:HD11	13:J:156:ARG:HG2	1.80	0.64
80:12:51:G:OP1	83:jj:508:ARG:NH1	2.30	0.64
4:9:1060:A:O2'	4:9:1062:A:N7	2.29	0.64
1:5:1198:G:H2'	1:5:1199:G:C8	2.32	0.64
1:5:2725:A:N6	21:R:88:ARG:O	2.31	0.64
32:c:82:GLY:HA2	32:c:91:VAL:HG12	1.79	0.64
1:5:2395:A:HO2'	1:5:2806:A:H1'	1.63	0.64
83:jj:220:SER:HB3	83:jj:245:THR:HG21	1.79	0.64
10:G:139:VAL:HG12	10:G:212:HIS:CE1	2.32	0.64
1:5:4035:G:H2'	1:5:4036:G:C8	2.33	0.64
4:9:750:C:N4	4:9:751:G:O6	2.30	0.64
4:9:925:G:H1	4:9:1017:U:H3	1.45	0.64
1:5:2760:G:O6	29:Z:64:LYS:NZ	2.30	0.64
78:gg:191:HIS:NE2	78:gg:215:GLN:O	2.30	0.64
1:5:265:C:O2	1:5:266:C:N4	2.31	0.63
1:5:4737:G:H2'	1:5:4738:C:C6	2.33	0.63
1:5:1072:C:N4	1:5:1239:C:H42	1.96	0.63
1:5:976:G:H1	1:5:1279:A:H2	1.46	0.63
1:5:4122:G:O2'	29:Z:136:PHE:OXT	2.17	0.63
4:9:1297:U:O4	61:PP:59:ARG:NH2	2.32	0.63
4:9:552:G:H5'	76:ee:116:VAL:HG11	1.81	0.63
83:jj:62:THR:HG1	83:jj:101:SER:HG	1.40	0.63
1:5:4303:C:H2'	1:5:4305:G:H8	1.63	0.63
4:9:536:A:H61	4:9:547:G:H1	1.47	0.63
1:5:1942:A:H2'	1:5:1943:A:C8	2.33	0.62
1:5:3911:C:H2'	1:5:3912:U:H6	1.62	0.62
55:JJ:85:GLY:O	55:JJ:108:ARG:NH1	2.33	0.62
1:5:1440:U:OP2	14:K:33:ARG:NH1	2.32	0.62
1:5:4084:G:O6	5:A:72:ARG:NH2	2.33	0.62
2:7:3:C:H2'	2:7:4:U:H6	1.65	0.62
81:13:53:G:H2'	81:13:54:A:H8	1.63	0.62
4:9:536:A:N6	4:9:547:G:H1	1.97	0.62
7:C:13:GLU:OE2	7:C:161:TYR:OH	2.14	0.62
81:11:43:G:H2'	81:11:44:A:C8	2.35	0.62
83:jj:106:TYR:O	83:jj:141:GLY:N	2.29	0.62
1:5:3599:A:H2'	1:5:3600:G:H8	1.64	0.62
4:9:898:U:H2'	4:9:899:U:H6	1.65	0.62
4:9:1834:A:H2	4:9:1837:G:N1	1.98	0.62
1:5:76:A:OP2	15:L:74:ARG:NH1	2.30	0.61
4:9:444:G:O6	54:II:26:LYS:NZ	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2553:A:H2	1:5:2765:A:H62	1.48	0.61
4:9:115:U:H2'	4:9:116:U:C6	2.36	0.61
1:5:510:U:OP2	30:a:85:GLN:NE2	2.28	0.61
1:5:2899:C:P	21:R:108:ARG:HH22	2.23	0.61
3:8:8:U:H2'	3:8:9:A:C8	2.36	0.61
4:9:1354:G:N2	4:9:1357:A:OP2	2.29	0.61
1:5:1441:C:H2'	1:5:1442:C:C6	2.35	0.61
1:5:2562:G:N2	1:5:2565:A:OP2	2.28	0.61
1:5:1411:C:H2'	1:5:1411(A):G:C8	2.34	0.61
4:9:1447:G:P	66:UU:87:ARG:HH22	2.24	0.61
1:5:2583:C:OP2	36:g:76:ARG:NH1	2.30	0.61
14:K:93:ARG:NH1	14:K:95:ARG:O	2.31	0.61
1:5:956:A:H8	1:5:957:G:C8	2.19	0.61
1:5:2639:U:HO2'	1:5:2694:G:H1	0.68	0.61
4:9:533:A:H2'	4:9:534:G:H8	1.64	0.61
4:9:1616:U:H3	4:9:1620:A:H2	1.46	0.61
1:5:2647:A:H62	1:5:2686:G:H8	1.48	0.61
1:5:3932:U:H2'	1:5:3933:G:C8	2.36	0.61
17:N:124:ASP:OD1	17:N:125:SER:N	2.30	0.60
48:CC:146:GLU:OE1	49:DD:120:TYR:OH	2.14	0.60
66:UU:41:ARG:NH1	66:UU:45:GLU:OE2	2.34	0.60
1:5:3938:G:N2	1:5:4171:C:OP2	2.33	0.60
10:G:218:GLU:OE1	17:N:26:ARG:NH2	2.29	0.60
4:9:689:U:OP1	53:HH:103:LYS:NZ	2.34	0.60
1:5:4061:G:H2'	1:5:4062:A:H8	1.65	0.60
4:9:570:C:O2	70:YY:34:THR:OG1	2.17	0.60
68:WW:90:GLN:HG3	68:WW:94:LEU:HD12	1.82	0.60
4:9:1653:U:H2'	4:9:1654:G:C8	2.35	0.60
1:5:4188:U:H2'	1:5:4189:U:C6	2.36	0.60
1:5:4570:G:H2'	1:5:4571:A:H8	1.66	0.60
4:9:507:G:OP2	70:YY:104:ARG:NH2	2.35	0.60
4:9:903:A:H2'	4:9:904:A:C8	2.36	0.60
57:LL:104:LYS:O	69:XX:11:ARG:NH2	2.34	0.60
78:gg:145:GLU:O	78:gg:175:LYS:NZ	2.32	0.60
81:13:62:C:H2'	81:13:63:A:C8	2.37	0.60
4:9:453:C:H2'	4:9:454:U:H5'	1.84	0.60
5:A:29:LEU:O	5:A:123:ARG:NH1	2.34	0.60
11:H:120:GLU:OE1	11:H:124:ARG:NH2	2.30	0.60
1:5:914:U:O2'	1:5:915:A:OP2	2.18	0.60
1:5:1865:G:N2	1:5:1868:A:OP2	2.34	0.59
1:5:4936:G:O2'	1:5:4937:C:OP1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:533:A:H2'	4:9:534:G:C8	2.37	0.59
4:9:1119:A:H2'	4:9:1120:U:C6	2.37	0.59
81:13:62:C:H2'	81:13:63:A:H8	1.67	0.59
1:5:910:G:H2'	1:5:911:U:H6	1.67	0.59
18:O:72:HIS:O	18:O:74:ARG:NH1	2.35	0.59
1:5:3910:C:H2'	1:5:3911:C:C6	2.38	0.59
74:cc:20:ARG:NH1	74:cc:25:GLY:O	2.28	0.59
1:5:1339:U:H2'	1:5:1340:C:C6	2.37	0.59
1:5:3961:G:C6	1:5:3963:A:H2'	2.37	0.59
1:5:4992:G:H2'	1:5:4993:G:C8	2.37	0.59
3:8:67:U:H2'	3:8:68:G:H8	1.66	0.59
1:5:1756:U:H2'	1:5:1757:U:C6	2.36	0.59
83:jj:511:ALA:HB3	83:jj:559:PHE:CZ	2.37	0.59
4:9:5:U:H2'	4:9:6:G:H8	1.67	0.59
1:5:2546:G:O2'	1:5:2547:G:OP1	2.18	0.59
4:9:107:A:H2'	4:9:108:G:C8	2.37	0.59
81:11:69:U:H2'	81:11:70:G:C8	2.38	0.59
83:jj:533:ARG:N	83:jj:536:ASP:OD2	2.33	0.59
81:13:23:C:H2'	81:13:24:G:C8	2.38	0.58
1:5:746:A:O2'	1:5:747:A:H5'	2.03	0.58
1:5:1188:C:H2'	1:5:1189:G:C8	2.38	0.58
1:5:1989:G:H2'	1:5:1990:A:H8	1.68	0.58
3:8:8:U:H2'	3:8:9:A:H8	1.69	0.58
4:9:898:U:H2'	4:9:899:U:C6	2.39	0.58
4:9:1597:C:OP2	71:ZZ:85:ARG:NH2	2.29	0.58
29:Z:5:MET:HG3	29:Z:77:TYR:OH	2.04	0.58
32:c:13:SER:O	32:c:17:ARG:NE	2.36	0.58
1:5:2685:C:OP1	36:g:57:ARG:NH1	2.36	0.58
1:5:2822:G:N7	21:R:20:LYS:NZ	2.49	0.58
1:5:4239:A:H2'	1:5:4240:G:C8	2.39	0.58
1:5:4960:G:H2'	1:5:4961:G:H8	1.68	0.58
4:9:1239:U:H5''	61:PP:124:LYS:HE2	1.86	0.58
1:5:1190:C:H2'	1:5:1191:C:C6	2.39	0.58
1:5:4039:G:H4'	1:5:4049:U:H2'	1.85	0.58
4:9:656:G:O2'	48:CC:227:ARG:NH1	2.35	0.58
4:9:1424:G:H2'	4:9:1425:G:H8	1.69	0.58
49:DD:70:THR:HG22	49:DD:86:LEU:HD13	1.85	0.58
1:5:456:C:H2'	1:5:457:G:C8	2.38	0.58
4:9:1337:C:H2'	4:9:1338:G:H8	1.69	0.58
83:jj:402:THR:O	83:jj:470:ARG:NH2	2.34	0.58
83:jj:512:MET:HA	83:jj:521:THR:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3904:G:O2'	1:5:3905:A:OP1	2.20	0.57
2:7:3:C:H2'	2:7:4:U:C6	2.39	0.57
7:C:335:MET:O	7:C:339:THR:HG23	2.04	0.57
63:RR:37:GLU:OE2	78:gg:106:LYS:NZ	2.30	0.57
1:5:280:G:H5''	17:N:14:LYS:HE2	1.85	0.57
17:N:178:HIS:HA	17:N:181:HIS:NE2	2.18	0.57
4:9:1228:A:H2'	4:9:1229:G:H8	1.68	0.57
4:9:1658:G:OP2	4:9:1660:C:N4	2.37	0.57
58:MM:75:ASN:HB3	58:MM:128:PHE:CZ	2.39	0.57
1:5:54:G:OP1	82:j:43:ARG:NH1	2.38	0.57
80:12:66:A:H2'	80:12:67:A:C8	2.39	0.57
4:9:866:U:H2'	4:9:867:G:C8	2.39	0.57
4:9:1293:A:N6	4:9:1306:U:H3	2.01	0.57
1:5:1238:A:O2'	1:5:1239:C:OP1	2.17	0.57
1:5:4077:A:N1	1:5:4171:C:N4	2.52	0.57
4:9:649:U:H2'	4:9:650:A:H8	1.70	0.57
1:5:3877:A:N3	1:5:4401:G:O2'	2.30	0.57
78:gg:42:MET:SD	78:gg:56:GLN:NE2	2.74	0.57
1:5:217:C:H4'	1:5:218:A:C8	2.40	0.57
1:5:1818:G:OP2	1:5:1818:G:N2	2.29	0.57
1:5:457:G:H2'	1:5:458:C:C6	2.40	0.57
1:5:1411:C:H2'	1:5:1411(A):G:H8	1.70	0.57
1:5:165:A:H2'	1:5:166:C:C6	2.40	0.56
1:5:3961:G:N1	1:5:3963:A:H2'	2.20	0.56
4:9:1227:G:C2	4:9:1228:A:C8	2.92	0.56
1:5:4942:C:H4'	1:5:4943:A:OP1	2.03	0.56
71:ZZ:79:ILE:HB	71:ZZ:83:LEU:HD23	1.86	0.56
1:5:478:G:H2'	1:5:479:G:H8	1.70	0.56
1:5:2465:C:H1'	1:5:3672:G:H22	1.70	0.56
1:5:3740:G:O2'	81:11:70:G:O2'	2.24	0.56
1:5:4239:A:H2'	1:5:4240:G:H8	1.71	0.56
1:5:4286:C:H2'	1:5:4287:G:H8	1.70	0.56
4:9:1101:U:H2'	4:9:1102:G:C8	2.41	0.56
10:G:229:LYS:HD3	38:i:43:MET:HE1	1.87	0.56
17:N:184:ILE:O	17:N:194:ARG:NH2	2.33	0.56
29:Z:5:MET:HG3	29:Z:77:TYR:CE2	2.39	0.56
47:BB:75:GLN:HG2	47:BB:78:GLU:OE2	2.06	0.56
83:jj:130:ASP:OD1	83:jj:152:ARG:NH2	2.38	0.56
1:5:264:C:H5''	1:5:265:C:OP2	2.04	0.56
1:5:3692:A:H62	1:5:3823:G:N2	2.03	0.56
3:8:93:C:OP1	82:j:76:HIS:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Z:4:PHE:CD2	29:Z:5:MET:HG2	2.40	0.56
49:DD:211:VAL:O	63:RR:20:TYR:OH	2.21	0.56
86:12:101:GTP:O1B	83:jj:475:LYS:NZ	2.27	0.56
1:5:3770:U:H2'	1:5:3771:C:C6	2.41	0.56
4:9:1868:U:O2'	72:aa:100:ARG:NH1	2.28	0.56
48:CC:196:ILE:HB	48:CC:223:TYR:HB2	1.87	0.56
50:EE:212:ASP:OD1	50:EE:213:ALA:N	2.37	0.56
1:5:1193:C:H2'	1:5:1194:G:C8	2.41	0.56
6:B:50:LYS:NZ	6:B:339:GLY:O	2.29	0.56
41:m:68:MET:HG2	41:m:79:PRO:HA	1.87	0.56
1:5:1961:G:O2'	1:5:2025:A:N6	2.39	0.56
1:5:3641:U:H5	1:5:3646:A:N7	2.04	0.56
1:5:3663:A:N6	1:5:4168:G:O2'	2.38	0.56
5:A:36:GLU:OE1	5:A:163:ARG:NH1	2.39	0.56
80:12:23:A:H2'	80:12:24:G:C8	2.40	0.56
1:5:2275:G:H2'	1:5:2276:A:C8	2.41	0.56
1:5:2478:C:N4	1:5:2479:G:O6	2.39	0.56
1:5:2503:G:N2	1:5:4084:G:O4'	2.39	0.56
1:5:2601:A:N6	1:5:2744:A:OP2	2.38	0.56
47:BB:107:ARG:NH1	60:OO:133:THR:O	2.35	0.56
1:5:1440:U:H2'	1:5:1441:C:C6	2.42	0.55
1:5:1558:A:H2'	1:5:1559:G:H8	1.71	0.55
1:5:1391:A:P	20:Q:181:ARG:HH22	2.29	0.55
1:5:1405:C:H2'	1:5:1406:G:C8	2.41	0.55
1:5:4459:U:H2'	1:5:4460:U:C6	2.42	0.55
22:S:161:ARG:NH1	22:S:164:LYS:O	2.39	0.55
81:13:23:C:H2'	81:13:24:G:H8	1.70	0.55
1:5:517:C:H2'	1:5:518:G:C8	2.41	0.55
1:5:2520:C:H2'	1:5:2521:G:C8	2.40	0.55
4:9:981:A:H2'	4:9:982:G:C8	2.40	0.55
4:9:1395:C:O2'	4:9:1396:A:OP1	2.21	0.55
57:LL:49:GLU:HG2	57:LL:118:ARG:HE	1.72	0.55
1:5:3707:U:H2'	1:5:3708:C:C6	2.42	0.55
4:9:1693:G:N2	4:9:1834:A:H8	2.05	0.55
62:QQ:16:LYS:NZ	62:QQ:123:ASP:OD2	2.40	0.55
67:VV:53:TYR:OH	67:VV:76:ASP:OD2	2.21	0.55
80:12:11:C:H2'	80:12:12:U:C6	2.41	0.55
4:9:649:U:H2'	4:9:650:A:C8	2.42	0.55
4:9:1305:C:OP2	77:ff:93:HIS:ND1	2.30	0.55
10:G:284:ASP:OD1	10:G:287:ARG:NH2	2.34	0.55
83:jj:350:THR:O	83:jj:354:PHE:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1311:G:H4'	34:e:50:LYS:HE2	1.89	0.55
30:a:72:THR:HG22	30:a:110:LYS:HB3	1.89	0.55
83:jj:555:GLN:HB3	83:jj:570:ILE:HD12	1.88	0.55
46:AA:36:GLN:O	46:AA:53:ARG:NH1	2.34	0.55
1:5:1195:G:H2'	1:5:1196:G:C8	2.42	0.55
4:9:674:C:H2'	4:9:675:U:C6	2.42	0.55
48:CC:275:LYS:HG3	48:CC:276:THR:HG23	1.89	0.55
1:5:1766:A:O2'	1:5:1767:A:O5'	2.20	0.54
1:5:4053:A:H2'	1:5:4054:C:C6	2.42	0.54
4:9:540:U:O2'	4:9:543:C:N4	2.41	0.54
63:RR:77:GLU:OE2	63:RR:80:ARG:NH2	2.39	0.54
1:5:2489:C:O2'	1:5:2491:C:N4	2.41	0.54
1:5:4303:C:H2'	1:5:4305:G:C8	2.43	0.54
4:9:862:A:C8	68:WW:107:SER:HA	2.42	0.54
26:W:105:ARG:NH2	52:GG:150:GLU:OE1	2.37	0.54
55:JJ:78:LEU:HB3	55:JJ:92:MET:HG3	1.88	0.54
62:QQ:19:ALA:HB2	62:QQ:75:GLY:HA3	1.88	0.54
3:8:75:G:OP2	28:Y:74:TYR:OH	2.22	0.54
4:9:536:A:H61	4:9:547:G:N2	2.05	0.54
29:Z:5:MET:HE2	29:Z:77:TYR:CE2	2.42	0.54
83:jj:501:HIS:H	83:jj:534:THR:HG22	1.72	0.54
1:5:1890:G:N2	1:5:1939:A:H61	2.05	0.54
61:PP:21:ASP:OD1	61:PP:22:LEU:N	2.41	0.54
10:G:201:GLU:OE2	17:N:6:TYR:OH	2.20	0.54
1:5:2097:A:OP1	1:5:2107:A:N6	2.41	0.54
1:5:3648:A:H1'	1:5:3785:A:N6	2.23	0.54
43:o:27:LYS:NZ	88:11:101:ATP:O2G	2.40	0.54
78:gg:116:ASP:OD2	78:gg:118:ARG:NH1	2.40	0.54
1:5:1177:U:H2'	1:5:1178:G:C8	2.42	0.54
1:5:2899:C:OP1	21:R:108:ARG:NH2	2.37	0.54
1:5:4260:U:H2'	1:5:4261:C:C6	2.43	0.54
1:5:679:C:OP1	45:r:84:LYS:NZ	2.33	0.54
1:5:981:C:P	9:E:48:ARG:HH22	2.30	0.54
1:5:1368:A:H1'	28:Y:1:MET:HE2	1.90	0.54
4:9:804:U:H2'	4:9:805:U:C6	2.43	0.54
4:9:1454:A:C2	4:9:1476:A:H1'	2.42	0.54
13:J:113:ILE:HD12	13:J:119:TYR:HB2	1.89	0.54
1:5:976:G:H21	7:C:323:ARG:CD	2.20	0.54
1:5:2477:A:H2'	1:5:2478:C:C6	2.43	0.54
1:5:4943:A:OP1	9:E:157:THR:HG22	2.08	0.54
4:9:1098:C:H2'	4:9:1099:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1588:A:H2'	4:9:1589:A:C8	2.43	0.54
19:P:54:LYS:HA	19:P:83:TRP:CD1	2.43	0.54
71:ZZ:100:VAL:HG21	71:ZZ:110:THR:HG23	1.89	0.54
1:5:1772:C:H2'	1:5:1773:U:O4'	2.08	0.54
1:5:4064:C:H2'	1:5:4065:G:C8	2.42	0.54
4:9:1037:G:H4'	4:9:1845:A:H4'	1.90	0.54
1:5:3868:G:H22	1:5:3900:G:H1'	1.73	0.53
12:I:66:GLU:OE1	12:I:69:ARG:NH1	2.36	0.53
1:5:1475:G:H2'	1:5:1476:C:C6	2.43	0.53
1:5:3968:U:O2'	1:5:3969:G:OP1	2.23	0.53
1:5:4258:C:H5'	13:J:68:ILE:HD11	1.90	0.53
1:5:4870:G:H2'	16:M:91:TRP:CZ2	2.43	0.53
16:M:89:THR:HG22	16:M:91:TRP:H	1.73	0.53
18:O:10:ASP:OD1	18:O:37:ARG:HD3	2.09	0.53
52:GG:223:LYS:NZ	52:GG:226:GLU:OE1	2.38	0.53
4:9:453:C:C2'	4:9:454:U:H5'	2.38	0.53
14:K:58:LYS:NZ	14:K:62:GLN:OE1	2.30	0.53
1:5:5029:C:H2'	1:5:5030:U:C6	2.44	0.53
4:9:165:G:OP2	4:9:165:G:N2	2.39	0.53
4:9:1438:A:H2'	4:9:1439:A:C8	2.43	0.53
4:9:942:G:H2'	4:9:943:U:C6	2.43	0.53
1:5:1200:G:H2'	1:5:1201:U:C6	2.44	0.53
4:9:527:C:H2'	4:9:528:A:H8	1.73	0.53
5:A:30:ARG:NH2	5:A:33:ASP:OD2	2.36	0.53
43:o:63:THR:O	43:o:87:ARG:NH1	2.41	0.53
80:12:66:A:H2'	80:12:67:A:H8	1.73	0.53
1:5:1198:G:H2'	1:5:1199:G:H8	1.74	0.53
1:5:4474:A:H5''	41:m:99:LYS:HG3	1.89	0.53
1:5:4935:C:H2'	1:5:4936:G:C8	2.44	0.53
4:9:5:U:H2'	4:9:6:G:C8	2.43	0.53
67:VV:20:SER:HB3	67:VV:59:ILE:HD11	1.91	0.53
4:9:1300:U:O2	61:PP:51:ARG:NH2	2.41	0.53
7:C:237:ILE:HD12	7:C:237:ILE:H	1.74	0.53
29:Z:77:TYR:CD1	29:Z:77:TYR:C	2.86	0.53
78:gg:105:THR:N	78:gg:126:ASP:OD2	2.37	0.53
1:5:4546:A:N7	5:A:215:ASN:ND2	2.57	0.53
1:5:4578:G:H2'	1:5:4579:U:C6	2.43	0.53
4:9:945:U:H2'	4:9:946:U:C6	2.44	0.53
10:G:217:ILE:O	10:G:221:VAL:HG13	2.08	0.53
70:YY:86:GLU:OE2	70:YY:90:ARG:NH1	2.31	0.53
1:5:979:C:OP1	9:E:49:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:688:U:OP1	53:HH:116:ARG:NH2	2.28	0.53
4:9:1303:C:O2	4:9:1303:C:H5'	2.09	0.53
4:9:1610:G:OP2	64:SS:132:ARG:NH1	2.42	0.53
78:gg:107:ASP:OD2	78:gg:125:ARG:NH1	2.41	0.53
1:5:2415:U:H2'	1:5:2416:G:C8	2.43	0.52
1:5:2864:A:H2'	1:5:2865:U:C6	2.43	0.52
1:5:3717:A:H2'	1:5:3718:A:H8	1.71	0.52
4:9:1776:G:H2'	4:9:1777:G:H8	1.73	0.52
29:Z:88:ASP:OD1	29:Z:121:ARG:NH2	2.32	0.52
80:12:18:G:O2'	80:12:57:G:N2	2.32	0.52
81:11:25:U:C2	81:11:26:G:C8	2.97	0.52
1:5:1246:G:N7	1:5:1247:U:N3	2.57	0.52
4:9:1692:U:H2'	4:9:1693:G:C8	2.43	0.52
65:TT:104:LEU:HD22	65:TT:121:ARG:HG3	1.90	0.52
1:5:1298:C:H2'	1:5:1299:G:H8	1.73	0.52
1:5:3923:A:H2'	1:5:3924:C:C6	2.44	0.52
4:9:1628:C:H2'	4:9:1629:C:C6	2.45	0.52
10:G:248:HIS:O	10:G:249:ARG:NH1	2.39	0.52
1:5:2478:C:H2'	1:5:2479:G:C8	2.45	0.52
1:5:152:U:P	17:N:49:ARG:HH12	2.33	0.52
1:5:1951:G:O2'	22:S:95:ARG:NH2	2.25	0.52
1:5:2755:A:P	29:Z:65:ARG:HH22	2.32	0.52
4:9:688:U:C5	53:HH:102:PRO:HA	2.44	0.52
4:9:1236:G:O2'	61:PP:131:PRO:O	2.19	0.52
4:9:1253:A:H4'	4:9:1254:C:H5''	1.92	0.52
80:12:69:U:H2'	80:12:70:C:C6	2.45	0.52
81:11:18:G:H21	81:11:57:G:H2'	1.74	0.52
1:5:136:C:H42	37:h:79:LYS:HE3	1.75	0.52
1:5:4238:G:H2'	1:5:4239:A:H8	1.74	0.52
83:jj:520:GLN:NE2	83:jj:549:GLU:OE2	2.42	0.52
47:BB:175:GLU:O	47:BB:187:LYS:NZ	2.43	0.52
50:EE:94:LYS:O	70:YY:16:ARG:NH2	2.29	0.52
1:5:100:C:H2'	1:5:101:A:H8	1.73	0.52
1:5:1643:A:H2'	1:5:1644:C:C6	2.45	0.52
1:5:4481:U:H2'	1:5:4482:U:C6	2.45	0.52
1:5:5053:U:H5'	1:5:5054:C:C5	2.44	0.52
4:9:507:G:P	70:YY:104:ARG:HH22	2.33	0.52
29:Z:100:VAL:HG13	29:Z:107:LYS:HA	1.92	0.52
73:bb:15:GLU:OE2	73:bb:18:LYS:NZ	2.34	0.52
1:5:1244:G:H2'	1:5:1245:C:C6	2.44	0.52
1:5:2079:G:H2'	1:5:2080:U:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3720:G:OP1	38:i:75:LYS:NZ	2.42	0.52
1:5:396:A:H2'	1:5:397:G:C8	2.45	0.51
1:5:2486:G:H2'	1:5:2487:G:C8	2.45	0.51
1:5:4370:G:H5''	43:o:64:LYS:HD2	1.91	0.51
1:5:4572:U:H2'	1:5:4573:G:C8	2.45	0.51
4:9:1527:C:OP1	62:QQ:142:GLN:NE2	2.30	0.51
6:B:80:GLU:OE1	6:B:323:TYR:OH	2.18	0.51
25:V:21:PRO:HA	25:V:54:ALA:HA	1.91	0.51
69:XX:68:LYS:HE2	76:ee:82:VAL:HG22	1.91	0.51
1:5:1617:G:H1'	1:5:2513:A:N6	2.26	0.51
1:5:156:G:N2	1:5:157:U:O4	2.42	0.51
1:5:4130:C:H2'	1:5:4131:G:H8	1.75	0.51
4:9:986:G:C8	60:OO:137:SER:O	2.63	0.51
60:OO:103:ASN:HB3	60:OO:139:SER:OG	2.10	0.51
1:5:1558:A:H2'	1:5:1559:G:C8	2.44	0.51
1:5:1942:A:H2'	1:5:1943:A:H8	1.75	0.51
1:5:2412:A:H2'	1:5:2413:U:C6	2.45	0.51
1:5:4233:A:C8	1:5:4235:G:C8	2.98	0.51
1:5:4623:G:OP1	6:B:19:ARG:NH2	2.43	0.51
4:9:186:C:H2'	4:9:187:G:H8	1.75	0.51
4:9:910:G:OP2	21:R:173:ARG:NH1	2.43	0.51
1:5:3944:G:H1	1:5:4069:U:H3	1.58	0.51
59:NN:25:TRP:CG	73:bb:82:LYS:HE2	2.45	0.51
1:5:1990:A:H2'	1:5:1991:A:H5''	1.93	0.51
1:5:4061:G:H2'	1:5:4062:A:C8	2.44	0.51
1:5:4950:U:O2'	1:5:4951:G:OP1	2.22	0.51
3:8:46:G:OP1	40:l:18:LYS:NZ	2.32	0.51
4:9:65:C:N4	52:GG:133:LEU:HB3	2.25	0.51
4:9:530:U:H3'	4:9:531:A:H8	1.75	0.51
58:MM:83:LYS:NZ	58:MM:87:GLU:OE2	2.37	0.51
78:gg:176:VAL:O	78:gg:185:LYS:N	2.36	0.51
1:5:1564:A:H2'	1:5:1565:A:C8	2.46	0.51
1:5:4274:A:H2'	1:5:4275:G:C8	2.45	0.51
4:9:886:A:H3'	4:9:887:U:H5''	1.91	0.51
58:MM:42:LEU:O	58:MM:45:ARG:NH1	2.44	0.51
1:5:4966:A:H5''	6:B:128:LYS:HG3	1.93	0.51
4:9:1144:A:H5'	4:9:1355:C:H41	1.76	0.51
4:9:1736:G:H2'	4:9:1737:G:H8	1.76	0.51
1:5:4064:C:H2'	1:5:4065:G:O4'	2.11	0.51
4:9:1541:G:N3	65:TT:12:GLN:NE2	2.58	0.51
4:9:1614:A:H2'	4:9:1615:U:H6	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:354:GLN:HG3	6:B:359:ALA:HB1	1.93	0.51
46:AA:5:LEU:HD21	67:VV:41:LYS:HA	1.92	0.51
1:5:1200:G:H2'	1:5:1201:U:H6	1.76	0.50
1:5:3948:C:H5''	1:5:3949:A:OP2	2.11	0.50
1:5:4301:U:H4'	23:T:54:HIS:CD2	2.45	0.50
4:9:895:G:H2'	4:9:896:U:C6	2.46	0.50
4:9:1115:U:O2'	4:9:1116:C:OP2	2.22	0.50
66:UU:21:ARG:HB3	66:UU:115:THR:HB	1.94	0.50
1:5:86:U:H2'	1:5:87:A:C8	2.46	0.50
78:gg:101:PHE:CE2	78:gg:136:GLY:HA2	2.46	0.50
83:jj:513:VAL:N	83:jj:520:GLN:O	2.41	0.50
1:5:668:C:H4'	7:C:6:PRO:HB3	1.92	0.50
1:5:2520:C:H2'	1:5:2521:G:H8	1.75	0.50
1:5:4925:U:H4'	1:5:4926:C:C5'	2.41	0.50
4:9:125:C:OP1	4:9:127:C:N4	2.44	0.50
57:LL:101:ARG:HB2	69:XX:7:LEU:O	2.12	0.50
1:5:1088:C:H2'	1:5:1089:G:H8	1.77	0.50
1:5:1932:A:OP2	18:O:49:ARG:NH2	2.39	0.50
3:8:141:C:OP1	17:N:38:ARG:NH1	2.45	0.50
46:AA:85:ARG:NH2	63:RR:82:ASP:O	2.38	0.50
73:bb:67:THR:HG21	73:bb:72:ARG:HH11	1.77	0.50
1:5:1989:G:H2'	1:5:1990:A:C8	2.47	0.50
1:5:2566:G:H2'	1:5:2567:G:C8	2.46	0.50
1:5:4045:G:H2'	1:5:4046:A:H3'	1.93	0.50
2:7:26:C:O2'	13:J:147:ARG:NH1	2.43	0.50
4:9:1693:G:H21	4:9:1834:A:H8	1.60	0.50
61:PP:18:ARG:NH1	64:SS:88:LYS:O	2.41	0.50
70:YY:7:ILE:HB	70:YY:47:MET:HE1	1.93	0.50
3:8:67:U:H2'	3:8:68:G:C8	2.45	0.50
4:9:877:C:H2'	4:9:878:G:C8	2.46	0.50
81:11:23:C:H2'	81:11:24:G:C8	2.47	0.50
13:J:109:ILE:HD13	13:J:115:LEU:HD21	1.93	0.50
29:Z:5:MET:SD	29:Z:82:PRO:HB3	2.52	0.50
49:DD:16:ILE:HD11	75:dd:36:LEU:HD23	1.94	0.50
1:5:973:G:N2	1:5:1282:G:C8	2.80	0.50
1:5:1077:C:OP1	1:5:1215:C:O2'	2.21	0.50
1:5:1244:G:C6	1:5:1245:C:N4	2.79	0.50
4:9:1291:A:OP2	4:9:1302:G:O2'	2.29	0.50
4:9:1407:U:H2'	4:9:1408:U:C6	2.46	0.50
4:9:1862:G:O2'	72:aa:5:ARG:NH2	2.45	0.50
1:5:1195:G:H2'	1:5:1196:G:H8	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2083:C:OP2	20:Q:14:ARG:NH2	2.42	0.50
1:5:2313:A:HO2'	1:5:2314:G:P	2.34	0.50
1:5:4037:C:H2'	1:5:4038:C:C6	2.47	0.50
1:5:4508:C:OP1	25:V:43:LYS:NZ	2.44	0.50
4:9:63:U:O2'	4:9:170:A:N3	2.41	0.50
4:9:821:G:C6	55:JJ:150:ARG:HG3	2.47	0.50
83:jj:64:LYS:NZ	83:jj:105:GLU:OE2	2.44	0.50
1:5:2079:G:H2'	1:5:2080:U:H6	1.77	0.49
4:9:1313:A:H4'	4:9:1314:U:O5'	2.12	0.49
6:B:381:THR:HG23	6:B:384:GLU:H	1.77	0.49
9:E:69:ALA:HA	9:E:71:TYR:CE2	2.46	0.49
49:DD:142:LEU:HD13	49:DD:150:MET:HG3	1.93	0.49
1:5:3947:A:H2'	1:5:3948:C:C6	2.47	0.49
1:5:4238:G:H2'	1:5:4239:A:C8	2.48	0.49
4:9:878:G:H1	4:9:908:A:H61	1.58	0.49
4:9:1285:G:O6	58:MM:82:ASN:ND2	2.44	0.49
4:9:1720:U:H3'	4:9:1721:U:H5''	1.95	0.49
12:I:38:ARG:NH1	12:I:45:GLU:OE1	2.43	0.49
25:V:48:ARG:HD2	25:V:49:LEU:H	1.77	0.49
59:NN:55:ARG:NH1	59:NN:56:ASP:OD1	2.45	0.49
1:5:424:U:H2'	1:5:425:U:C6	2.46	0.49
1:5:1402:C:H2'	1:5:1403:G:H8	1.76	0.49
1:5:4286:C:H2'	1:5:4287:G:C8	2.46	0.49
4:9:581:U:H4'	70:YY:66:GLY:CA	2.43	0.49
4:9:1285:G:OP1	58:MM:107:SER:OG	2.25	0.49
54:II:38:ILE:HD11	54:II:81:VAL:HG23	1.94	0.49
81:11:53:G:H2'	81:11:54:A:C8	2.43	0.49
4:9:344:U:H2'	4:9:345:U:C6	2.47	0.49
4:9:1337:C:H2'	4:9:1338:G:C8	2.48	0.49
4:9:1801:A:H2'	4:9:1802:C:C6	2.48	0.49
14:K:216:ARG:O	14:K:245:ARG:NH1	2.41	0.49
1:5:520:U:H2'	1:5:521:C:C6	2.47	0.49
1:5:1358:G:H2'	1:5:1360:G:O6	2.12	0.49
1:5:3606:U:H2'	1:5:3607:U:C6	2.48	0.49
1:5:3930:U:H2'	1:5:3931:C:C6	2.48	0.49
4:9:1855:G:OP2	60:OO:147:ARG:NH1	2.44	0.49
83:jj:501:HIS:ND1	83:jj:502:PRO:HD2	2.28	0.49
1:5:2503:G:H5''	1:5:2503:G:H8	1.78	0.49
1:5:2504:C:O2'	1:5:2505:C:O2	2.25	0.49
1:5:2664:G:H4'	1:5:2677:G:H4'	1.94	0.49
1:5:4926:C:H5'	1:5:4926:C:O2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:10:GLY:O	16:M:62:LEU:N	2.43	0.49
50:EE:199:GLU:OE2	50:EE:209:HIS:NE2	2.43	0.49
81:13:18:G:H21	81:13:57:G:H2'	1.78	0.49
1:5:2409:U:H5	1:5:2783:A:N1	2.11	0.49
1:5:4038:C:H2'	1:5:4039:G:C8	2.47	0.49
1:5:4099:G:H22	1:5:4109:G:N2	2.11	0.49
4:9:107:A:H2'	4:9:108:G:H8	1.78	0.49
8:D:202:GLN:NE2	8:D:237:GLU:OE1	2.44	0.49
59:NN:19:ARG:NH2	73:bb:84:HIS:OXT	2.44	0.49
62:QQ:146:ARG:NH1	81:13:35:A:OP2	2.46	0.49
1:5:490:C:H2'	1:5:491:G:C8	2.48	0.49
1:5:1509:C:H5''	30:a:2:PRO:HD2	1.94	0.49
58:MM:85:LEU:HD21	58:MM:109:VAL:HG23	1.94	0.49
1:5:655:C:P	7:C:268:ARG:HE	2.35	0.49
1:5:1380:G:H4'	1:5:1381:U:O2	2.12	0.49
1:5:1967:A:C2	1:5:2021:G:C5	3.01	0.49
1:5:2567:G:H2'	1:5:2568:C:C6	2.48	0.49
1:5:2602:G:H2'	1:5:2603:C:C6	2.47	0.49
1:5:3860:A:H61	1:5:4560:C:H5	1.59	0.49
1:5:4504:C:H2'	1:5:4505:C:C6	2.48	0.49
1:5:4911:A:OP2	6:B:100:ARG:NH1	2.40	0.49
1:5:4935:C:H2'	1:5:4936:G:H8	1.77	0.49
1:5:1402:C:H2'	1:5:1403:G:C8	2.47	0.49
1:5:2062:C:OP1	22:S:2:LYS:HG3	2.13	0.49
1:5:4772:C:N4	1:5:4864:U:O2	2.42	0.49
4:9:29:G:H2'	4:9:30:C:C6	2.48	0.49
4:9:1698:C:O2'	4:9:1699:A:OP1	2.29	0.49
19:P:42:ARG:NH1	19:P:110:ASP:OD1	2.46	0.49
1:5:1332:C:H2'	1:5:1333:A:C8	2.48	0.48
1:5:1332:C:H2'	1:5:1333:A:H8	1.78	0.48
1:5:2895:A:H2'	1:5:2896:G:C8	2.48	0.48
1:5:3736:A:H2'	1:5:3737:A:C8	2.48	0.48
1:5:3949:A:H2'	1:5:3950:U:C6	2.48	0.48
4:9:571:U:H5'	70:YY:37:LYS:HE2	1.95	0.48
6:B:56:ILE:O	6:B:73:VAL:HA	2.13	0.48
10:G:139:VAL:HG11	10:G:238:LYS:HE3	1.95	0.48
36:g:15:THR:HG22	36:g:16:ALA:H	1.78	0.48
55:JJ:155:LYS:HE3	55:JJ:156:HIS:CE1	2.48	0.48
1:5:981:C:OP2	9:E:48:ARG:NH2	2.43	0.48
1:5:1920:C:H3'	1:5:1921:C:H5''	1.95	0.48
1:5:2440:U:O2'	1:5:2441:C:OP1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2517:A:O2'	36:g:66:ARG:NH2	2.45	0.48
1:5:4188:U:H2'	1:5:4189:U:H6	1.77	0.48
4:9:186:C:H2'	4:9:187:G:C8	2.48	0.48
4:9:1597:C:H4'	4:9:1603:G:O6	2.12	0.48
4:9:1856:C:H2'	4:9:1857:G:C8	2.48	0.48
83:jj:173:LYS:NZ	90:jj:700:GCP:O2G	2.33	0.48
1:5:2053:C:O3'	18:O:18:ARG:NH1	2.44	0.48
1:5:4099:G:H1	1:5:4109:G:N2	2.09	0.48
4:9:126:G:OP1	52:GG:198:ARG:NH1	2.33	0.48
4:9:1781:A:H2'	4:9:1782:G:C8	2.48	0.48
4:9:1854:U:OP1	60:OO:150:ARG:NH2	2.45	0.48
19:P:39:MET:O	19:P:114:ILE:HG22	2.13	0.48
78:gg:258:ILE:O	78:gg:267:VAL:N	2.35	0.48
1:5:3873:G:H2'	1:5:3874:G:C8	2.49	0.48
1:5:5066:U:OP1	19:P:43:LYS:NZ	2.44	0.48
4:9:72:C:H41	52:GG:170:ARG:NH1	2.11	0.48
63:RR:99:ASP:HB2	63:RR:100:PRO:HD2	1.96	0.48
68:WW:6:VAL:HG12	68:WW:34:ILE:HD11	1.95	0.48
1:5:3911:C:H2'	1:5:3912:U:C6	2.47	0.48
4:9:1292:C:H2'	4:9:1293:A:H5''	1.95	0.48
4:9:1507:G:H1	77:ff:88:PRO:HA	1.79	0.48
14:K:114:ARG:NH1	20:Q:4:ASP:O	2.43	0.48
47:BB:168:MET:HG2	47:BB:197:ILE:HG21	1.95	0.48
53:HH:170:VAL:HG13	53:HH:187:PHE:HB2	1.95	0.48
1:5:433:A:C2	1:5:3867:A:H4'	2.48	0.48
1:5:1534:A:C8	82:j:15:THR:HG23	2.48	0.48
1:5:3681:G:N1	5:A:118:GLU:OE2	2.46	0.48
2:7:7:G:OP1	8:D:33:ARG:NE	2.30	0.48
4:9:1736:G:H2'	4:9:1737:G:C8	2.49	0.48
81:11:70:G:H2'	81:11:71:C:C6	2.47	0.48
1:5:470:A:H61	1:5:684:G:H1'	1.78	0.48
1:5:1964:A:H3'	1:5:1965:G:H8	1.78	0.48
1:5:2088:A:C5'	1:5:2089:G:H3'	2.44	0.48
1:5:4594:U:H2'	1:5:4595:G:H8	1.78	0.48
8:D:278:ASP:OD2	8:D:282:GLN:NE2	2.41	0.48
55:JJ:136:ARG:HD3	55:JJ:160:SER:HA	1.95	0.48
1:5:1075:G:H22	1:5:1235:G:N2	2.12	0.48
1:5:4481:U:H2'	1:5:4482:U:H6	1.79	0.48
1:5:5003:U:H2'	1:5:5004:C:C6	2.48	0.48
4:9:106:C:H2'	4:9:107:A:H8	1.79	0.48
4:9:496:C:OP1	50:EE:29:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:156:LEU:HD11	9:E:198:ILE:HG13	1.96	0.48
32:c:47:ILE:HD12	32:c:94:LEU:HD12	1.95	0.48
1:5:1502:G:O6	20:Q:89:ASP:HA	2.14	0.48
1:5:3692:A:H62	1:5:3823:G:H21	1.62	0.48
1:5:4520:G:H2'	1:5:4521:U:O4'	2.14	0.48
4:9:57:U:OP1	4:9:504:G:O2'	2.25	0.48
4:9:1623:A:H5''	64:SS:133:GLY:HA3	1.96	0.48
8:D:68:ARG:NH1	8:D:70:GLU:OE1	2.47	0.48
29:Z:5:MET:HG3	29:Z:77:TYR:CZ	2.48	0.48
39:k:24:LYS:HA	39:k:67:LYS:O	2.13	0.48
52:GG:48:TYR:OH	52:GG:119:LYS:O	2.29	0.48
53:HH:75:ILE:HG22	53:HH:79:LEU:HB2	1.96	0.48
1:5:691:C:H2'	1:5:692:A:C8	2.48	0.48
1:5:3965:A:N1	1:5:4047:A:H2'	2.29	0.48
1:5:4266:G:N3	1:5:4266:G:H2'	2.29	0.48
4:9:412:G:O2'	4:9:812:A:N6	2.46	0.48
15:L:21:ARG:HB3	17:N:197:THR:HG22	1.96	0.48
51:FF:73:THR:O	51:FF:89:THR:HG21	2.14	0.48
83:jj:420:LEU:HD13	83:jj:456:ARG:HG2	1.96	0.48
1:5:660:G:H2'	1:5:661:C:C6	2.48	0.47
1:5:1961:G:O2'	1:5:2024:G:N2	2.46	0.47
1:5:2695:A:OP1	39:k:35:LYS:NZ	2.34	0.47
1:5:2714:G:OP2	39:k:70:LYS:NZ	2.39	0.47
6:B:384:GLU:OE2	26:W:14:TYR:OH	2.30	0.47
17:N:80:THR:HB	17:N:87:HIS:HB3	1.96	0.47
43:o:24:THR:O	43:o:69:ARG:N	2.45	0.47
47:BB:208:HIS:CG	47:BB:209:ASP:H	2.32	0.47
53:HH:192:PHE:CD2	73:bb:12:PRO:HB3	2.48	0.47
72:aa:45:VAL:HG21	72:aa:64:LEU:HD13	1.96	0.47
1:5:86:U:H2'	1:5:87:A:H8	1.78	0.47
1:5:1457:G:O2'	1:5:1458:C:H5''	2.14	0.47
1:5:4957:C:H3'	1:5:4958:C:H5''	1.96	0.47
4:9:68:A:OP2	52:GG:164:LYS:NZ	2.32	0.47
47:BB:136:ARG:HB2	47:BB:218:LEU:HD11	1.96	0.47
48:CC:169:TYR:OH	48:CC:175:GLY:O	2.31	0.47
1:5:1811:G:H2'	1:5:1812:C:C6	2.48	0.47
1:5:3799:A:OP1	25:V:64:THR:HG21	2.14	0.47
1:5:4621:C:OP1	25:V:48:ARG:NH1	2.38	0.47
10:G:153:HIS:CE1	10:G:156:ARG:HH11	2.32	0.47
18:O:168:TYR:CE2	18:O:172:LYS:HE3	2.50	0.47
51:FF:179:ASN:HB3	51:FF:187:SER:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:aa:87:ARG:NH2	72:aa:94:ASP:O	2.33	0.47
1:5:407:A:O2'	1:5:410:A:OP1	2.32	0.47
1:5:660:G:H2'	1:5:661:C:H6	1.80	0.47
1:5:1472:C:H2'	1:5:1473:U:C6	2.50	0.47
1:5:2673:G:N3	1:5:2673:G:H5'	2.29	0.47
4:9:1017:U:H2'	4:9:1018:U:H6	1.78	0.47
51:FF:38:TYR:OH	74:cc:54:ASP:OD1	2.20	0.47
1:5:1406:G:H2'	1:5:1406(A):G:H8	1.79	0.47
1:5:2415:U:H2'	1:5:2416:G:N9	2.30	0.47
1:5:2638:G:H1	1:5:2697:A:H61	1.63	0.47
4:9:1277:C:H2'	4:9:1278:A:H8	1.80	0.47
20:Q:69:LYS:O	20:Q:75:ARG:NH1	2.47	0.47
57:LL:40:ILE:HD11	57:LL:44:PHE:HB2	1.96	0.47
80:12:63:C:H2'	80:12:64:A:H8	1.79	0.47
1:5:2478:C:H2'	1:5:2479:G:H8	1.79	0.47
1:5:4485:C:O2'	41:m:88:LYS:NZ	2.43	0.47
4:9:225:G:O5'	4:9:225:G:H8	1.97	0.47
4:9:693:A:H61	4:9:733:C:N4	2.13	0.47
48:CC:254:ASP:N	48:CC:254:ASP:OD1	2.46	0.47
52:GG:126:ASP:OD1	52:GG:127:THR:N	2.47	0.47
61:PP:14:LYS:NZ	61:PP:23:ASP:OD2	2.45	0.47
81:11:43:G:H2'	81:11:44:A:H8	1.78	0.47
1:5:325:U:H2'	1:5:326:C:C6	2.50	0.47
1:5:1397:A:N1	1:5:1498:G:O2'	2.45	0.47
1:5:2088:A:H5''	1:5:2089:G:H3'	1.97	0.47
1:5:2574:G:N7	1:5:2760:G:N2	2.62	0.47
1:5:4572:U:H2'	1:5:4573:G:H8	1.80	0.47
4:9:74:G:N2	4:9:78:C:OP2	2.38	0.47
4:9:1503:C:H2'	4:9:1504:U:C6	2.49	0.47
4:9:1839:U:H1'	4:9:1863:A:H2	1.79	0.47
18:O:37:ARG:HD2	18:O:108:ILE:HD11	1.96	0.47
39:k:37:ARG:HD3	39:k:38:CYS:O	2.15	0.47
49:DD:105:LEU:HB2	49:DD:122:VAL:HG21	1.97	0.47
52:GG:52:ILE:HG23	52:GG:52:ILE:O	2.15	0.47
1:5:1344:C:H2'	1:5:1345:A:C8	2.50	0.47
1:5:1727:U:H2'	1:5:1728:U:C6	2.50	0.47
4:9:527:C:H2'	4:9:528:A:C8	2.50	0.47
4:9:640:A:H2'	4:9:641:A:C8	2.50	0.47
78:gg:249:CYS:SG	78:gg:289:LEU:HD13	2.54	0.47
81:13:18:G:N2	81:13:57:G:H2'	2.30	0.47
1:5:136:C:N4	37:h:79:LYS:HE3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1440:U:H2'	1:5:1441:C:C5	2.50	0.47
1:5:2404:A:H61	1:5:2787:A:H61	1.63	0.47
1:5:2404:A:H61	1:5:2787:A:N6	2.13	0.47
1:5:2876:G:OP1	44:p:7:LYS:N	2.37	0.47
4:9:141:A:H61	4:9:177:G:H1'	1.80	0.47
4:9:221:A:H2'	4:9:222:U:C6	2.49	0.47
4:9:1134:G:H2'	4:9:1135:C:C6	2.50	0.47
4:9:1774:C:H2'	4:9:1775:U:C6	2.50	0.47
18:O:79:ILE:O	18:O:83:THR:HG23	2.15	0.47
45:r:105:ASP:OD1	45:r:105:ASP:N	2.47	0.47
52:GG:7:PHE:HB2	52:GG:113:ILE:HD12	1.97	0.47
64:SS:92:ASP:HB3	64:SS:94:LYS:HE2	1.97	0.47
78:gg:245:ARG:HD3	78:gg:247:TRP:CH2	2.50	0.47
1:5:980:U:O2	1:5:1275:G:N2	2.32	0.47
1:5:1405:C:H2'	1:5:1406:G:H8	1.80	0.47
1:5:3961:G:H2'	1:5:3962:A:H2'	1.97	0.47
1:5:4591:U:H2'	1:5:4592:C:C6	2.50	0.47
80:12:65:G:H2'	80:12:66:A:H8	1.79	0.47
1:5:1358:G:N2	1:5:1381:U:O4	2.48	0.46
4:9:1347:U:OP1	48:CC:121:ARG:NH2	2.33	0.46
4:9:1782:G:H5''	4:9:1783:C:OP2	2.15	0.46
49:DD:28:GLU:OE1	56:KK:61:GLN:NE2	2.43	0.46
58:MM:52:LEU:HD21	58:MM:62:VAL:HG13	1.97	0.46
83:jj:135:ARG:HH11	83:jj:135:ARG:HA	1.80	0.46
1:5:262:G:H2'	1:5:263:G:H8	1.80	0.46
1:5:519:C:H2'	1:5:520:U:C6	2.51	0.46
1:5:1818:G:H2'	1:5:1820:U:OP2	2.16	0.46
11:H:40:HIS:ND1	11:H:41:ILE:HG13	2.29	0.46
47:BB:23:ASP:OD2	60:OO:16:SER:OG	2.27	0.46
1:5:1411(C):C:H2'	1:5:1412:G:C8	2.50	0.46
4:9:894:G:H2'	4:9:895:G:C8	2.51	0.46
4:9:1614:A:H2'	4:9:1615:U:C6	2.50	0.46
5:A:137:ILE:HD11	5:A:149:LYS:HB2	1.97	0.46
13:J:43:LEU:HD13	13:J:117:ILE:HD11	1.98	0.46
46:AA:44:ASP:HA	63:RR:128:PHE:HB3	1.97	0.46
1:5:100:C:H2'	1:5:101:A:C8	2.51	0.46
4:9:869:A:N6	53:HH:115:LYS:O	2.43	0.46
7:C:339:THR:HG22	7:C:342:ARG:HH22	1.80	0.46
27:X:72:ASP:OD1	27:X:73:HIS:N	2.43	0.46
1:5:134:G:C8	1:5:134:G:H5'	2.50	0.46
1:5:678:C:H2'	1:5:679:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1502:G:H5'	1:5:1502:G:H8	1.81	0.46
1:5:2540:C:H2'	1:5:2541:G:H8	1.81	0.46
1:5:5006:U:H4'	1:5:5007:A:H5'	1.97	0.46
4:9:547:G:O5'	4:9:547:G:H8	1.98	0.46
46:AA:134:LEU:CD2	46:AA:144:THR:HG21	2.46	0.46
52:GG:58:LYS:HA	52:GG:107:SER:HB2	1.97	0.46
55:JJ:59:GLU:O	55:JJ:62:THR:OG1	2.32	0.46
65:TT:126:GLN:OE1	65:TT:129:ARG:NH1	2.48	0.46
72:aa:44:ILE:HG13	72:aa:45:VAL:HG23	1.98	0.46
1:5:1098:G:C6	1:5:1198:G:N2	2.84	0.46
1:5:2732:G:H2'	1:5:2733:C:C6	2.51	0.46
1:5:4862:G:H2'	1:5:4863:G:C8	2.51	0.46
1:5:4927:G:H3'	1:5:4928:C:O2	2.15	0.46
4:9:221:A:H2'	4:9:222:U:H6	1.80	0.46
4:9:907:G:H2'	4:9:908:A:C8	2.51	0.46
11:H:51:LYS:HB2	11:H:53:LYS:HG2	1.97	0.46
58:MM:75:ASN:HB3	58:MM:128:PHE:CE2	2.51	0.46
81:11:5:A:H2'	81:11:6:G:H8	1.80	0.46
1:5:1173:G:H2'	1:5:1174:G:C8	2.50	0.46
1:5:1468:C:H2'	1:5:1469:C:C6	2.51	0.46
1:5:4254:G:O2'	1:5:4255:A:OP1	2.32	0.46
1:5:4746:C:H2'	1:5:4747:C:C6	2.51	0.46
1:5:4960:G:H2'	1:5:4961:G:C8	2.48	0.46
4:9:1485:U:OP1	49:DD:151:LYS:NZ	2.48	0.46
1:5:1198:G:N2	1:5:1199:G:C6	2.84	0.46
1:5:1596:U:O2'	19:P:135:ARG:NH2	2.31	0.46
1:5:4751:G:H1	1:5:4948:C:H5	1.62	0.46
4:9:1447:G:O5'	66:UU:87:ARG:NH2	2.47	0.46
4:9:1622:U:OP1	64:SS:120:HIS:ND1	2.40	0.46
4:9:1737:G:H2'	4:9:1738:C:C6	2.51	0.46
29:Z:9:LYS:HB2	29:Z:25:ILE:HD12	1.97	0.46
1:5:4760:G:H2'	1:5:4761:G:O4'	2.16	0.46
4:9:17:C:H2'	4:9:18:C:C6	2.51	0.46
4:9:616:A:OP1	69:XX:68:LYS:NZ	2.47	0.46
4:9:804:U:H2'	4:9:805:U:H6	1.81	0.46
4:9:1863:A:H1'	72:aa:79:ILE:HD13	1.97	0.46
51:FF:136:ARG:CZ	81:11:32:C:H4'	2.46	0.46
80:12:9:A:N6	80:12:22:G:N7	2.63	0.46
81:13:47:U:H3'	81:13:48:C:H5'	1.98	0.46
81:11:48:C:C4	81:11:59:A:C8	3.03	0.46
1:5:664:G:H2'	1:5:665:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2089:G:O2'	7:C:307:LYS:NZ	2.36	0.46
1:5:3859:G:OP2	19:P:25:HIS:HE1	1.99	0.46
4:9:1397:U:O2	4:9:1397:U:H2'	2.16	0.46
55:JJ:58:ARG:O	55:JJ:62:THR:HG23	2.16	0.46
80:12:50:U:O2'	83:jj:510:GLN:OE1	2.34	0.46
1:5:982:U:O2	1:5:1273:G:N2	2.25	0.45
4:9:1004:U:H2'	4:9:1005:G:H8	1.81	0.45
50:EE:45:ILE:HD12	50:EE:80:ILE:HD12	1.98	0.45
63:RR:36:GLU:OE2	63:RR:47:ARG:NH1	2.42	0.45
1:5:164:G:H2'	1:5:165:A:C8	2.51	0.45
1:5:1298:C:H2'	1:5:1299:G:C8	2.51	0.45
1:5:1577:G:O5'	5:A:181:LYS:NZ	2.49	0.45
4:9:633:C:H1'	76:ee:89:THR:HG21	1.97	0.45
4:9:1169:G:OP1	42:n:6:ARG:NH2	2.48	0.45
6:B:288:GLY:HA3	6:B:330:PHE:CZ	2.52	0.45
11:H:16:VAL:HG21	11:H:81:ILE:HG23	1.97	0.45
35:f:88:PHE:CE1	35:f:92:LEU:HD11	2.50	0.45
49:DD:57:ASN:O	49:DD:65:ARG:NH1	2.45	0.45
1:5:1406:G:H2'	1:5:1406(A):G:C8	2.51	0.45
1:5:2864:A:H2'	1:5:2865:U:H6	1.81	0.45
1:5:3652:A:H2'	1:5:3653:A:C5	2.51	0.45
1:5:3827:G:O2'	1:5:3829:G:OP2	2.30	0.45
4:9:74:G:O6	52:GG:159:ARG:NH2	2.48	0.45
4:9:145:G:C5	4:9:175:A:C2	3.03	0.45
4:9:626:G:H3'	4:9:627:U:C5'	2.47	0.45
4:9:989:C:OP2	47:BB:155:TYR:OH	2.33	0.45
4:9:1088:U:H4'	4:9:1089:G:OP2	2.17	0.45
4:9:1119:A:H2'	4:9:1120:U:H6	1.80	0.45
24:U:42:PHE:CZ	24:U:46:ARG:HG3	2.51	0.45
46:AA:2:SER:O	46:AA:8:LEU:HB2	2.17	0.45
54:II:34:ALA:HB2	54:II:56:ARG:HD2	1.98	0.45
78:gg:36:ARG:C	78:gg:38:LYS:H	2.24	0.45
1:5:638:G:H2'	1:5:639:U:C6	2.51	0.45
1:5:1421:G:OP1	20:Q:68:ARG:NH2	2.45	0.45
6:B:89:ILE:HD11	6:B:150:PHE:CE1	2.52	0.45
48:CC:191:VAL:HG11	48:CC:236:PHE:HA	1.98	0.45
81:11:4:C:H2'	81:11:5:A:C8	2.52	0.45
4:9:536:A:N6	4:9:547:G:H22	2.11	0.45
4:9:880:G:C6	4:9:907:G:C6	3.04	0.45
4:9:1863:A:OP2	72:aa:4:LYS:NZ	2.42	0.45
5:A:180:LEU:HD23	5:A:180:LEU:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:84:PRO:HA	17:N:87:HIS:NE2	2.31	0.45
53:HH:37:LYS:O	53:HH:41:ARG:HB2	2.16	0.45
81:11:15:A:H61	81:11:21:A:H2	1.64	0.45
1:5:1411(B):C:H2'	1:5:1411(C):C:C6	2.51	0.45
1:5:2833:A:OP2	33:d:44:ARG:NH2	2.41	0.45
1:5:2869:U:O2'	1:5:2881:A:N7	2.48	0.45
1:5:4413:C:H5	1:5:4429:C:H42	1.64	0.45
1:5:4761:G:H2'	1:5:4762:A:C8	2.52	0.45
4:9:1004:U:H2'	4:9:1005:G:C8	2.51	0.45
4:9:1240:A:H8	4:9:1267:C:O2'	2.00	0.45
36:g:15:THR:HG22	36:g:16:ALA:N	2.31	0.45
81:11:48:C:H6	81:11:48:C:O5'	1.99	0.45
1:5:223:G:H4'	1:5:225:G:N7	2.32	0.45
1:5:2579:G:N2	1:5:2582:A:OP2	2.33	0.45
1:5:3642:A:C4	82:j:3:LYS:HB3	2.51	0.45
1:5:3788:C:N4	1:5:3812:C:OP2	2.41	0.45
3:8:150:C:N4	10:G:105:THR:O	2.49	0.45
4:9:145:G:H2'	4:9:146:G:C8	2.50	0.45
4:9:1229:G:H2'	4:9:1230:C:O4'	2.17	0.45
4:9:1839:U:H2'	4:9:1840:U:C6	2.52	0.45
8:D:37:VAL:HG12	8:D:50:ARG:HD2	1.99	0.45
64:SS:86:ARG:NH2	64:SS:89:ASP:OD1	2.35	0.45
83:jj:162:ARG:HB3	83:jj:251:ILE:HD11	1.99	0.45
1:5:1314:C:C2	1:5:1315:C:C5	3.05	0.45
1:5:2065:G:H2'	1:5:2066:C:O4'	2.17	0.45
1:5:2671:C:H2'	1:5:2672:C:C6	2.52	0.45
1:5:2837:U:OP1	6:B:249:ARG:NH1	2.46	0.45
1:5:3682:A:H5''	5:A:132:ASN:OD1	2.16	0.45
1:5:3934:G:H2'	1:5:3935:C:C6	2.52	0.45
4:9:153:G:C2	4:9:154:U:C4	3.05	0.45
4:9:1611:G:OP2	64:SS:121:ARG:NH2	2.32	0.45
17:N:80:THR:HB	17:N:87:HIS:CB	2.47	0.45
26:W:101:ARG:NH2	52:GG:145:PHE:O	2.49	0.45
58:MM:95:ASP:OD2	58:MM:101:ARG:NE	2.36	0.45
1:5:127:G:H2'	1:5:128:C:C6	2.52	0.45
1:5:510:U:H5''	30:a:86:THR:HG22	1.99	0.45
1:5:653:C:H2'	1:5:654:C:C6	2.51	0.45
1:5:3607:U:H2'	1:5:3608:A:H8	1.81	0.45
1:5:4562:C:H2'	1:5:4563:U:C6	2.52	0.45
4:9:106:C:H2'	4:9:107:A:C8	2.52	0.45
4:9:1284:A:H5'	4:9:1286:G:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:c:20:LEU:HD23	32:c:102:SER:HA	1.99	0.45
62:QQ:53:GLU:OE1	62:QQ:85:ARG:NH1	2.46	0.45
65:TT:75:MET:HA	65:TT:78:ILE:HG22	1.99	0.45
80:12:54:U:H5'	80:12:55:U:OP2	2.17	0.45
1:5:717:U:H2'	1:5:718:C:C6	2.52	0.45
1:5:2566:G:H2'	1:5:2567:G:H8	1.80	0.45
1:5:3607:U:H2'	1:5:3608:A:C8	2.52	0.45
1:5:3625:G:O2'	1:5:3626:G:OP1	2.33	0.45
1:5:4127:A:N3	1:5:4128:A:C8	2.85	0.45
1:5:4737:G:H2'	1:5:4738:C:H6	1.79	0.45
4:9:96:C:H2'	4:9:97:U:C6	2.52	0.45
1:5:175:C:H2'	1:5:176:G:C8	2.53	0.44
1:5:1210:C:H42	14:K:65:ARG:NH2	2.14	0.44
1:5:1236:C:H2'	1:5:1238:A:C8	2.52	0.44
1:5:2683:C:H2'	1:5:2684:C:C6	2.52	0.44
4:9:996:A:H2'	4:9:997:A:C8	2.52	0.44
14:K:148:SER:HA	14:K:244:ARG:NH2	2.31	0.44
64:SS:24:ARG:HB2	64:SS:29:ALA:HB2	1.98	0.44
81:11:23:C:H2'	81:11:24:G:H8	1.81	0.44
81:11:62:C:H2'	81:11:63:A:H8	1.82	0.44
83:jj:130:ASP:CG	83:jj:152:ARG:HE	2.25	0.44
1:5:1786:A:H2'	1:5:1789:C:C5	2.51	0.44
1:5:4130:C:H2'	1:5:4131:G:C8	2.53	0.44
4:9:1776:G:H2'	4:9:1777:G:C8	2.53	0.44
10:G:111:PRO:HD2	10:G:114:ILE:HD12	1.99	0.44
69:XX:68:LYS:HG2	76:ee:82:VAL:HG22	1.98	0.44
1:5:2899:C:H2'	1:5:2900:U:C6	2.52	0.44
1:5:4629:U:C2	1:5:4630:G:C8	3.06	0.44
2:7:62:U:OP2	8:D:276:LYS:NZ	2.45	0.44
4:9:928:G:H1	4:9:1013:U:H3	1.65	0.44
4:9:1070:A:H2'	4:9:1071:G:O4'	2.17	0.44
41:m:51:ILE:CG2	41:m:52:ILE:H	2.26	0.44
73:bb:42:LYS:HD2	73:bb:57:VAL:HG11	1.99	0.44
81:13:74:C:O2'	81:13:75:C:OP1	2.30	0.44
4:9:17:C:O2'	4:9:1194:A:N1	2.45	0.44
4:9:381:C:H2'	4:9:382:C:C6	2.52	0.44
4:9:1217:A:H2'	4:9:1218:C:C6	2.53	0.44
4:9:1679:A:OP1	51:FF:60:ARG:NH2	2.46	0.44
7:C:29:LYS:HB2	7:C:267:TRP:HH2	1.81	0.44
51:FF:127:ARG:NH1	51:FF:128:ILE:O	2.50	0.44
60:OO:43:HIS:CD2	60:OO:52:THR:HG1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1662:C:H2'	1:5:1663:C:C6	2.52	0.44
1:5:2429:A:H5''	40:l:43:HIS:NE2	2.33	0.44
3:8:144:U:H2'	3:8:145:C:C6	2.53	0.44
4:9:122:G:OP1	50:EE:75:LYS:NZ	2.35	0.44
10:G:230:MET:HE2	10:G:230:MET:HA	2.00	0.44
25:V:43:LYS:HE2	25:V:62:MET:SD	2.58	0.44
51:FF:51:HIS:O	62:QQ:50:LYS:HE3	2.17	0.44
53:HH:69:LEU:HD22	53:HH:96:ALA:HB2	2.00	0.44
78:gg:192:THR:OG1	78:gg:213:ASP:OD2	2.21	0.44
1:5:1727:U:OP1	14:K:130:ASN:ND2	2.50	0.44
1:5:2100:G:O2'	1:5:2101:A:OP2	2.33	0.44
1:5:2340:C:H5'	7:C:42:THR:HG21	1.99	0.44
1:5:2730:U:H2'	1:5:2731:C:C6	2.52	0.44
1:5:2874:U:O2	44:p:19:GLY:HA2	2.17	0.44
1:5:4173:G:H2'	1:5:4174:U:C6	2.53	0.44
4:9:349:A:H2'	4:9:350:C:C6	2.53	0.44
4:9:735:C:H2'	4:9:736:C:C6	2.52	0.44
4:9:920:A:H4'	68:WW:57:ARG:HG2	2.00	0.44
4:9:955:A:N3	4:9:956:G:H1'	2.33	0.44
4:9:1822:A:H2'	4:9:1823:A:H5''	1.99	0.44
18:O:157:GLU:OE1	18:O:160:ARG:NH1	2.51	0.44
52:GG:148:SER:N	52:GG:151:ASP:OD2	2.33	0.44
58:MM:36:ARG:HA	58:MM:36:ARG:HD2	1.79	0.44
1:5:478:G:H2'	1:5:479:G:C8	2.51	0.44
1:5:727:C:OP1	14:K:65:ARG:NH2	2.42	0.44
1:5:1772:C:H5''	1:5:1773:U:OP2	2.17	0.44
1:5:1893:C:H1'	1:5:1937:C:O2	2.17	0.44
1:5:3725:G:N2	1:5:3728:A:OP2	2.40	0.44
1:5:4740:G:N2	1:5:4960:G:C5	2.86	0.44
1:5:4944:C:OP1	1:5:4944:C:H4'	2.17	0.44
4:9:1117:C:O2	4:9:1117:C:H2'	2.18	0.44
4:9:1597:C:H4'	4:9:1603:G:C6	2.53	0.44
1:5:2495:U:H2'	1:5:2496:G:H8	1.83	0.44
4:9:346:C:H5''	4:9:347:G:OP2	2.18	0.44
4:9:878:G:H2'	4:9:879:C:H6	1.82	0.44
4:9:910:G:H2'	4:9:911:C:C6	2.53	0.44
4:9:1454:A:H2	4:9:1476:A:H1'	1.83	0.44
4:9:1670:C:H2'	4:9:1671:G:C8	2.53	0.44
30:a:103:VAL:CG1	30:a:108:TYR:HB2	2.48	0.44
48:CC:272:HIS:NE2	48:CC:276:THR:HG21	2.32	0.44
81:11:62:C:H2'	81:11:63:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:231:U:H4'	28:Y:100:HIS:CD2	2.53	0.44
1:5:1245:C:N4	1:5:1246:G:O6	2.51	0.44
1:5:4293:U:O4	1:5:4329:G:H8	2.01	0.44
1:5:4508:C:H5''	25:V:43:LYS:HD3	2.00	0.44
2:7:23:A:N3	2:7:118:C:O2'	2.40	0.44
4:9:407:G:H2'	4:9:407:G:N3	2.32	0.44
16:M:91:TRP:HA	16:M:94:LYS:HE3	1.99	0.44
30:a:59:ARG:HH11	30:a:59:ARG:HG3	1.83	0.44
38:i:45:ARG:NH1	38:i:49:GLY:O	2.49	0.44
80:12:62:A:H2'	80:12:63:C:C6	2.53	0.44
81:11:12:C:H2'	81:11:13:G:H8	1.83	0.44
83:jj:499:LEU:HD11	83:jj:567:VAL:HG13	1.99	0.44
83:jj:501:HIS:CG	83:jj:502:PRO:HD2	2.53	0.44
83:jj:561:GLU:HB3	83:jj:565:LYS:HG3	1.99	0.44
1:5:1346:C:H2'	1:5:1347:G:H8	1.83	0.43
1:5:2632:U:H2'	1:5:2633:U:C6	2.53	0.43
1:5:3732:A:H2'	1:5:3733:A:C8	2.53	0.43
4:9:216:C:C4	4:9:217:A:N7	2.86	0.43
17:N:94:PHE:CE2	17:N:96:ARG:HB2	2.53	0.43
30:a:79:TRP:CE3	30:a:87:ARG:HG2	2.53	0.43
54:II:60:LEU:HD23	54:II:185:ALA:HB2	2.00	0.43
60:OO:21:VAL:HG22	60:OO:25:GLU:HB3	2.00	0.43
80:12:15:G:H2'	80:12:16:U:C6	2.53	0.43
81:11:65:C:H2'	81:11:66:C:C6	2.53	0.43
83:jj:403:TYR:N	83:jj:411:VAL:O	2.40	0.43
1:5:129:C:H2'	1:5:130:C:C6	2.53	0.43
1:5:270:U:H2'	1:5:271:C:C6	2.53	0.43
1:5:940:C:OP1	14:K:241:ARG:NH2	2.49	0.43
1:5:1372:A:OP1	17:N:202:ARG:NH2	2.48	0.43
1:5:2342:G:OP2	30:a:2:PRO:HA	2.19	0.43
1:5:5016:A:H5''	1:5:5017:G:OP2	2.17	0.43
4:9:312:G:OP2	52:GG:195:LYS:NZ	2.38	0.43
4:9:1260:A:C2	4:9:1620:A:C8	3.06	0.43
13:J:119:TYR:CE1	64:SS:12:ILE:HD12	2.53	0.43
1:5:2275:G:H2'	1:5:2276:A:H8	1.82	0.43
1:5:4472:G:O2'	41:m:74:TYR:O	2.30	0.43
1:5:4524:G:N3	6:B:252:ALA:HB1	2.33	0.43
81:11:9:U:H5'	81:11:49:G:H5'	2.01	0.43
1:5:52:G:H4'	1:5:1529:G:H4'	1.99	0.43
1:5:1069:G:H5''	1:5:1070:G:OP2	2.18	0.43
4:9:352:U:H2'	4:9:353:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:561:A:H2'	4:9:562:U:C6	2.53	0.43
4:9:916:A:C5	59:NN:73:ARG:HD3	2.53	0.43
4:9:1323:U:H2'	4:9:1324:G:C8	2.52	0.43
4:9:1390:U:H2'	4:9:1391:C:C6	2.53	0.43
4:9:1536:G:H2'	4:9:1537:A:C8	2.53	0.43
19:P:128:ARG:HD2	19:P:136:ILE:HG21	2.01	0.43
29:Z:77:TYR:CZ	32:c:39:ARG:HG3	2.54	0.43
65:TT:11:GLN:OE1	65:TT:62:ARG:NH1	2.41	0.43
83:jj:64:LYS:NZ	83:jj:107:GLY:O	2.46	0.43
1:5:6:C:H2'	1:5:7:C:C6	2.53	0.43
1:5:1484:G:N3	1:5:1484:G:H2'	2.33	0.43
1:5:1501:C:C6	20:Q:68:ARG:HD2	2.54	0.43
1:5:1851:G:H4'	1:5:2283:G:H5'	2.00	0.43
1:5:2258:C:H5'	1:5:2258:C:C6	2.54	0.43
1:5:4488:A:H4'	1:5:4489:G:H8	1.83	0.43
3:8:153:C:OP1	10:G:238:LYS:NZ	2.44	0.43
4:9:379:C:H5'	54:II:33:ALA:HA	1.99	0.43
4:9:1513:C:H2'	4:9:1514:G:H8	1.83	0.43
4:9:1630:A:H5''	64:SS:37:GLY:H	1.83	0.43
4:9:1797:U:H2'	4:9:1798:C:C6	2.53	0.43
10:G:156:ARG:HH21	10:G:248:HIS:CE1	2.36	0.43
11:H:41:ILE:HG22	11:H:43:VAL:HG13	2.01	0.43
43:o:44:LYS:HE3	43:o:52:THR:HB	2.01	0.43
52:GG:34:THR:O	52:GG:52:ILE:HG22	2.19	0.43
57:LL:48:LYS:NZ	57:LL:52:GLU:OE1	2.42	0.43
81:11:29:G:C6	81:11:42:A:C6	3.07	0.43
1:5:966:A:H5'	1:5:967:C:H2'	2.01	0.43
1:5:1202:C:H2'	1:5:1203:G:H8	1.84	0.43
1:5:3968:U:HO2'	1:5:3969:G:P	2.41	0.43
1:5:5047:C:O2'	1:5:5050:C:OP2	2.28	0.43
4:9:1617:G:H4'	75:dd:14:PHE:CZ	2.53	0.43
4:9:1731:A:H2'	4:9:1732:G:C8	2.53	0.43
12:I:91:LEU:HD12	12:I:135:ILE:HG23	2.01	0.43
37:h:4:ILE:HD12	37:h:53:SER:HB2	2.00	0.43
46:AA:15:VAL:HG21	63:RR:111:PHE:CD2	2.54	0.43
58:MM:86:GLY:HA3	58:MM:104:VAL:O	2.17	0.43
64:SS:15:VAL:HG12	64:SS:16:LEU:HG	2.00	0.43
78:gg:196:ASN:HD21	78:gg:235:ILE:HD11	1.83	0.43
81:11:47:U:H3'	81:11:48:C:H5'	1.99	0.43
1:5:120:A:H2'	1:5:149:A:N6	2.32	0.43
1:5:665:C:H5''	1:5:666:G:O5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:679:C:H2'	1:5:680:G:H8	1.82	0.43
1:5:742:G:C6	1:5:922(A):G:C6	3.07	0.43
1:5:935:A:N3	16:M:44:ARG:HA	2.34	0.43
1:5:1502:G:H5''	1:5:1502:G:C8	2.54	0.43
1:5:4751:G:H22	1:5:4948:C:H5	1.66	0.43
4:9:562:U:H2'	4:9:563:G:C8	2.54	0.43
4:9:908:A:H2'	4:9:909:G:O4'	2.18	0.43
53:HH:64:VAL:HG13	53:HH:65:PRO:HD2	2.00	0.43
57:LL:101:ARG:NH1	69:XX:5:ARG:O	2.51	0.43
81:13:12:C:H2'	81:13:13:G:C8	2.53	0.43
81:11:5:A:H2'	81:11:6:G:C8	2.54	0.43
1:5:2095:A:H2'	1:5:2096:G:C8	2.54	0.43
1:5:2519:U:C2	1:5:2520:C:C5	3.07	0.43
1:5:3723:A:H2'	1:5:3724:A:C8	2.53	0.43
1:5:5041:G:OP2	26:W:61:LYS:NZ	2.45	0.43
4:9:1667:U:H2'	4:9:1668:U:C6	2.53	0.43
29:Z:115:LYS:NZ	29:Z:119:GLU:OE2	2.50	0.43
44:p:13:LYS:HE3	44:p:14:TYR:CZ	2.53	0.43
47:BB:126:ASP:OD1	47:BB:136:ARG:HD3	2.19	0.43
51:FF:122:ARG:HA	51:FF:146:ARG:HD3	1.99	0.43
80:12:63:C:H2'	80:12:64:A:C8	2.54	0.43
83:jj:133:LEU:HA	83:jj:147:TYR:CD1	2.54	0.43
1:5:1302:U:C5	1:5:1303:A:C6	3.06	0.43
1:5:1320:U:O2'	1:5:1891:A:N1	2.43	0.43
1:5:1468:C:H2'	1:5:1469:C:H6	1.84	0.43
1:5:1973:G:H2'	1:5:1974:U:C6	2.54	0.43
1:5:3710:G:H1'	1:5:3712:A:H61	1.79	0.43
1:5:4088:C:H2'	1:5:4089:G:C8	2.54	0.43
1:5:4088:C:H2'	1:5:4089:G:H8	1.84	0.43
4:9:181:A:H5''	4:9:182:C:OP2	2.19	0.43
4:9:1113:A:H2'	4:9:1114:U:C6	2.54	0.43
4:9:1624:U:H2'	4:9:1625:U:C6	2.54	0.43
52:GG:7:PHE:CZ	52:GG:9:ALA:HB3	2.54	0.43
77:ff:125:GLU:O	77:ff:143:LYS:NZ	2.28	0.43
1:5:67:C:OP2	1:5:312:G:N2	2.52	0.43
1:5:217:C:H6	1:5:217:C:H2'	1.72	0.43
1:5:484:U:O2'	1:5:485:C:OP1	2.29	0.43
1:5:4458:C:H2'	1:5:4459:U:C6	2.53	0.43
4:9:523:A:P	55:JJ:127:ARG:HH21	2.41	0.43
4:9:1101:U:H2'	4:9:1102:G:H8	1.81	0.43
4:9:1531:A:H2'	4:9:1532:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:185:ASN:ND2	9:E:274:LEU:O	2.51	0.43
19:P:29:THR:HA	19:P:32:THR:HG22	2.00	0.43
34:e:35:TRP:CE2	34:e:56:PRO:HD2	2.54	0.43
43:o:72:CYS:HB3	43:o:77:CYS:O	2.19	0.43
80:12:19:G:O3'	80:12:20:G:N2	2.52	0.43
1:5:975:C:H2'	1:5:976:G:C8	2.53	0.42
1:5:1088:C:H2'	1:5:1089:G:C8	2.53	0.42
1:5:1455:G:H2'	1:5:1456:C:C6	2.54	0.42
1:5:3653:A:H4'	5:A:179:ILE:O	2.18	0.42
1:5:4978:G:H2'	1:5:4979:A:H5''	2.01	0.42
3:8:9:A:H2'	3:8:10:G:H8	1.83	0.42
4:9:65:C:C5	52:GG:133:LEU:HD13	2.54	0.42
4:9:1246:A:O2'	66:UU:72:GLU:OE2	2.31	0.42
34:e:89:LEU:HD13	34:e:118:LEU:HD22	2.01	0.42
57:LL:17:PHE:CZ	57:LL:19:ASN:HB2	2.53	0.42
58:MM:52:LEU:O	58:MM:79:VAL:N	2.45	0.42
80:12:76:A:OP1	83:jj:449:ARG:NH2	2.44	0.42
1:5:63:G:P	17:N:169:ARG:HH22	2.42	0.42
1:5:99:A:H2'	1:5:100:C:O2	2.19	0.42
1:5:1766:A:O2'	1:5:1767:A:P	2.77	0.42
1:5:1846:G:H2'	1:5:1847:C:C6	2.54	0.42
1:5:4048:A:O2'	1:5:4049:U:OP2	2.35	0.42
4:9:533:A:C6	4:9:552:G:C6	3.07	0.42
4:9:1566:G:O3'	4:9:1567:G:N2	2.52	0.42
7:C:293:LEU:HD22	20:Q:34:PHE:CD2	2.54	0.42
17:N:51:LEU:HD11	17:N:119:TYR:HB3	2.01	0.42
23:T:28:ALA:HA	23:T:31:MET:HG2	2.01	0.42
52:GG:127:THR:HG22	52:GG:128:THR:N	2.34	0.42
69:XX:63:ASN:ND2	69:XX:114:ASP:OD1	2.45	0.42
82:j:27:TYR:HA	82:j:34:CYS:HA	2.01	0.42
1:5:40:G:N2	1:5:4380:A:H62	2.17	0.42
1:5:1836:G:H4'	1:5:1837:A:O5'	2.19	0.42
1:5:1975:G:N2	1:5:1983:A:OP1	2.37	0.42
1:5:2475:G:C2	27:X:50:LYS:HE2	2.54	0.42
1:5:3611:A:H2	1:5:5016:A:C8	2.37	0.42
4:9:28:U:H2'	4:9:29:G:H8	1.85	0.42
4:9:217:A:C6	4:9:218:U:C5	3.07	0.42
4:9:1397:U:C6	4:9:1442:U:H4'	2.55	0.42
4:9:1567:G:P	4:9:1567:G:H21	2.41	0.42
4:9:1776:G:C2	4:9:1777:G:C5	3.07	0.42
8:D:37:VAL:HG12	8:D:50:ARG:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:173:ASN:ND2	22:S:175:PHE:O	2.49	0.42
25:V:87:SER:HA	25:V:97:TYR:HB3	2.01	0.42
39:k:17:ARG:NH1	39:k:19:ASP:OD1	2.51	0.42
70:YY:29:HIS:O	70:YY:29:HIS:CG	2.73	0.42
1:5:1344:C:H2'	1:5:1345:A:H8	1.84	0.42
1:5:2517:A:N3	1:5:2539:C:O2'	2.51	0.42
1:5:2638:G:H22	1:5:2697:A:N6	2.16	0.42
1:5:4636:U:O4	33:d:78:ARG:NE	2.52	0.42
1:5:4674:C:H2'	1:5:4675:U:C6	2.55	0.42
1:5:4759:C:H2'	1:5:4760:G:C8	2.55	0.42
4:9:563:G:C4	4:9:564:A:C8	3.07	0.42
4:9:1136:U:H2'	4:9:1137:U:C6	2.55	0.42
4:9:1190:A:H2'	4:9:1191:C:O4'	2.19	0.42
4:9:1309:C:H2'	4:9:1310:U:C6	2.55	0.42
4:9:1603:G:N3	4:9:1603:G:H5'	2.34	0.42
17:N:193:ARG:O	17:N:197:THR:HG23	2.19	0.42
51:FF:79:HIS:O	51:FF:81:ARG:N	2.52	0.42
1:5:956:A:C8	1:5:957:G:C8	3.05	0.42
1:5:1907:A:H4'	14:K:222:LYS:HE3	2.00	0.42
1:5:2756:G:C6	1:5:2757:A:C6	3.08	0.42
1:5:2848:G:O2'	1:5:3838:U:O4	2.28	0.42
1:5:3598:C:H2'	1:5:3599:A:C8	2.55	0.42
1:5:3717:A:OP2	1:5:3735:G:N2	2.52	0.42
1:5:4573:G:H2'	1:5:4574:U:C6	2.54	0.42
4:9:355:G:OP1	57:LL:105:ARG:NH1	2.46	0.42
4:9:1320:G:H2'	4:9:1321:G:O4'	2.19	0.42
4:9:1455:A:C2	4:9:1456:G:C8	3.07	0.42
51:FF:179:ASN:CB	51:FF:187:SER:HB3	2.50	0.42
65:TT:39:LEU:HD23	65:TT:56:ARG:CZ	2.50	0.42
78:gg:220:ASP:OD1	78:gg:222:ASN:N	2.53	0.42
80:12:67:A:C6	80:12:68:U:C4	3.07	0.42
1:5:288:G:H2'	1:5:289:C:C6	2.54	0.42
1:5:1353:G:N7	20:Q:104:ARG:NH2	2.65	0.42
1:5:4274:A:H2'	1:5:4275:G:H8	1.83	0.42
4:9:380:G:O5'	4:9:380:G:H8	2.03	0.42
4:9:871:U:OP1	57:LL:153:LYS:NZ	2.45	0.42
4:9:1139:C:H5	4:9:1149:A:N6	2.18	0.42
20:Q:43:PHE:CD1	20:Q:133:GLY:HA3	2.54	0.42
50:EE:18:TRP:HH2	50:EE:31:PRO:HD3	1.84	0.42
1:5:2559:G:H2'	1:5:2560:C:C6	2.55	0.42
1:5:2691:U:H2'	1:5:2692:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3813:A:N3	1:5:4538:G:O2'	2.47	0.42
4:9:581:U:H4'	70:YY:66:GLY:HA3	2.01	0.42
4:9:1491:G:H2'	4:9:1492:U:C6	2.55	0.42
4:9:1692:U:H2'	4:9:1693:G:H8	1.84	0.42
49:DD:148:LYS:HG3	49:DD:149:SER:H	1.85	0.42
65:TT:108:GLU:OE2	65:TT:115:LYS:NZ	2.36	0.42
78:gg:174:VAL:HB	78:gg:188:HIS:HB2	2.02	0.42
1:5:457:G:H2'	1:5:458:C:H6	1.84	0.42
1:5:976:G:H21	7:C:323:ARG:HD3	1.83	0.42
1:5:1534:A:C4	82:j:13:ASN:O	2.72	0.42
1:5:1727:U:H2'	1:5:1728:U:H6	1.84	0.42
1:5:4524:G:C2	6:B:252:ALA:HB1	2.55	0.42
1:5:4761:G:H2'	1:5:4762:A:H8	1.84	0.42
1:5:4897:G:C6	1:5:4924:C:N3	2.88	0.42
4:9:459:C:H2'	4:9:460:A:C8	2.54	0.42
4:9:793:G:H2'	4:9:794:A:H8	1.84	0.42
4:9:1144:A:H5'	4:9:1355:C:N4	2.35	0.42
5:A:101:VAL:HG22	5:A:165:VAL:HG22	2.01	0.42
14:K:148:SER:HA	14:K:244:ARG:HH22	1.84	0.42
25:V:111:GLU:OE2	25:V:131:ARG:NH1	2.45	0.42
65:TT:116:ASP:CG	65:TT:117:GLN:H	2.26	0.42
80:12:16:U:H4'	80:12:17:U:O4	2.20	0.42
1:5:64:A:C4	1:5:109:G:N7	2.88	0.42
1:5:1238:A:HO2'	1:5:1239:C:P	2.37	0.42
1:5:1850:A:H2'	1:5:1851:G:C8	2.55	0.42
1:5:1890:G:H22	1:5:1939:A:H61	1.68	0.42
4:9:549:C:H5''	4:9:550:C:OP2	2.19	0.42
4:9:1411:G:C6	4:9:1431:G:C6	3.08	0.42
4:9:1630:A:C6	4:9:1631:U:C4	3.08	0.42
4:9:1656:G:C2	4:9:1657:G:C8	3.08	0.42
4:9:1700:C:C2	4:9:1834:A:N6	2.88	0.42
4:9:1784:G:C6	4:9:1785:C:C4	3.08	0.42
5:A:207:VAL:HG13	5:A:208:GLU:HG3	2.02	0.42
8:D:184:ASP:O	8:D:188:LYS:N	2.53	0.42
50:EE:54:TYR:OH	50:EE:97:GLU:OE1	2.35	0.42
83:jj:92:GLU:CG	83:jj:148:LEU:HD11	2.50	0.42
83:jj:102:ASP:OD1	83:jj:103:GLY:N	2.53	0.42
83:jj:138:GLN:HE22	83:jj:142:GLY:HA2	1.85	0.42
83:jj:431:PRO:HA	83:jj:436:ASN:O	2.19	0.42
1:5:1460:C:H2'	1:5:1461:C:C6	2.55	0.42
1:5:1670:G:H2'	1:5:1855:G:H5''	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4488:A:H4'	1:5:4489:G:C8	2.55	0.42
1:5:4884:G:H2'	1:5:4885:U:O4'	2.20	0.42
1:5:4938:A:OP1	9:E:186:ARG:NE	2.40	0.42
4:9:67:C:C5	52:GG:162:LEU:HG	2.54	0.42
4:9:793:G:H2'	4:9:794:A:C8	2.54	0.42
4:9:1083:A:H4'	4:9:1085:C:C4	2.55	0.42
6:B:35:ASP:HB3	6:B:186:ASN:CG	2.45	0.42
19:P:94:MET:HE1	19:P:146:ILE:HB	2.01	0.42
47:BB:181:LEU:HA	47:BB:184:VAL:HG22	2.01	0.42
1:5:1211:G:O2'	1:5:1212:G:OP1	2.32	0.41
1:5:1983:A:H1'	1:5:2010:A:H4'	2.02	0.41
1:5:2475:G:C6	27:X:50:LYS:HG3	2.55	0.41
3:8:46:G:O2'	3:8:61:A:N1	2.52	0.41
4:9:634:A:H2'	4:9:635:G:H8	1.84	0.41
4:9:1609:C:OP2	64:SS:132:ARG:HD3	2.20	0.41
7:C:5:ARG:NH1	7:C:24:LEU:O	2.51	0.41
7:C:13:GLU:HG3	7:C:155:GLU:OE2	2.20	0.41
7:C:179:ASP:O	7:C:183:VAL:HG23	2.20	0.41
47:BB:25:PHE:HA	47:BB:28:LYS:HG2	2.02	0.41
47:BB:30:TRP:CE2	47:BB:48:LEU:HD13	2.55	0.41
81:11:65:C:H2'	81:11:66:C:H6	1.85	0.41
83:jj:97:ILE:HD11	83:jj:120:VAL:HG21	2.02	0.41
1:5:2370:A:N7	33:d:39:LYS:NZ	2.63	0.41
1:5:2502:A:H4'	1:5:2503:G:OP1	2.20	0.41
1:5:2553:A:H1'	1:5:2554:U:O4'	2.20	0.41
1:5:5029:C:H2'	1:5:5030:U:H6	1.83	0.41
4:9:1395:C:H1'	4:9:1474:A:C5	2.55	0.41
4:9:1405:A:H2'	4:9:1406:G:O4'	2.20	0.41
5:A:117:GLU:HG2	5:A:124:GLY:N	2.35	0.41
6:B:89:ILE:HD11	6:B:150:PHE:HE1	1.85	0.41
29:Z:5:MET:HG3	29:Z:77:TYR:HE2	1.85	0.41
45:r:84:LYS:HD3	45:r:88:ALA:HB1	2.02	0.41
46:AA:37:TYR:OH	67:VV:66:ASP:OD2	2.30	0.41
47:BB:205:TYR:CD1	47:BB:206:PRO:HD2	2.54	0.41
60:OO:95:ILE:HB	60:OO:129:ILE:HG23	2.02	0.41
69:XX:89:GLY:HA2	76:ee:82:VAL:HG12	2.03	0.41
78:gg:59:LEU:HD13	78:gg:90:TRP:CG	2.55	0.41
80:12:39:U:H2'	80:12:40:C:C6	2.55	0.41
83:jj:193:ARG:NH1	90:jj:700:GCP:O2A	2.35	0.41
83:jj:420:LEU:HD11	83:jj:454:GLU:HB2	2.02	0.41
1:5:516:C:H2'	1:5:517:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1554:A:OP2	44:p:4:ARG:NH1	2.40	0.41
1:5:2099:C:H4'	1:5:2100:G:OP2	2.19	0.41
1:5:4247:G:H5'	8:D:4:VAL:HG21	2.01	0.41
1:5:4517:A:N7	6:B:2:SER:N	2.67	0.41
1:5:4887:C:H2'	1:5:4888:C:C6	2.54	0.41
4:9:1424:G:H2'	4:9:1425:G:C8	2.51	0.41
6:B:189:THR:HG23	6:B:192:GLU:H	1.85	0.41
12:I:54:SER:HB2	12:I:135:ILE:HD11	2.01	0.41
23:T:36:LYS:HE2	23:T:36:LYS:HB3	1.87	0.41
26:W:50:ASN:HA	26:W:55:TYR:CG	2.55	0.41
27:X:63:LYS:HE2	27:X:63:LYS:HB3	1.88	0.41
35:f:65:ASN:OD1	35:f:66:LYS:N	2.53	0.41
83:jj:402:THR:HG22	83:jj:470:ARG:HG3	2.02	0.41
1:5:740:G:H2'	1:5:741:C:C6	2.56	0.41
1:5:975:C:H2'	1:5:976:G:H8	1.85	0.41
1:5:1169:G:H2'	1:5:1170:G:H8	1.85	0.41
1:5:4093:G:N1	1:5:4094:G:C5	2.88	0.41
1:5:4128:A:H3'	1:5:4129:G:H8	1.84	0.41
3:8:94:G:H1'	82:j:82:THR:O	2.20	0.41
4:9:30:C:O2'	4:9:596:U:OP1	2.33	0.41
8:D:209:ARG:NH2	8:D:234:ASP:OD1	2.38	0.41
9:E:264:ILE:HG23	9:E:270:LEU:HD23	2.02	0.41
45:r:38:PHE:O	45:r:45:HIS:HE1	2.03	0.41
48:CC:102:LEU:HG	48:CC:130:ILE:HG12	2.01	0.41
48:CC:253:PRO:HA	48:CC:256:TRP:CD1	2.56	0.41
1:5:927:G:C6	1:5:928:C:C4	3.09	0.41
1:5:959:G:C8	1:5:959:G:H5'	2.54	0.41
1:5:978:G:N2	1:5:1277:G:N1	2.58	0.41
1:5:2422:C:P	19:P:127:ARG:HH22	2.44	0.41
1:5:2654:C:H2'	1:5:2655:C:C6	2.55	0.41
1:5:2744:A:H2'	1:5:2745:A:C8	2.56	0.41
3:8:66:A:H2'	3:8:67:U:C6	2.55	0.41
4:9:589:G:O6	4:9:591:U:O2'	2.36	0.41
4:9:1017:U:H2'	4:9:1018:U:C6	2.55	0.41
4:9:1244:U:H2'	4:9:1245:G:H8	1.86	0.41
6:B:19:ARG:HD2	6:B:235:TRP:CH2	2.56	0.41
15:L:63:THR:HG21	30:a:66:ASN:HD22	1.85	0.41
15:L:174:LYS:O	30:a:138:LYS:HE2	2.20	0.41
60:OO:95:ILE:HD11	60:OO:126:ILE:HD12	2.02	0.41
61:PP:116:LEU:HD23	61:PP:116:LEU:HA	1.85	0.41
63:RR:41:ILE:HD13	63:RR:47:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:gg:147:HIS:HD1	78:gg:171:ASP:CG	2.29	0.41
81:13:53:G:H2'	81:13:54:A:C8	2.50	0.41
81:11:10:G:N1	81:11:46:G:C6	2.88	0.41
83:jj:92:GLU:OE2	83:jj:150:ARG:NH2	2.44	0.41
1:5:54:G:HO2'	17:N:108:ARG:HH22	1.68	0.41
1:5:1098:G:C6	1:5:1099:C:C4	3.09	0.41
1:5:1765:A:C4	1:5:1766:A:C8	3.09	0.41
1:5:1975:G:H22	1:5:1983:A:P	2.41	0.41
1:5:3611:A:C2	1:5:5016:A:H8	2.39	0.41
1:5:4594:U:H2'	1:5:4595:G:C8	2.54	0.41
4:9:501:C:H2'	4:9:502:C:H5''	2.03	0.41
4:9:641:A:OP1	55:JJ:40:LYS:HD2	2.20	0.41
4:9:1158:G:OP1	69:XX:5:ARG:NH2	2.53	0.41
4:9:1288:U:H5''	77:ff:95:ARG:HH22	1.86	0.41
4:9:1835:A:HO2'	4:9:1836:G:P	2.44	0.41
12:I:38:ARG:HD2	12:I:41:ALA:HB2	2.01	0.41
14:K:221:LYS:HB3	14:K:230:GLY:HA2	2.01	0.41
22:S:7:LEU:O	22:S:103:ALA:HB1	2.21	0.41
25:V:92:ASP:OD1	25:V:92:ASP:N	2.53	0.41
32:c:82:GLY:CA	32:c:91:VAL:HG12	2.50	0.41
51:FF:60:ARG:HD3	51:FF:61:PHE:CE1	2.56	0.41
53:HH:98:ARG:CZ	53:HH:128:ALA:HB1	2.51	0.41
56:KK:57:TYR:HB3	56:KK:75:GLY:HA2	2.03	0.41
1:5:700:G:H2'	1:5:701:G:H8	1.86	0.41
1:5:1176:C:H2'	1:5:1177:U:H6	1.86	0.41
1:5:1308:C:H2'	1:5:1309:C:C6	2.56	0.41
1:5:4372:U:OP2	43:o:61:LYS:HG2	2.20	0.41
1:5:5002:U:H2'	1:5:5003:U:C6	2.55	0.41
2:7:24:C:H2'	2:7:25:G:O4'	2.20	0.41
4:9:1010:G:H2'	4:9:1011:A:C8	2.55	0.41
4:9:1524:G:O2'	81:13:30:G:OP1	2.34	0.41
4:9:1698:C:HO2'	4:9:1699:A:P	2.42	0.41
10:G:139:VAL:HG11	10:G:238:LYS:CE	2.50	0.41
15:L:9:ILE:HG23	15:L:9:ILE:O	2.21	0.41
18:O:12:ARG:O	22:S:171:ARG:NH2	2.52	0.41
47:BB:30:TRP:CZ2	47:BB:48:LEU:HD13	2.56	0.41
47:BB:178:THR:C	47:BB:179:ASN:HD22	2.27	0.41
1:5:128:C:H2'	1:5:129:C:C6	2.56	0.41
1:5:1477:C:O2'	1:5:1478:C:OP1	2.37	0.41
1:5:1755:C:O2'	1:5:1757:U:OP2	2.20	0.41
1:5:2474:G:O2'	1:5:2475:G:OP1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2846:G:OP1	25:V:85:ARG:NH2	2.53	0.41
1:5:4637:G:OP1	33:d:30:HIS:HE1	2.03	0.41
4:9:141:A:N6	4:9:177:G:H1'	2.35	0.41
4:9:524:U:H5''	4:9:525:A:O4'	2.21	0.41
4:9:789:G:H2'	4:9:790:C:C6	2.56	0.41
4:9:1520:G:H2'	4:9:1520:G:N3	2.35	0.41
4:9:1656:G:H2'	4:9:1657:G:H8	1.85	0.41
4:9:1680:G:H2'	4:9:1681:U:C6	2.55	0.41
16:M:24:LEU:HD11	16:M:86:TRP:CG	2.56	0.41
20:Q:75:ARG:HA	20:Q:78:LYS:HE2	2.02	0.41
21:R:28:GLU:HG3	21:R:49:LEU:HD22	2.03	0.41
81:11:12:C:H2'	81:11:13:G:C8	2.55	0.41
1:5:310:G:C4	1:5:311:G:C8	3.08	0.41
1:5:1176:C:H2'	1:5:1177:U:C6	2.55	0.41
1:5:1272:C:H4'	14:K:36:PHE:CG	2.56	0.41
1:5:2466:G:O5'	1:5:2466:G:H8	2.03	0.41
1:5:3597:G:O2'	1:5:3598:C:OP1	2.35	0.41
1:5:3717:A:N1	1:5:3933:G:H1'	2.36	0.41
1:5:4915:G:N1	1:5:4916:G:C5	2.89	0.41
3:8:13:G:C5	3:8:14:U:C4	3.08	0.41
4:9:419:G:N2	4:9:661:U:O2	2.54	0.41
4:9:648:A:H4'	69:XX:104:GLY:O	2.20	0.41
4:9:681:U:H4'	69:XX:9:THR:HG22	2.03	0.41
6:B:154:LYS:HE3	6:B:154:LYS:HB2	1.86	0.41
19:P:37:LYS:O	19:P:114:ILE:HG23	2.21	0.41
19:P:54:LYS:HB3	19:P:54:LYS:HE2	1.87	0.41
30:a:59:ARG:NH2	30:a:61:TYR:OH	2.54	0.41
41:m:51:ILE:HG23	41:m:52:ILE:N	2.25	0.41
53:HH:135:PHE:CG	53:HH:136:PRO:HA	2.56	0.41
58:MM:85:LEU:HD11	58:MM:109:VAL:HG21	2.03	0.41
68:WW:30:CYS:SG	68:WW:31:SER:N	2.93	0.41
70:YY:29:HIS:HE1	70:YY:33:ALA:O	2.04	0.41
83:jj:525:LEU:HD11	83:jj:543:ARG:HB2	2.02	0.41
1:5:123:C:H2'	1:5:124:C:C6	2.56	0.41
1:5:1198:G:N2	1:5:1199:G:O6	2.54	0.41
1:5:2895:A:H2'	1:5:2896:G:H8	1.85	0.41
1:5:4065:G:C6	1:5:4066:U:C4	3.09	0.41
1:5:4232:U:H4'	1:5:4233:A:O5'	2.21	0.41
1:5:4305:G:H22	23:T:87:LYS:CD	2.34	0.41
1:5:4598:C:O2'	11:H:121:LYS:HE2	2.21	0.41
1:5:4685:U:H2'	1:5:4686:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:2:U:H2'	2:7:3:C:C6	2.56	0.41
4:9:616:A:H1'	76:ee:85:VAL:HG23	2.03	0.41
4:9:669:A:H5'	4:9:669:A:H8	1.84	0.41
4:9:693:A:H61	4:9:733:C:H42	1.69	0.41
4:9:1454:A:C8	63:RR:3:ARG:HD3	2.56	0.41
4:9:1521:C:OP2	64:SS:136:THR:OG1	2.29	0.41
4:9:1714:U:H2'	4:9:1715:A:C8	2.56	0.41
27:X:147:LEU:O	27:X:151:ASN:ND2	2.40	0.41
78:gg:175:LYS:HE2	78:gg:177:TRP:CH2	2.56	0.41
79:10:13:A:H2'	79:10:14:G:H8	1.86	0.41
1:5:750:U:H2'	1:5:751:G:O4'	2.21	0.40
1:5:1247:U:C2	1:5:1248:C:H5	2.39	0.40
1:5:1404:G:H2'	1:5:1405:C:C6	2.56	0.40
1:5:1985:G:H1'	1:5:2003:G:H2'	2.03	0.40
1:5:2544:G:C2	1:5:2545:U:C4	3.09	0.40
1:5:3726:A:O5'	1:5:3726:A:H8	2.03	0.40
4:9:79:A:H3'	4:9:80:G:H8	1.86	0.40
4:9:216:C:C2	4:9:217:A:C8	3.09	0.40
4:9:547:G:N3	4:9:548:C:H5	2.20	0.40
4:9:1656:G:N3	4:9:1657:G:C8	2.89	0.40
7:C:283:LYS:HE3	7:C:283:LYS:HB2	1.91	0.40
52:GG:52:ILE:HD11	52:GG:109:LEU:HD21	2.03	0.40
55:JJ:111:GLN:NE2	55:JJ:127:ARG:HB2	2.36	0.40
74:cc:7:GLN:N	74:cc:7:GLN:OE1	2.54	0.40
81:11:26:G:C5	81:11:27:C:C5	3.09	0.40
1:5:165:A:H2'	1:5:166:C:H6	1.84	0.40
1:5:686:A:C8	1:5:688:U:C4	3.09	0.40
1:5:1348:U:H2'	1:5:1349:G:H8	1.86	0.40
1:5:1358:G:O2'	1:5:1359:G:O5'	2.36	0.40
1:5:1590:C:H5''	1:5:1591:U:O5'	2.22	0.40
1:5:3969:G:C6	1:5:4053:A:C2	3.10	0.40
4:9:1679:A:C2	51:FF:60:ARG:HA	2.56	0.40
6:B:168:MET:HG2	6:B:178:ALA:HA	2.02	0.40
9:E:180:GLY:O	9:E:181:PRO:C	2.65	0.40
13:J:86:GLY:HA2	13:J:109:ILE:HD11	2.03	0.40
52:GG:73:VAL:HG12	52:GG:74:ARG:N	2.36	0.40
53:HH:63:PHE:HA	53:HH:95:ILE:O	2.20	0.40
1:5:423:G:H5'	19:P:26:PHE:HZ	1.86	0.40
1:5:983:C:C6	9:E:73:ARG:HD3	2.56	0.40
1:5:1186:U:H2'	1:5:1187:G:N3	2.36	0.40
1:5:1973:G:H2'	1:5:1974:U:C5	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2503:G:H3'	1:5:2504:C:O4'	2.22	0.40
1:5:4672:A:OP1	25:V:15:ARG:NH2	2.54	0.40
4:9:70:G:H1'	4:9:79:A:H61	1.86	0.40
4:9:379:C:H4'	54:II:31:ARG:O	2.21	0.40
4:9:448:A:H62	54:II:29:LEU:HD13	1.82	0.40
4:9:527:C:OP1	55:JJ:122:SER:OG	2.31	0.40
4:9:537:C:C2	4:9:538:U:C5	3.10	0.40
4:9:821:G:C6	55:JJ:147:PHE:CZ	3.10	0.40
4:9:894:G:H2'	4:9:895:G:H8	1.87	0.40
21:R:106:LEU:HD23	21:R:106:LEU:HA	1.90	0.40
66:UU:59:LYS:HD2	66:UU:84:ILE:HD11	2.03	0.40
1:5:466:A:C6	1:5:468:U:C4	3.10	0.40
1:5:712:C:OP1	9:E:142:LYS:HE2	2.22	0.40
1:5:956:A:N6	1:5:1283:G:O2'	2.45	0.40
1:5:1080:C:H2'	1:5:1081:C:C6	2.55	0.40
1:5:1866:U:OP1	12:I:4:ARG:NH1	2.44	0.40
1:5:4066:U:H2'	1:5:4067:U:C6	2.56	0.40
1:5:4324:A:H2'	1:5:4325:A:C8	2.57	0.40
1:5:4474:A:H5''	41:m:99:LYS:CG	2.52	0.40
4:9:1617:G:H4'	75:dd:14:PHE:CE2	2.56	0.40
6:B:95:THR:HG22	6:B:97:ARG:H	1.86	0.40
11:H:40:HIS:CE1	11:H:41:ILE:HG13	2.56	0.40
47:BB:49:VAL:HA	60:OO:51:GLU:OE2	2.22	0.40
1:5:755:C:C2	1:5:756:G:C8	3.09	0.40
1:5:966:A:H1'	1:5:968:C:N4	2.37	0.40
1:5:1169:G:H2'	1:5:1170:G:C8	2.56	0.40
1:5:1196:G:C6	1:5:1197:C:N4	2.90	0.40
1:5:1312:A:O2'	34:e:44:ARG:NH2	2.54	0.40
1:5:4886:C:H2'	1:5:4887:C:C6	2.57	0.40
4:9:90:G:H2'	4:9:91:A:O4'	2.21	0.40
4:9:182:C:H5'	4:9:183:G:C8	2.56	0.40
4:9:481:C:H5''	4:9:482:G:OP2	2.21	0.40
4:9:572:U:OP1	70:YY:59:GLY:N	2.54	0.40
5:A:10:LYS:HA	5:A:16:PHE:CD2	2.57	0.40
10:G:216:PRO:HG2	10:G:219:LEU:HD12	2.04	0.40
23:T:19:PHE:CE2	23:T:20:ARG:HD3	2.57	0.40
50:EE:141:THR:OG1	50:EE:143:ASP:OD1	2.32	0.40
55:JJ:38:ARG:N	55:JJ:42:GLU:OE1	2.33	0.40
55:JJ:155:LYS:HG3	55:JJ:156:HIS:CD2	2.56	0.40
58:MM:42:LEU:HD12	58:MM:68:LEU:HD23	2.03	0.40
81:11:59:A:H2'	81:11:60:A:C8	2.56	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%)	237 (96%)	9 (4%)	0	100	100
6	B	392/403 (97%)	379 (97%)	13 (3%)	0	100	100
7	C	360/425 (85%)	354 (98%)	6 (2%)	0	100	100
8	D	291/297 (98%)	285 (98%)	6 (2%)	0	100	100
9	E	208/291 (72%)	200 (96%)	8 (4%)	0	100	100
10	G	229/319 (72%)	222 (97%)	7 (3%)	0	100	100
11	H	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
12	I	201/214 (94%)	196 (98%)	5 (2%)	0	100	100
13	J	168/178 (94%)	166 (99%)	2 (1%)	0	100	100
14	K	223/247 (90%)	217 (97%)	6 (3%)	0	100	100
15	L	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
16	M	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
17	N	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
18	O	197/203 (97%)	190 (96%)	7 (4%)	0	100	100
19	P	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
20	Q	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
21	R	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
22	S	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
23	T	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
24	U	97/128 (76%)	92 (95%)	5 (5%)	0	100	100
25	V	127/140 (91%)	125 (98%)	2 (2%)	0	100	100
26	W	102/157 (65%)	101 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	X	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
28	Y	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
29	Z	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
30	a	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
31	b	94/245 (38%)	92 (98%)	2 (2%)	0	100	100
32	c	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
33	d	105/125 (84%)	99 (94%)	6 (6%)	0	100	100
34	e	126/135 (93%)	123 (98%)	3 (2%)	0	100	100
35	f	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
36	g	112/116 (97%)	112 (100%)	0	0	100	100
37	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
38	i	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
39	k	67/70 (96%)	67 (100%)	0	0	100	100
40	l	48/51 (94%)	48 (100%)	0	0	100	100
41	m	50/102 (49%)	46 (92%)	4 (8%)	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%)	85 (96%)	4 (4%)	0	100	100
45	r	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
46	AA	215/295 (73%)	207 (96%)	8 (4%)	0	100	100
47	BB	211/264 (80%)	203 (96%)	8 (4%)	0	100	100
48	CC	219/293 (75%)	214 (98%)	5 (2%)	0	100	100
49	DD	222/243 (91%)	218 (98%)	4 (2%)	0	100	100
50	EE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
51	FF	180/204 (88%)	171 (95%)	9 (5%)	0	100	100
52	GG	235/249 (94%)	225 (96%)	10 (4%)	0	100	100
53	HH	181/194 (93%)	178 (98%)	3 (2%)	0	100	100
54	II	194/208 (93%)	193 (100%)	1 (0%)	0	100	100
55	JJ	179/194 (92%)	175 (98%)	4 (2%)	0	100	100
56	KK	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
57	LL	139/158 (88%)	137 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	MM	108/132 (82%)	105 (97%)	3 (3%)	0	100	100
59	NN	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
60	OO	134/168 (80%)	132 (98%)	2 (2%)	0	100	100
61	PP	127/145 (88%)	124 (98%)	3 (2%)	0	100	100
62	QQ	140/146 (96%)	137 (98%)	3 (2%)	0	100	100
63	RR	130/135 (96%)	128 (98%)	2 (2%)	0	100	100
64	SS	138/152 (91%)	134 (97%)	4 (3%)	0	100	100
65	TT	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
66	UU	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
67	VV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
68	WW	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
69	XX	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
70	YY	122/130 (94%)	119 (98%)	3 (2%)	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%)	76 (94%)	5 (6%)	0	100	100
74	cc	60/69 (87%)	59 (98%)	1 (2%)	0	100	100
75	dd	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
76	ee	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
77	ff	66/156 (42%)	63 (96%)	3 (4%)	0	100	100
78	gg	311/317 (98%)	297 (96%)	14 (4%)	0	100	100
82	j	84/97 (87%)	81 (96%)	3 (4%)	0	100	100
83	jj	511/703 (73%)	498 (98%)	13 (2%)	0	100	100
All	All	11657/13594 (86%)	11344 (97%)	313 (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%)	200 (100%)	0	100	100
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
14	K	196/215 (91%)	196 (100%)	0	100	100
15	L	175/176 (99%)	175 (100%)	0	100	100
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%)	171 (100%)	0	100	100
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	93
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	94
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%)	106 (100%)	0	100	100
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	122/132 (92%)	122 (100%)	0	100	100
65	TT	111/115 (96%)	111 (100%)	0	100	100
66	UU	92/107 (86%)	92 (100%)	0	100	100
67	VV	67/67 (100%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
76	ee	47/106 (44%)	47 (100%)	0	100	100
77	ff	61/140 (44%)	61 (100%)	0	100	100
78	gg	272/275 (99%)	272 (100%)	0	100	100
82	j	73/80 (91%)	73 (100%)	0	100	100
83	jj	445/586 (76%)	445 (100%)	0	100	100
All	All	10181/11529 (88%)	10179 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	S	84	TYR
48	CC	248	TYR

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	216	HIS
6	B	11	HIS
6	B	55	HIS
6	B	109	HIS
6	B	167	GLN
6	B	204	GLN
6	B	276	HIS
6	B	376	HIS
7	C	21	ASN
7	C	89	GLN
7	C	245	HIS
7	C	346	ASN

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Mol	Chain	Res	Type
9	E	131	HIS
9	E	185	ASN
9	E	194	GLN
9	E	253	GLN
10	G	96	GLN
10	G	134	ASN
10	G	202	ASN
11	H	8	GLN
11	H	78	GLN
11	H	98	HIS
12	I	59	GLN
12	I	73	ASN
12	I	144	ASN
12	I	202	ASN
13	J	98	ASN
13	J	104	ASN
14	K	55	HIS
14	K	79	ASN
14	K	199	HIS
16	M	20	HIS
16	M	70	GLN
17	N	8	GLN
17	N	87	HIS
18	O	50	ASN
18	O	150	GLN
19	P	25	HIS
19	P	34	GLN
19	P	116	HIS
20	Q	7	HIS
20	Q	57	ASN
20	Q	160	HIS
21	R	141	HIS
22	S	50	GLN
22	S	156	HIS
23	T	98	HIS
25	V	77	HIS
26	W	59	HIS
26	W	63	GLN
27	X	73	HIS
28	Y	72	GLN
30	a	14	HIS
30	a	34	ASN

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Mol	Chain	Res	Type
30	a	39	HIS
30	a	120	GLN
31	b	58	GLN
33	d	30	HIS
35	f	24	HIS
37	h	65	GLN
38	i	20	ASN
38	i	80	HIS
39	k	31	ASN
43	o	90	HIS
45	r	30	ASN
45	r	45	HIS
46	AA	169	HIS
47	BB	179	ASN
49	DD	145	GLN
49	DD	159	HIS
49	DD	174	HIS
49	DD	226	GLN
50	EE	188	ASN
50	EE	201	HIS
51	FF	65	GLN
51	FF	203	ASN
52	GG	146	ASN
52	GG	225	GLN
53	HH	186	ASN
54	II	165	GLN
55	JJ	111	GLN
55	JJ	124	HIS
57	LL	11	GLN
57	LL	94	HIS
57	LL	106	HIS
58	MM	19	GLN
59	NN	5	HIS
59	NN	36	GLN
59	NN	69	ASN
59	NN	105	ASN
62	QQ	80	GLN
63	RR	62	GLN
64	SS	11	HIS
64	SS	135	HIS
68	WW	113	HIS
68	WW	120	HIS

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Mol	Chain	Res	Type
69	XX	16	HIS
70	YY	29	HIS
70	YY	94	HIS
72	aa	17	HIS
74	cc	7	GLN
74	cc	29	GLN
74	cc	45	ASN
76	ee	131	ASN
78	gg	133	ASN
82	j	57	ASN
82	j	66	HIS
82	j	76	HIS
83	jj	99	GLN
83	jj	138	GLN
83	jj	367	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3580/3601 (99%)	537 (15%)	165 (4%)
2	7	118/120 (98%)	7 (5%)	1 (0%)
3	8	149/156 (95%)	21 (14%)	4 (2%)
4	9	1685/1869 (90%)	233 (13%)	57 (3%)
79	10	10/185 (5%)	2 (20%)	0
80	12	74/76 (97%)	8 (10%)	3 (4%)
81	11	73/75 (97%)	11 (15%)	4 (5%)
81	13	73/75 (97%)	9 (12%)	3 (4%)
All	All	5762/6157 (93%)	828 (14%)	237 (4%)

All (828) 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

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Mol	Chain	Res	Type
1	5	93	G
1	5	109	G
1	5	119	G
1	5	120	A
1	5	122	U
1	5	126	C
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	197	A
1	5	200	U
1	5	201	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	295	A
1	5	296	A
1	5	297	U
1	5	306	A
1	5	309	C
1	5	310	G
1	5	315	G

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Mol	Chain	Res	Type
1	5	316	U
1	5	334	A
1	5	340	C
1	5	379	G
1	5	387	G
1	5	407	A
1	5	408	A
1	5	409	G
1	5	410	A
1	5	412	G
1	5	413	G
1	5	431	G
1	5	446	C
1	5	449	C
1	5	450	G
1	5	453	G
1	5	454	U
1	5	466	A
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	499	G
1	5	505	G
1	5	510	U
1	5	649	A
1	5	650	C
1	5	666	G
1	5	683	C
1	5	685	C
1	5	686	A
1	5	687	U
1	5	696	C
1	5	697	G
1	5	704	C

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Mol	Chain	Res	Type
1	5	730	G
1	5	731	G
1	5	738	C
1	5	739	G
1	5	747	A
1	5	749	G
1	5	758	G
1	5	913	U
1	5	914	U
1	5	915	A
1	5	917	A
1	5	923	C
1	5	924	C
1	5	925	C
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	943	A
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	983	C
1	5	1070	G
1	5	1072	C
1	5	1073	G
1	5	1076	C
1	5	1079	C
1	5	1179	U
1	5	1180	C
1	5	1195	G
1	5	1204	C
1	5	1211	G
1	5	1212	G

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Mol	Chain	Res	Type
1	5	1214	C
1	5	1215	C
1	5	1234	G
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	1249	C
1	5	1250	C
1	5	1272	C
1	5	1273	G
1	5	1280	C
1	5	1284	G
1	5	1287	G
1	5	1292	C
1	5	1293	G
1	5	1296	G
1	5	1301	C
1	5	1304	C
1	5	1326	A
1	5	1337	A
1	5	1354	A
1	5	1359	G
1	5	1360	G
1	5	1370	G
1	5	1371	A
1	5	1377	G
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	1436	C
1	5	1441	C
1	5	1445	U
1	5	1446	C
1	5	1456	C

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Mol	Chain	Res	Type
1	5	1458	C
1	5	1477	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	1547	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	1654	G
1	5	1661	C
1	5	1676	C
1	5	1677	U
1	5	1691	G
1	5	1734	G
1	5	1741	G
1	5	1742	A
1	5	1750	G
1	5	1753	G
1	5	1754	U
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	1767	A
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	1918	U
1	5	1920	C
1	5	1921	C
1	5	1922	G
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	1977	C
1	5	1978	C
1	5	1980	U
1	5	1981	G
1	5	1984	A
1	5	1987	C
1	5	1991	A
1	5	1993	C
1	5	2001	G
1	5	2002	A
1	5	2004	U
1	5	2005	G
1	5	2011	C
1	5	2023	C
1	5	2024	G
1	5	2026	A
1	5	2044	U

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Mol	Chain	Res	Type
1	5	2048	U
1	5	2055	G
1	5	2056	G
1	5	2069	A
1	5	2084	U
1	5	2089	G
1	5	2090	U
1	5	2093	G
1	5	2094	C
1	5	2097	A
1	5	2098	G
1	5	2100	G
1	5	2101	A
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	2279	A
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	2422	C
1	5	2441	C
1	5	2475	G
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2503	G

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Mol	Chain	Res	Type
1	5	2504	C
1	5	2505	C
1	5	2506	G
1	5	2507	A
1	5	2513	A
1	5	2546	G
1	5	2547	G
1	5	2553	A
1	5	2554	U
1	5	2555	G
1	5	2560	C
1	5	2566	G
1	5	2587	A
1	5	2601	A
1	5	2627	C
1	5	2669	C
1	5	2686	G
1	5	2687	U
1	5	2695	A
1	5	2696	A
1	5	2697	A
1	5	2705	G
1	5	2708	U
1	5	2711	G
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	2787	A
1	5	2788	U
1	5	2790	U
1	5	2794	C
1	5	2795	A
1	5	2796	G
1	5	2826	U

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Mol	Chain	Res	Type
1	5	2827	G
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	3653	A
1	5	3662	A
1	5	3672	G
1	5	3673	C
1	5	3711	A
1	5	3712	A
1	5	3748	A
1	5	3750	G
1	5	3753	G
1	5	3777	G
1	5	3783	A
1	5	3784	A
1	5	3786	U
1	5	3811	G
1	5	3812	C
1	5	3817	A
1	5	3819	G
1	5	3840	U
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

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Mol	Chain	Res	Type
1	5	3949	A
1	5	3950	U
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	4065	G
1	5	4069	U
1	5	4070	U
1	5	4076	G
1	5	4084	G
1	5	4085	A
1	5	4119	C
1	5	4120	U
1	5	4122	G
1	5	4125	C
1	5	4127	A
1	5	4128	A
1	5	4163	U
1	5	4170	A
1	5	4171	C
1	5	4183	G
1	5	4184	G
1	5	4191	G
1	5	4203	A
1	5	4213	A
1	5	4229	U
1	5	4233	A
1	5	4251	A
1	5	4255	A

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Mol	Chain	Res	Type
1	5	4258	C
1	5	4266	G
1	5	4267	G
1	5	4268	A
1	5	4271	A
1	5	4273	A
1	5	4280	A
1	5	4281	A
1	5	4291	G
1	5	4305	G
1	5	4306	U
1	5	4330	G
1	5	4339	A
1	5	4349	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	4419	U
1	5	4422	A
1	5	4438	U
1	5	4448	G
1	5	4449	A
1	5	4452	U
1	5	4453	C
1	5	4464	A
1	5	4476	C
1	5	4488	A
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	4548	A
1	5	4549	G
1	5	4560	C

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Mol	Chain	Res	Type
1	5	4567	G
1	5	4572	U
1	5	4573	G
1	5	4575	G
1	5	4590	A
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	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	4758	U
1	5	4759	C
1	5	4765	G
1	5	4771	C
1	5	4870	G
1	5	4871	C
1	5	4875	G
1	5	4882	U
1	5	4883	C
1	5	4885	U
1	5	4902	C
1	5	4909	A
1	5	4910	A
1	5	4913	G
1	5	4914	G
1	5	4915	G
1	5	4919	G
1	5	4921	C
1	5	4922	C
1	5	4925	U
1	5	4926	C

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Mol	Chain	Res	Type
1	5	4931	G
1	5	4937	C
1	5	4943	A
1	5	4944	C
1	5	4945	G
1	5	4947	U
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	5007	A
1	5	5017	G
1	5	5041	G
1	5	5047	C
1	5	5048	A
1	5	5050	C
1	5	5054	C
1	5	5058	A
1	5	5061	A
1	5	5062	G
2	7	7	G
2	7	42	A
2	7	53	U
2	7	64	G
2	7	97	G
2	7	100	A
2	7	110	G
3	8	2	G
3	8	3	A
3	8	34	U
3	8	51	U
3	8	52	A
3	8	59	A
3	8	62	A
3	8	63	U
3	8	87	G
3	8	94	G
3	8	95	A

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Mol	Chain	Res	Type
3	8	104	A
3	8	105	C
3	8	109	C
3	8	110	U
3	8	114	G
3	8	123	U
3	8	124	U
3	8	125	C
3	8	126	C
3	8	137	A
4	9	4	C
4	9	17	C
4	9	25	A
4	9	26	U
4	9	33	G
4	9	41	G
4	9	42	A
4	9	46	A
4	9	56	G
4	9	59	U
4	9	67	C
4	9	68	A
4	9	72	C
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	130	G
4	9	143	U
4	9	147	A
4	9	155	G
4	9	161	U
4	9	182	C
4	9	183	G
4	9	184	G
4	9	188	C

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Mol	Chain	Res	Type
4	9	192	C
4	9	215	G
4	9	294	U
4	9	307	G
4	9	308	G
4	9	312	G
4	9	319	C
4	9	347	G
4	9	362	C
4	9	364	A
4	9	369	C
4	9	370	G
4	9	385	G
4	9	386	C
4	9	400	C
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	454	U
4	9	464	A
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	496	C
4	9	516	A
4	9	517	C
4	9	532	C
4	9	533	A
4	9	541	U
4	9	544	G
4	9	550	C
4	9	551	U
4	9	554	A

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Mol	Chain	Res	Type
4	9	555	A
4	9	556	U
4	9	559	G
4	9	561	A
4	9	562	U
4	9	564	A
4	9	571	U
4	9	587	A
4	9	588	G
4	9	589	G
4	9	590	A
4	9	591	U
4	9	606	G
4	9	607	U
4	9	608	C
4	9	609	U
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	752	G
4	9	753	C
4	9	754	G
4	9	799	U
4	9	811	A
4	9	821	G
4	9	822	U
4	9	830	A
4	9	844	U
4	9	847	A
4	9	859	G
4	9	867	G
4	9	868	G
4	9	869	A
4	9	870	A

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Mol	Chain	Res	Type
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	913	A
4	9	914	U
4	9	920	A
4	9	922	A
4	9	933	G
4	9	943	U
4	9	990	A
4	9	992	A
4	9	999	G
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	1116	C
4	9	1117	C
4	9	1118	C
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
4	9	1254	C
4	9	1256	G
4	9	1257	G

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Mol	Chain	Res	Type
4	9	1259	A
4	9	1274	G
4	9	1275	G
4	9	1293	A
4	9	1301	A
4	9	1302	G
4	9	1303	C
4	9	1309	C
4	9	1314	U
4	9	1371	U
4	9	1372	U
4	9	1378	A
4	9	1396	A
4	9	1397	U
4	9	1428	G
4	9	1429	G
4	9	1454	A
4	9	1462	U
4	9	1463	U
4	9	1476	A
4	9	1477	U
4	9	1490	G
4	9	1497	G
4	9	1498	A
4	9	1521	C
4	9	1522	A
4	9	1533	A
4	9	1548	G
4	9	1552	G
4	9	1556	A
4	9	1557	C
4	9	1579	A
4	9	1580	A
4	9	1581	C
4	9	1582	C
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

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Mol	Chain	Res	Type
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	1758	G
4	9	1783	C
4	9	1785	C
4	9	1823	A
4	9	1824	A
4	9	1826	G
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	1851	A
4	9	1852	C
4	9	1861	G
4	9	1862	G
4	9	1863	A
4	9	1865	C
4	9	1869	A
79	10	19	U
79	10	23	A
80	12	13	C
80	12	18	G
80	12	19	G
80	12	20	G
80	12	45	G
80	12	47	U
80	12	48	C

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Mol	Chain	Res	Type
80	12	55	U
81	13	17	C
81	13	18	G
81	13	20	A
81	13	22	G
81	13	47	U
81	13	48	C
81	13	74	C
81	13	75	C
81	13	76	A
81	11	10	G
81	11	11	G
81	11	17	C
81	11	18	G
81	11	20	A
81	11	22	G
81	11	47	U
81	11	48	C
81	11	74	C
81	11	75	C
81	11	76	A

All (237) 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	200	U
1	5	217	C
1	5	218	A
1	5	219	G
1	5	224	U
1	5	226	G
1	5	245	C
1	5	265	C
1	5	266	C
1	5	275	C
1	5	294	G
1	5	296	A
1	5	309	C

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Mol	Chain	Res	Type
1	5	315	G
1	5	406	C
1	5	408	A
1	5	449	C
1	5	466	A
1	5	480	C
1	5	481	G
1	5	484	U
1	5	492	U
1	5	504	G
1	5	649	A
1	5	667	A
1	5	685	C
1	5	696	C
1	5	913	U
1	5	914	U
1	5	916	C
1	5	924	C
1	5	930	G
1	5	933	G
1	5	935(A)	G
1	5	955	G
1	5	956	A
1	5	959	G
1	5	966	A
1	5	971(A)	G
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
1	5	1324	A
1	5	1325	C
1	5	1358	G
1	5	1359	G
1	5	1370	G
1	5	1380	G

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Mol	Chain	Res	Type
1	5	1387	A
1	5	1437	C
1	5	1440	U
1	5	1445	U
1	5	1455	G
1	5	1477	C
1	5	1485	C
1	5	1502	G
1	5	1578	U
1	5	1590	C
1	5	1613	A
1	5	1633	G
1	5	1654	G
1	5	1733	G
1	5	1753	G
1	5	1766	A
1	5	1773	U
1	5	1804	A
1	5	1818	G
1	5	1835	G
1	5	1836	G
1	5	1918	U
1	5	1921	C
1	5	1977	C
1	5	1990	A
1	5	1992	U
1	5	2001	G
1	5	2010	A
1	5	2023	C
1	5	2088	A
1	5	2089	G
1	5	2093	G
1	5	2106	G
1	5	2258	C
1	5	2266	C
1	5	2267	U
1	5	2278	G
1	5	2313	A
1	5	2333	G
1	5	2421	G
1	5	2428	A
1	5	2474	G

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Mol	Chain	Res	Type
1	5	2490	U
1	5	2502	A
1	5	2505	C
1	5	2506	G
1	5	2546	G
1	5	2553	A
1	5	2587	A
1	5	2696	A
1	5	2724	G
1	5	2761	U
1	5	2763	U
1	5	2794	C
1	5	3603	G
1	5	3614	G
1	5	3625	G
1	5	3672	G
1	5	3710	G
1	5	3810	C
1	5	3876	A
1	5	3888	G
1	5	3904	G
1	5	3949	A
1	5	3959	U
1	5	3966	A
1	5	3968	U
1	5	3972	A
1	5	4041	C
1	5	4046	A
1	5	4047	A
1	5	4064	C
1	5	4069	U
1	5	4119	C
1	5	4121	G
1	5	4124	G
1	5	4127	A
1	5	4162	C
1	5	4170	A
1	5	4232	U
1	5	4254	G
1	5	4266	G
1	5	4291	G
1	5	4348	A

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Mol	Chain	Res	Type
1	5	4448	G
1	5	4452	U
1	5	4488	A
1	5	4527	G
1	5	4572	U
1	5	4626	A
1	5	4635	A
1	5	4719	G
1	5	4881	U
1	5	4882	U
1	5	4884	G
1	5	4894	A
1	5	4909	A
1	5	4913	G
1	5	4921	C
1	5	4925	U
1	5	4936	G
1	5	4938	A
1	5	4942	C
1	5	4944	C
1	5	5047	C
1	5	5061	A
2	7	109	U
3	8	2	G
3	8	51	U
3	8	94	G
3	8	124	U
4	9	24	C
4	9	33	G
4	9	41	G
4	9	72	C
4	9	110	U
4	9	126	G
4	9	160	U
4	9	182	C
4	9	407	G
4	9	448	A
4	9	465	A
4	9	516	A
4	9	532	C
4	9	553	U
4	9	555	A

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Mol	Chain	Res	Type
4	9	561	A
4	9	606	G
4	9	620	G
4	9	752	G
4	9	821	G
4	9	858	A
4	9	867	G
4	9	869	A
4	9	870	A
4	9	872	A
4	9	875	A
4	9	919	A
4	9	1016	U
4	9	1061	U
4	9	1137	U
4	9	1138	C
4	9	1165	G
4	9	1215	C
4	9	1253	A
4	9	1274	G
4	9	1303	C
4	9	1308	U
4	9	1313	A
4	9	1395	C
4	9	1396	A
4	9	1428	G
4	9	1454	A
4	9	1476	A
4	9	1489	A
4	9	1497	G
4	9	1580	A
4	9	1581	C
4	9	1622	U
4	9	1637	A
4	9	1638	G
4	9	1664	A
4	9	1679	A
4	9	1757	G
4	9	1835	A
4	9	1837	G
4	9	1863	A
4	9	1868	U

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Mol	Chain	Res	Type
80	12	19	G
80	12	44	A
80	12	46	G
81	13	16	G
81	13	19	G
81	13	74	C
81	11	10	G
81	11	16	G
81	11	19	G
81	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 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	$\# Z > 2$
87	PHE	12	102	80	10,11,12	0.37	0	8,13,15	0.23	0
88	ATP	11	101	81	28,33,33	0.69	0	34,52,52	0.79	1 (2%)
89	MET	13	102	81	6,7,8	0.55	0	2,7,9	0.30	0
86	GTP	12	101	80	29,34,34	1.17	2 (6%)	35,54,54	1.28	4 (11%)
84	SPD	5	5101	-	9,9,9	0.35	0	8,8,8	0.81	0
90	GCP	jj	700	91	27,34,34	2.38	4 (14%)	35,54,54	2.42	8 (22%)
88	ATP	13	101	81	28,33,33	0.71	0	34,52,52	0.78	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	PHE	12	102	80	-	2/5/6/8	0/1/1/1
88	ATP	11	101	81	-	3/18/38/38	0/3/3/3
89	MET	13	102	81	-	0/5/6/8	-
86	GTP	12	101	80	-	4/18/38/38	0/3/3/3
84	SPD	5	5101	-	-	1/7/7/7	-
90	GCP	jj	700	91	-	1/15/38/38	0/3/3/3
88	ATP	13	101	81	-	4/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	PB-O3A	9.95	1.69	1.58
86	12	101	GTP	C5-C6	-4.24	1.39	1.47
90	jj	700	GCP	C6-N1	4.12	1.40	1.33
90	jj	700	GCP	C8-N7	-2.51	1.30	1.34
90	jj	700	GCP	PB-O2B	-2.34	1.50	1.56
86	12	101	GTP	C2-N3	2.07	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C5-C6-N1	-9.77	110.36	123.42
90	jj	700	GCP	C2-N1-C6	7.18	125.94	115.96
86	12	101	GTP	C8-N7-C5	3.66	108.78	102.55
90	jj	700	GCP	O2B-PB-C3B	3.25	120.20	106.73
86	12	101	GTP	C2-N1-C6	-3.09	119.45	125.11
90	jj	700	GCP	N3-C2-N1	-2.93	123.48	127.21
86	12	101	GTP	C5-C6-N1	2.93	119.66	114.07
90	jj	700	GCP	C2-N3-C4	-2.58	112.71	115.48
90	jj	700	GCP	O2A-PA-O3A	2.49	114.00	107.27
88	11	101	ATP	C5-C6-N6	2.34	123.87	120.31
88	13	101	ATP	C5-C6-N6	2.27	123.77	120.31
90	jj	700	GCP	O1G-PG-C3B	-2.27	106.42	111.37
86	12	101	GTP	O6-C6-C5	-2.09	120.18	124.32
90	jj	700	GCP	O2B-PB-O1B	2.08	116.72	109.95

There are no chirality outliers.

All (15) torsion outliers are listed below:

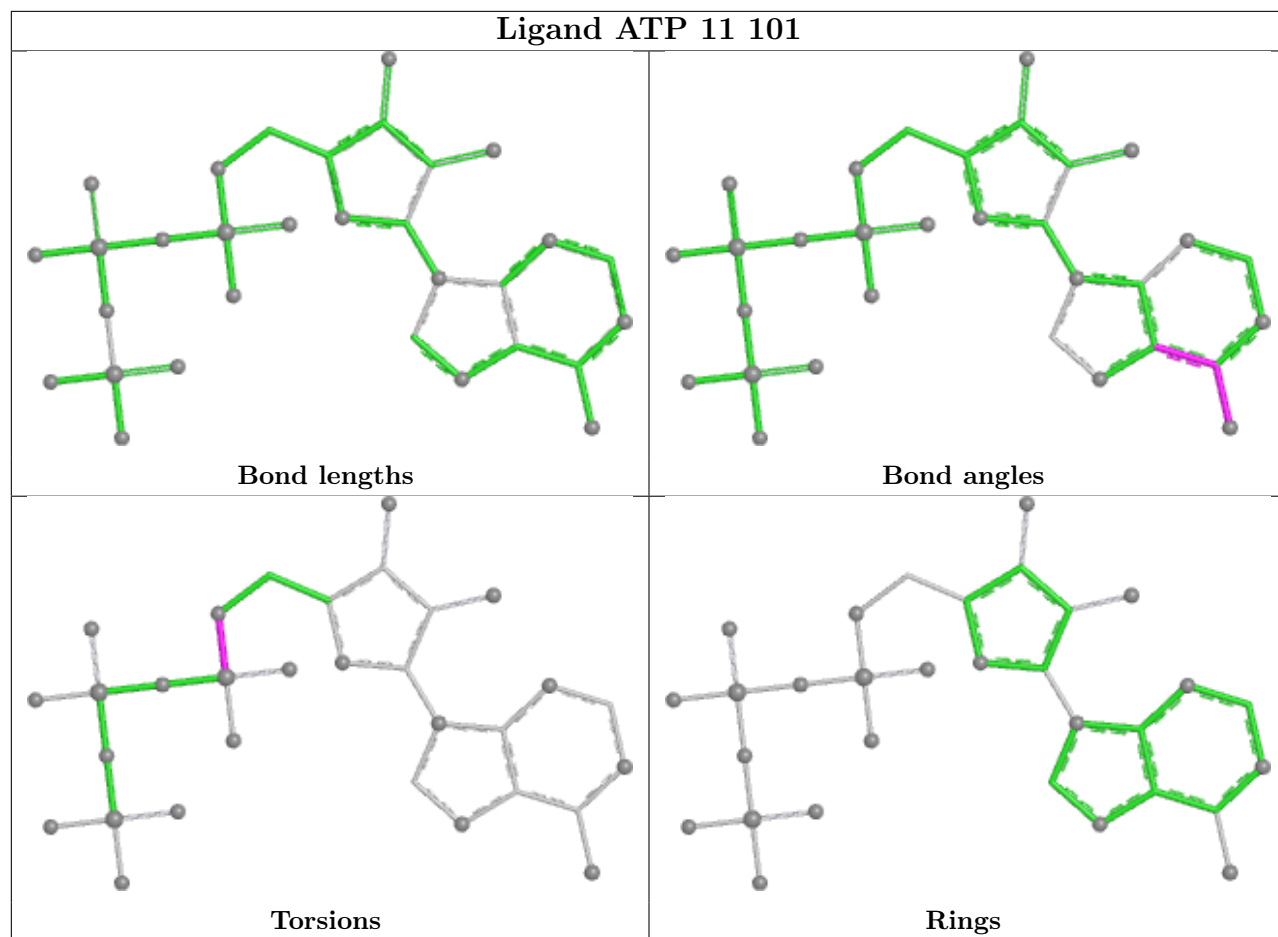
Mol	Chain	Res	Type	Atoms
86	12	101	GTP	PB-O3B-PG-O2G
86	12	101	GTP	C5'-O5'-PA-O2A
88	13	101	ATP	C5'-O5'-PA-O3A
88	11	101	ATP	C5'-O5'-PA-O1A
88	11	101	ATP	C5'-O5'-PA-O2A
88	11	101	ATP	C5'-O5'-PA-O3A
90	jj	700	GCP	PG-C3B-PB-O1B
84	5	5101	SPD	N6-C7-C8-C9
87	12	102	PHE	CA-CB-CG-CD1
87	12	102	PHE	CA-CB-CG-CD2
86	12	101	GTP	C5'-O5'-PA-O3A
86	12	101	GTP	C5'-O5'-PA-O1A
88	13	101	ATP	C5'-O5'-PA-O1A
88	13	101	ATP	PB-O3A-PA-O1A
88	13	101	ATP	PB-O3A-PA-O2A

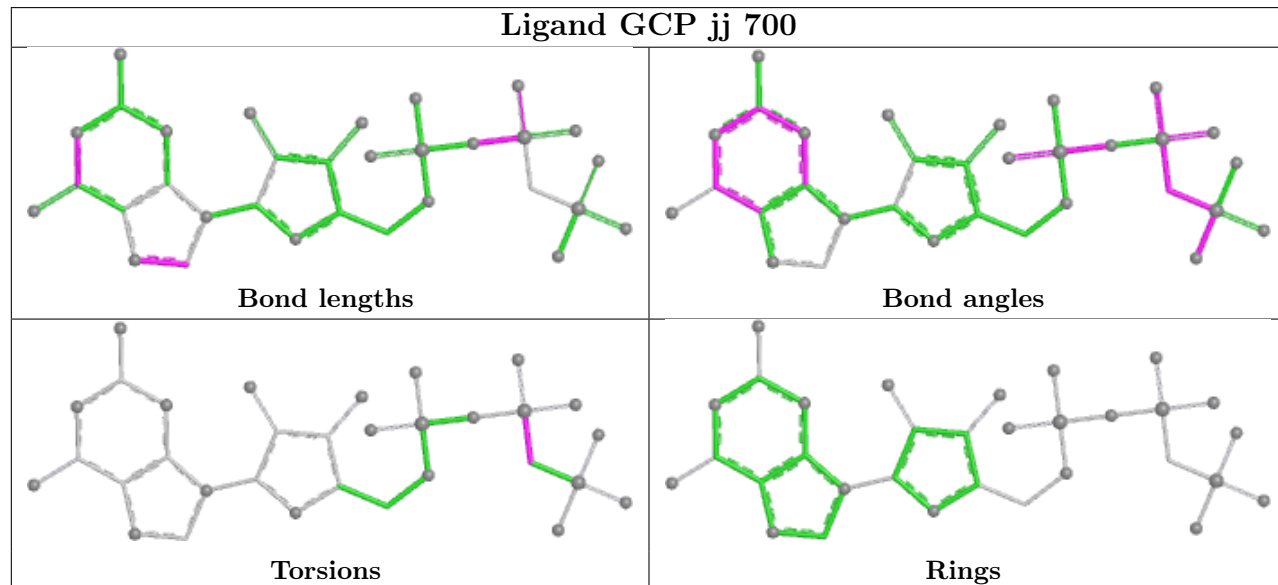
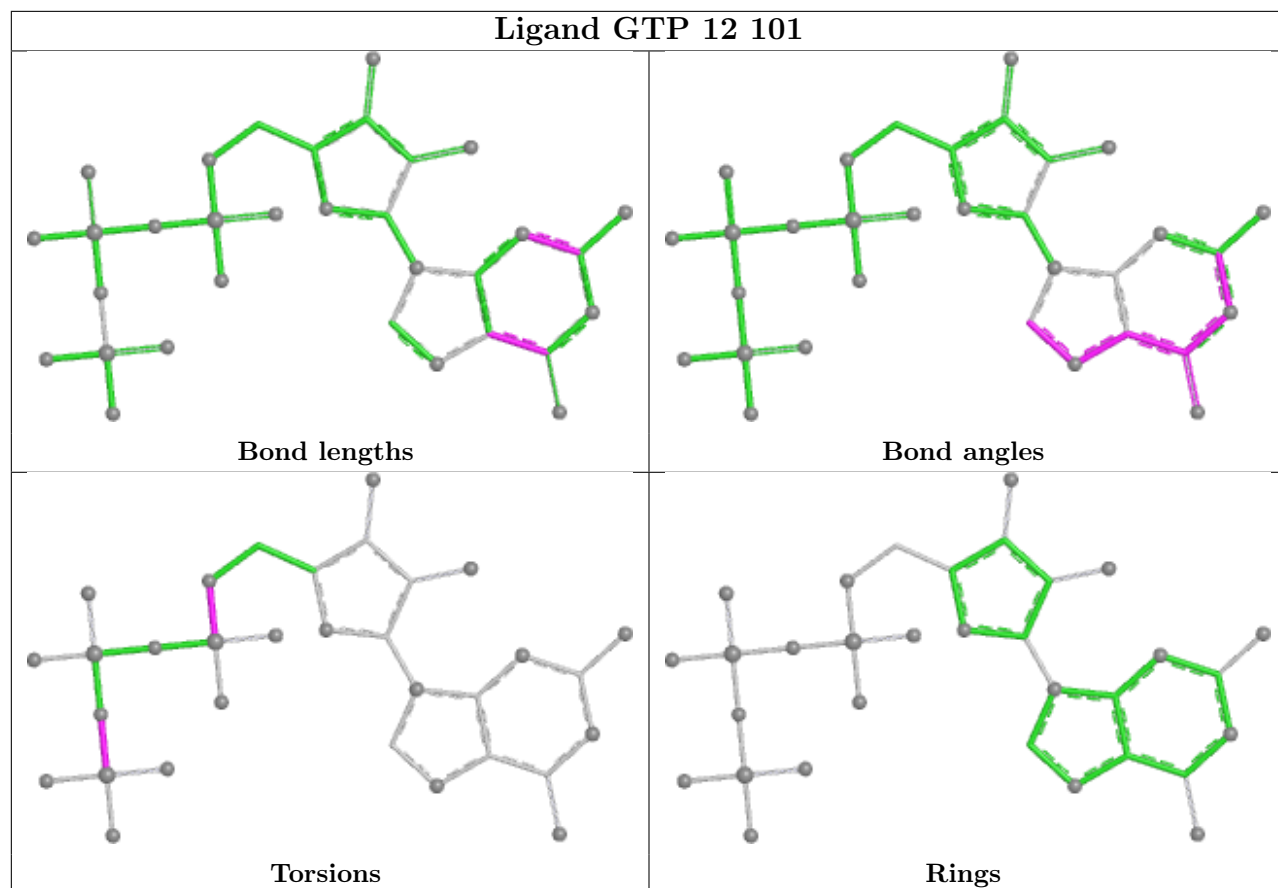
There are no ring outliers.

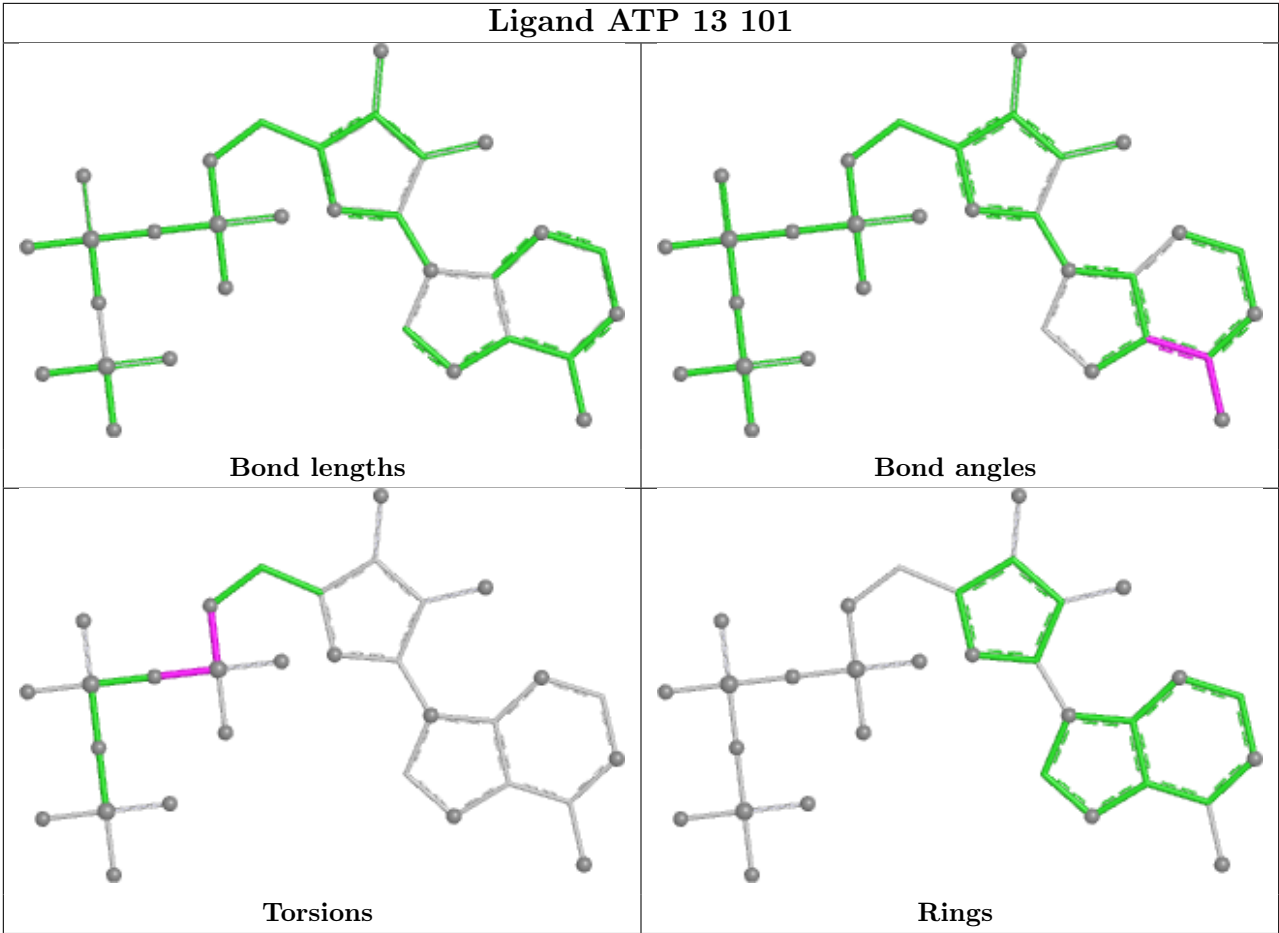
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	11	101	ATP	1	0
86	12	101	GTP	1	0
90	jj	700	GCP	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	42.08
1	5	1252:C	O3'	1271:G	P	35.85
1	5	1219:G	O3'	1233:G	P	21.05
1	5	1406(C):G	O3'	1411:C	P	17.84
1	5	4101:C	O3'	4107:G	P	17.51

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	3976:C	O3'	4035:G	P	16.47
1	5	4777:C	O3'	4859:C	P	16.37
1	5	523:C	O3'	638:G	P	16.35
1	5	990:C	O3'	1064:G	P	16.22
1	5	4138:C	O3'	4146:G	P	15.98
1	5	760:G	O3'	904:C	P	15.31
1	5	182:G	O3'	189:G	P	14.89
1	5	1696:C	O3'	1720:C	P	14.40
1	5	1364:U	O3'	1368:A	P	14.28
1	5	5022:U	O3'	5028:G	P	14.08
1	5	2901:G	O3'	3597:G	P	12.71
1	5	1180:C	O3'	1183:C	P	9.74
1	5	4729:A	O3'	4735:G	P	9.59
1	5	512:U	O3'	515:C	P	7.55
1	5	4740:G	O3'	4743:G	P	7.19
1	5	500:G	O3'	504:G	P	6.31
1	5	1100:U	O3'	1168:G	P	6.31
1	5	4899:G	O3'	4902:C	P	3.24

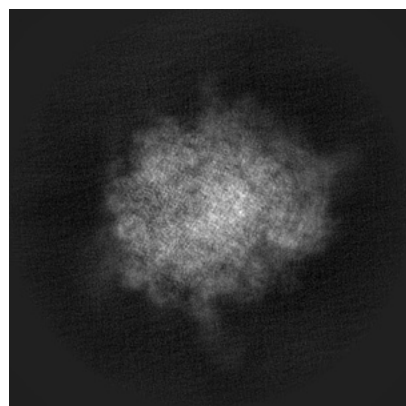
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73302. These allow visual inspection of the internal detail of the map and identification of artifacts.

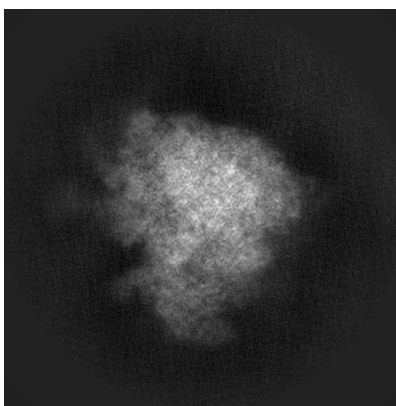
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

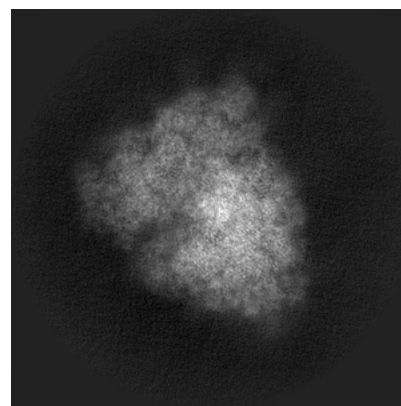
6.1.1 Primary map



X

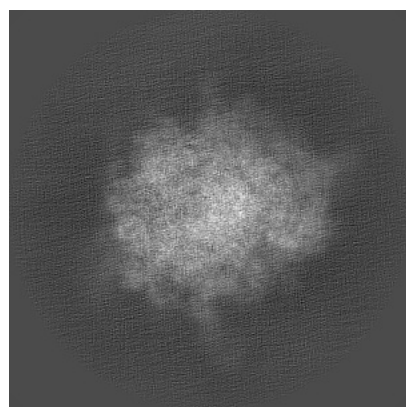


Y

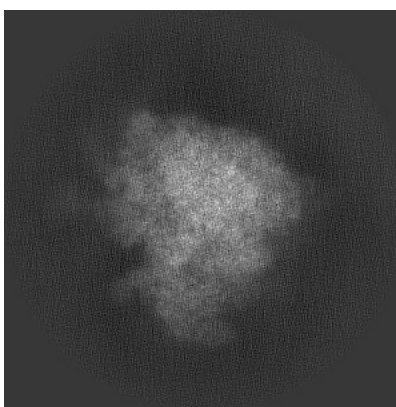


Z

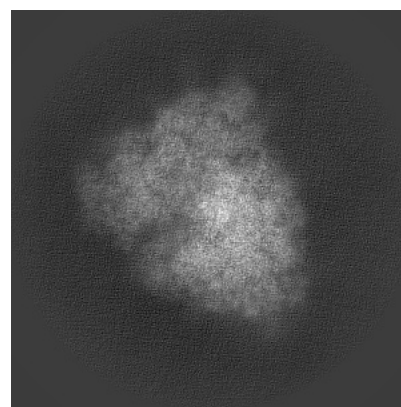
6.1.2 Raw map



X



Y

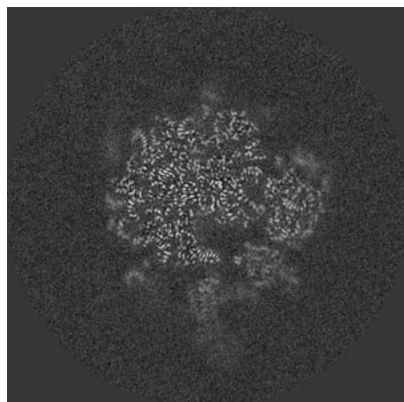


Z

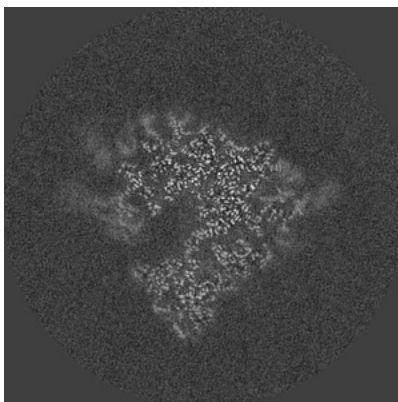
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

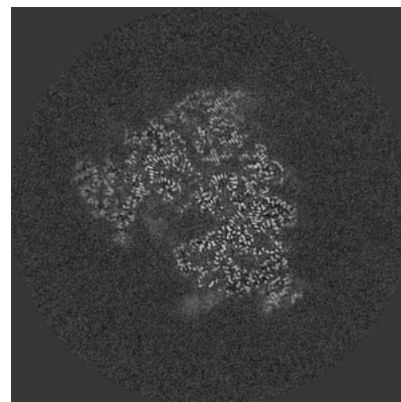
6.2.1 Primary map



X Index: 200

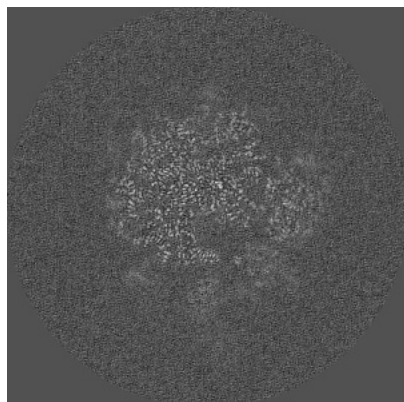


Y Index: 200

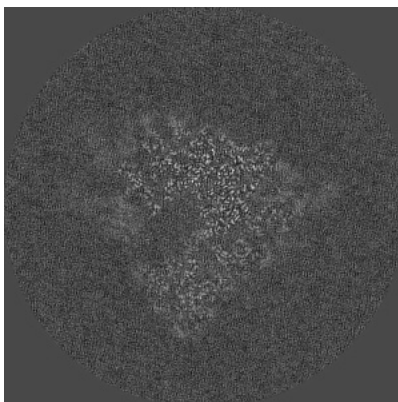


Z Index: 200

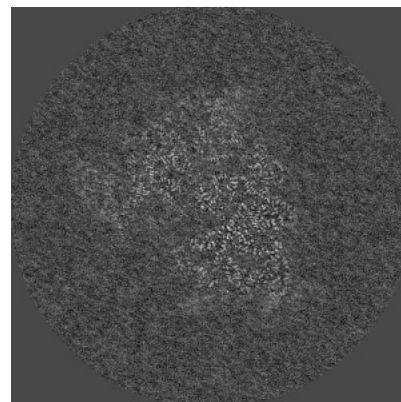
6.2.2 Raw map



X Index: 200



Y Index: 200

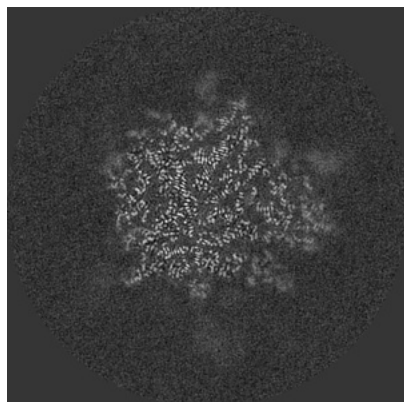


Z Index: 200

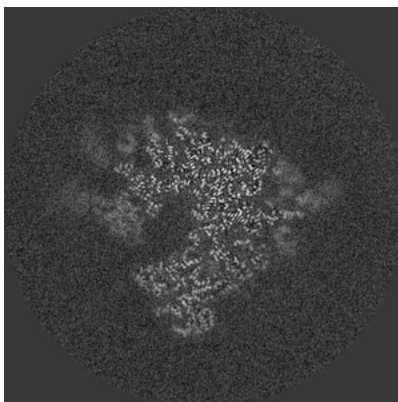
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

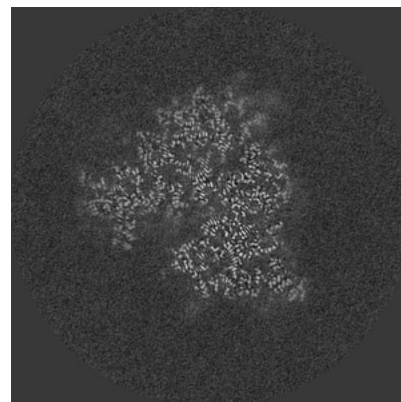
6.3.1 Primary map



X Index: 215

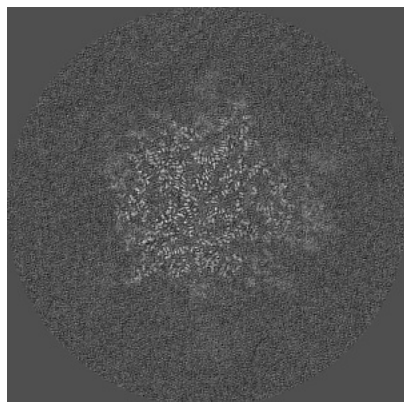


Y Index: 203

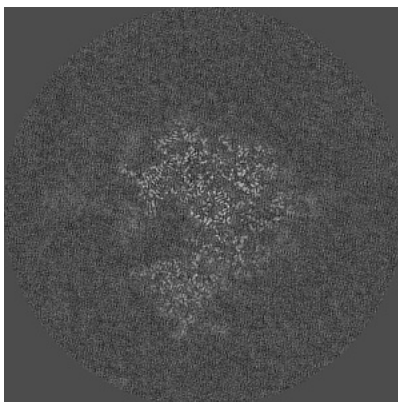


Z Index: 192

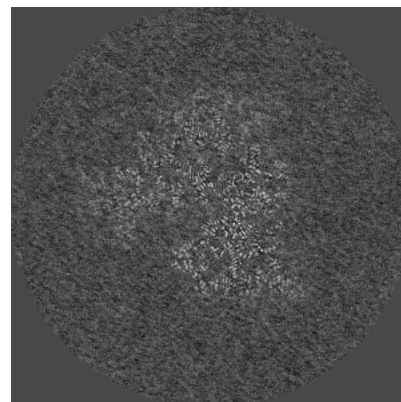
6.3.2 Raw map



X Index: 215



Y Index: 209

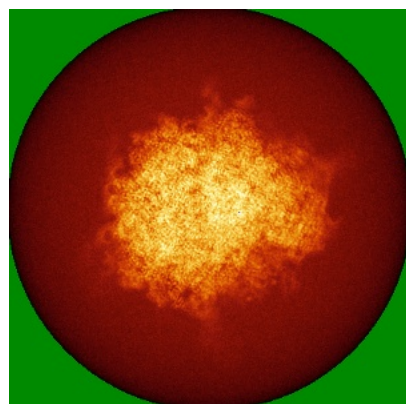


Z Index: 192

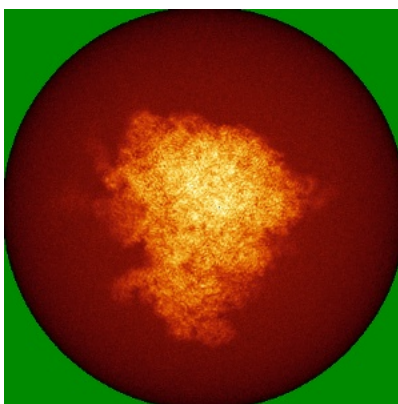
The images above show the largest variance slices of the map in three orthogonal directions.

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

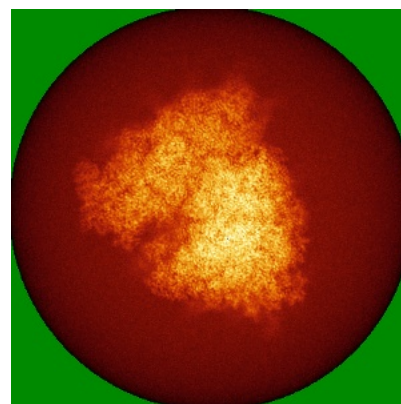
6.4.1 Primary map



X

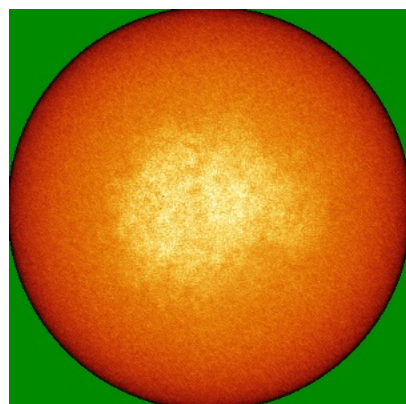


Y

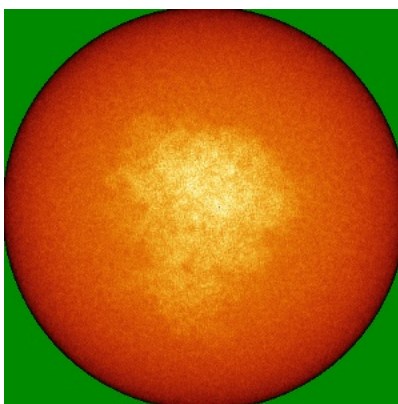


Z

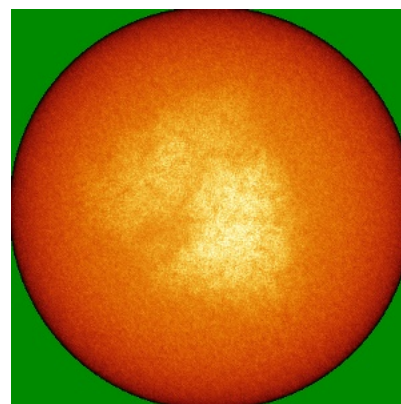
6.4.2 Raw map



X



Y

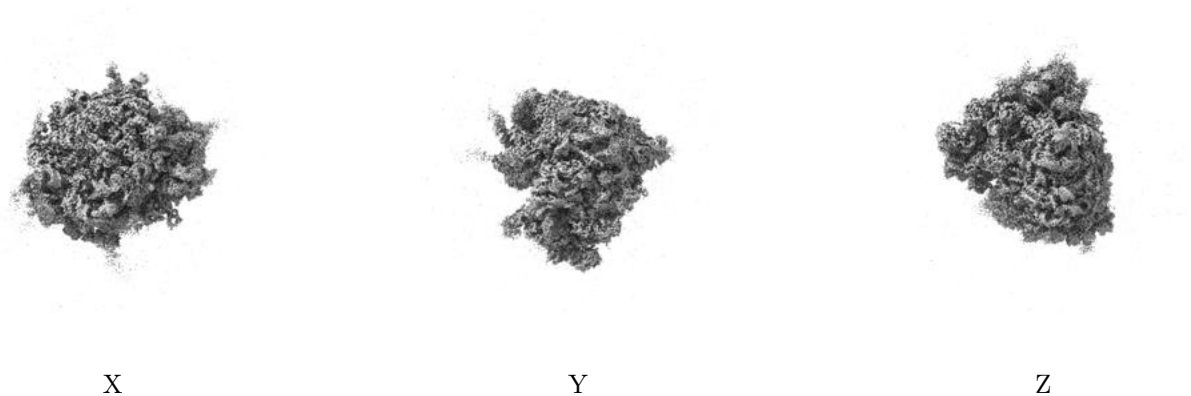


Z

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.

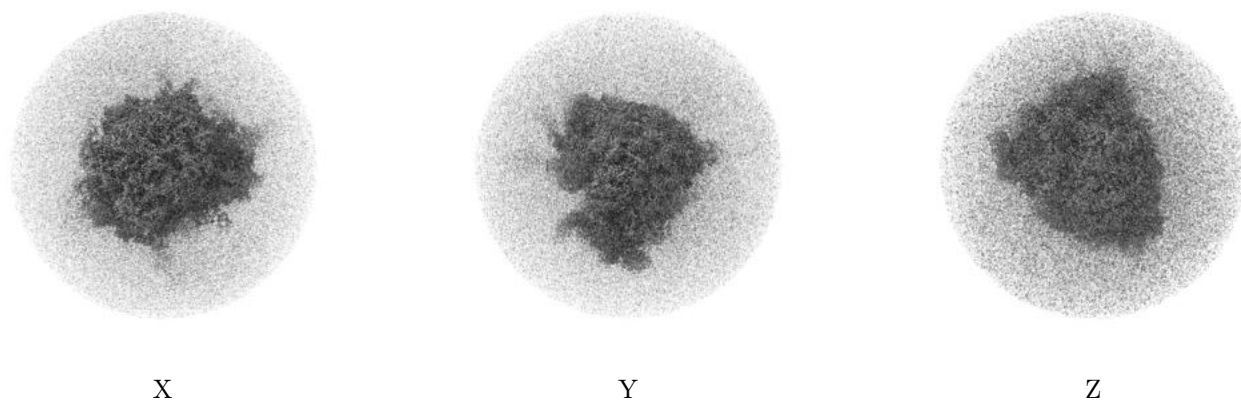
6.5 Orthogonal surface views [i](#)

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.

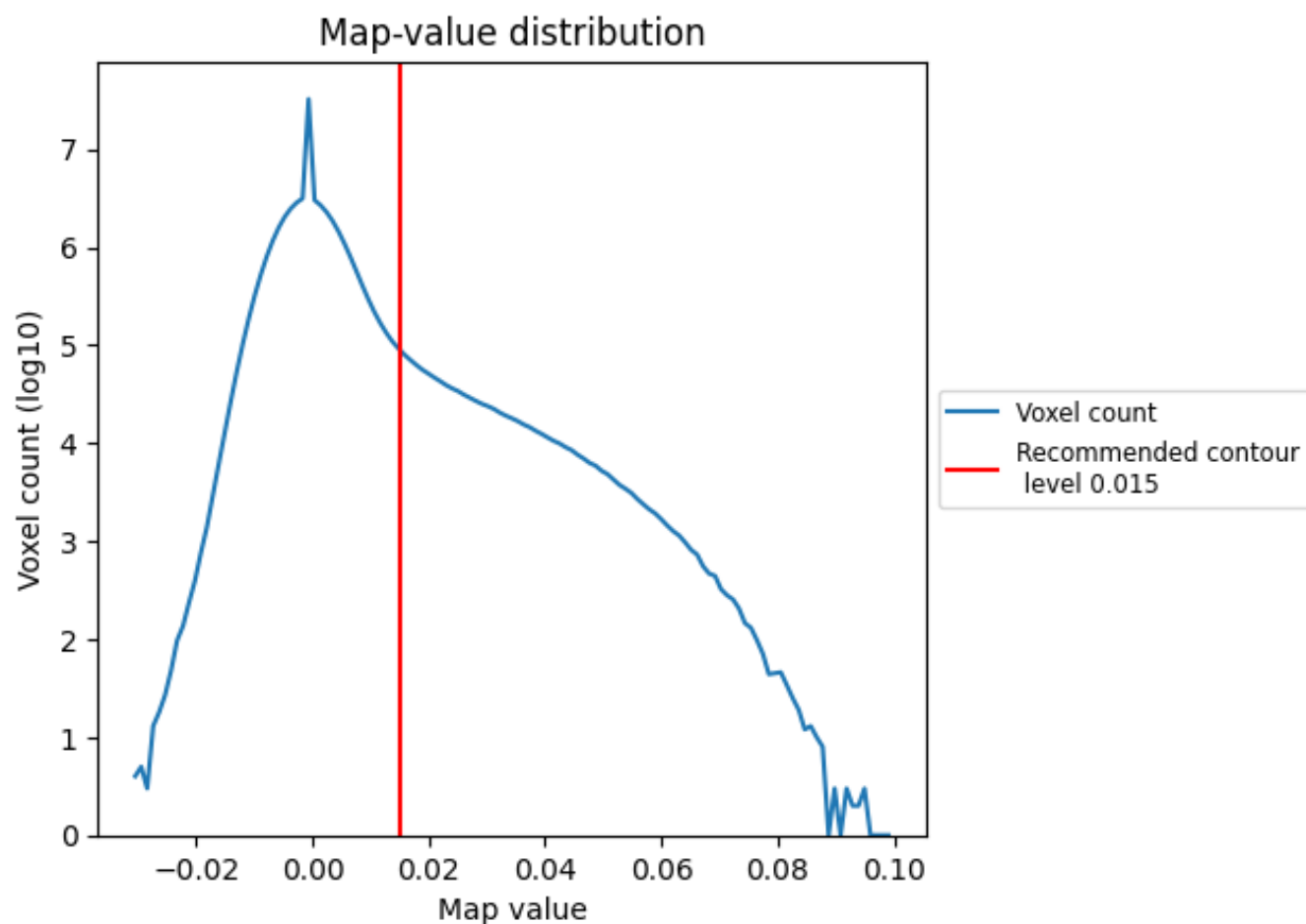
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

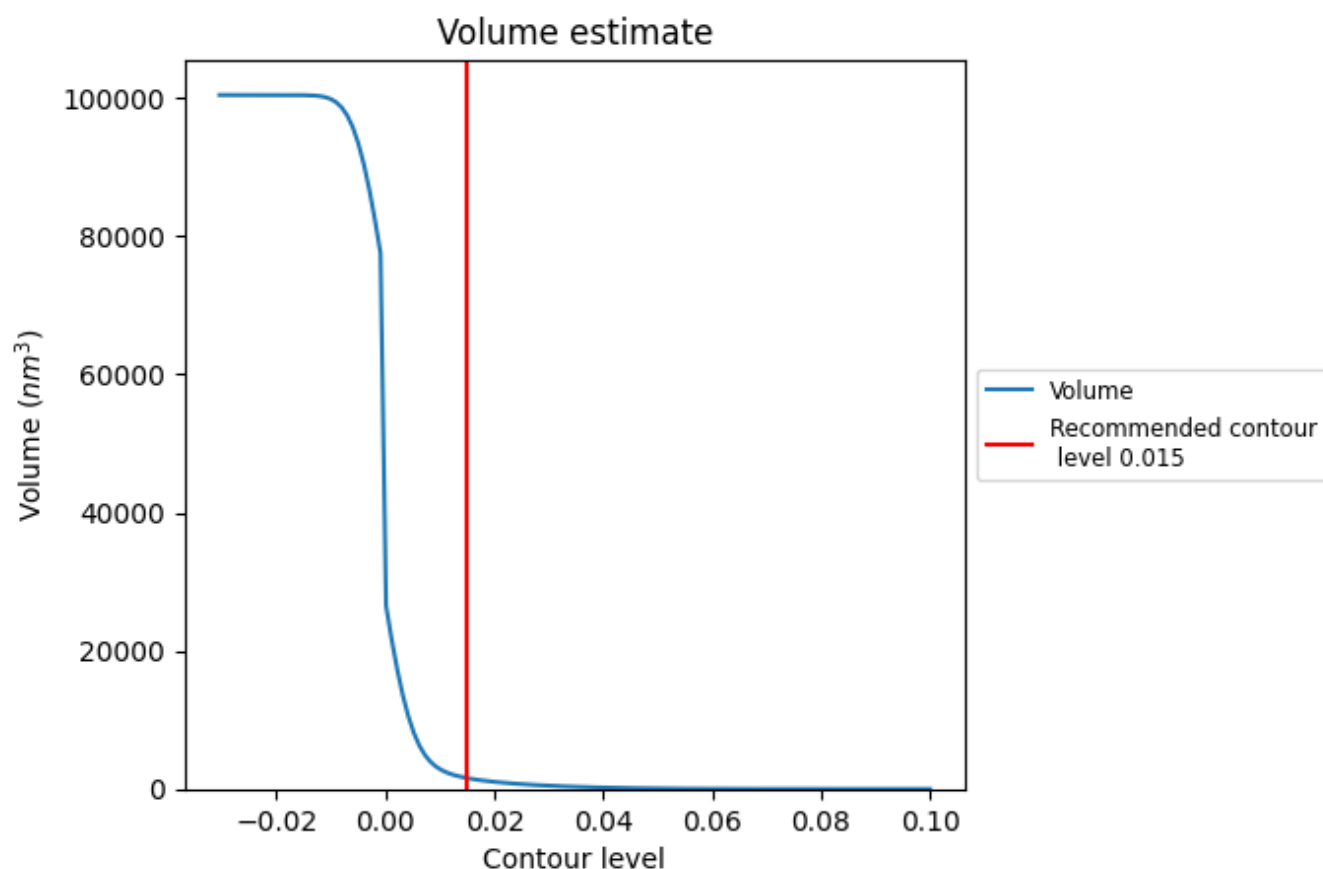
This section contains the results of statistical analysis of the map.

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.

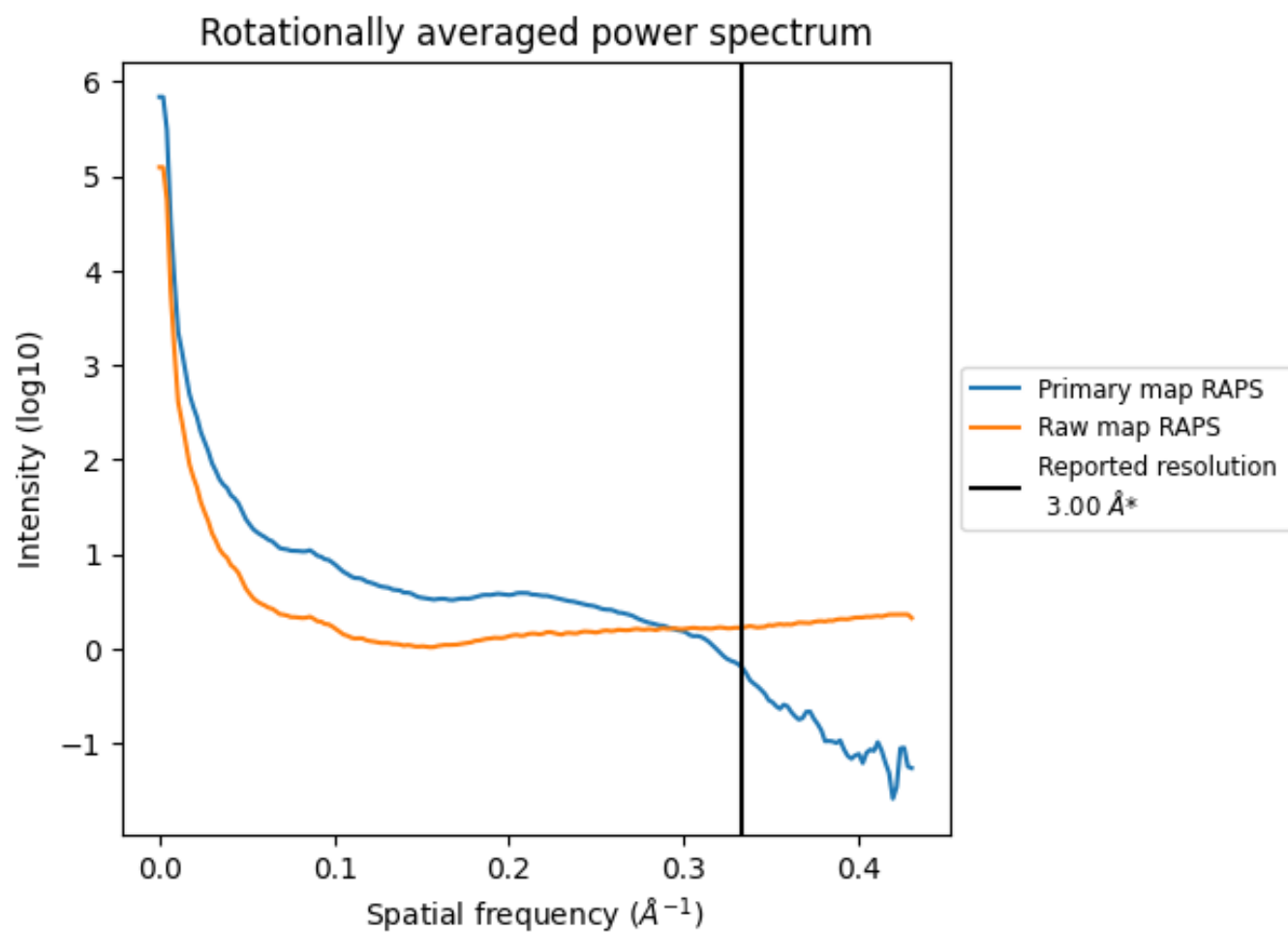
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1580 nm^3 ; this corresponds to an approximate mass of 1427 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 ⓘ

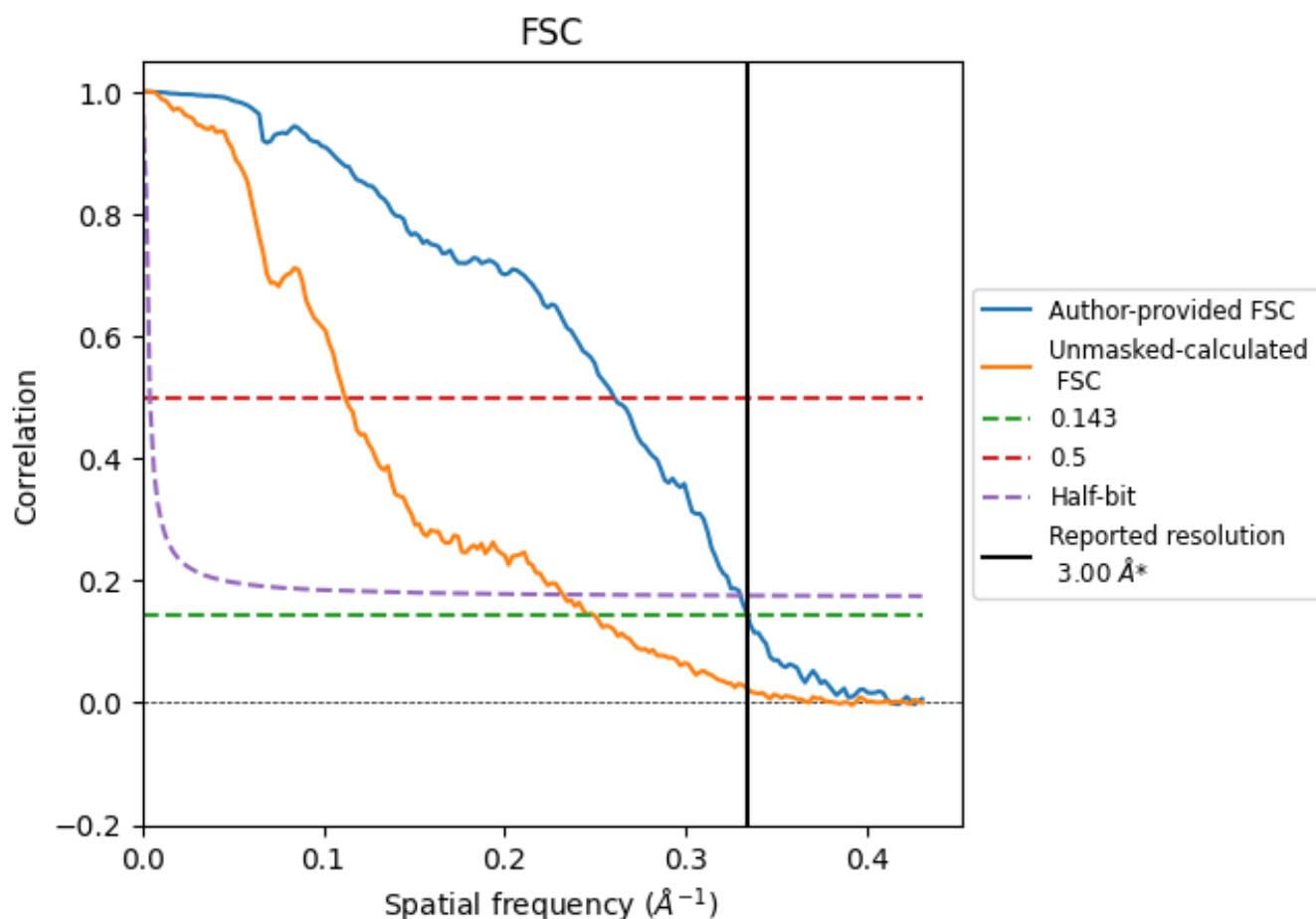


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

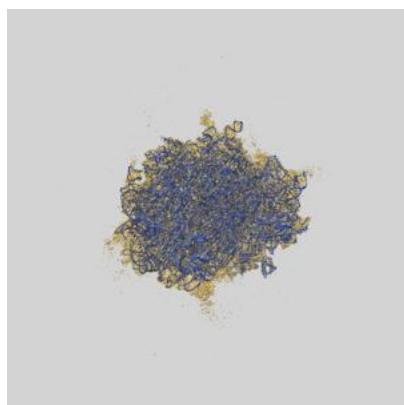
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.84	3.03
Unmasked-calculated*	4.01	8.94	4.31

*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 4.01 differs from the reported value 3.0 by more than 10 %

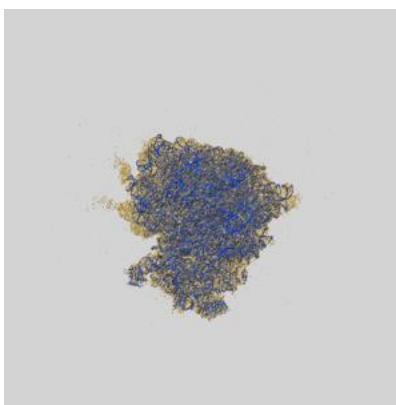
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73302 and PDB model 9YPO. Per-residue inclusion information can be found in section [3](#) on page [31](#).

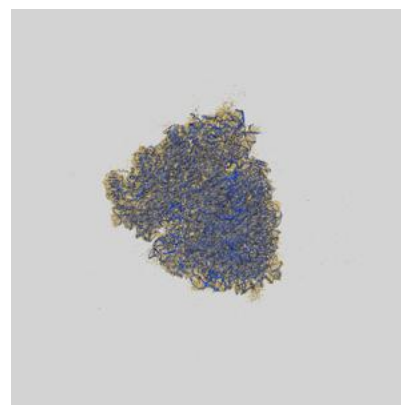
9.1 Map-model overlay [i](#)



X



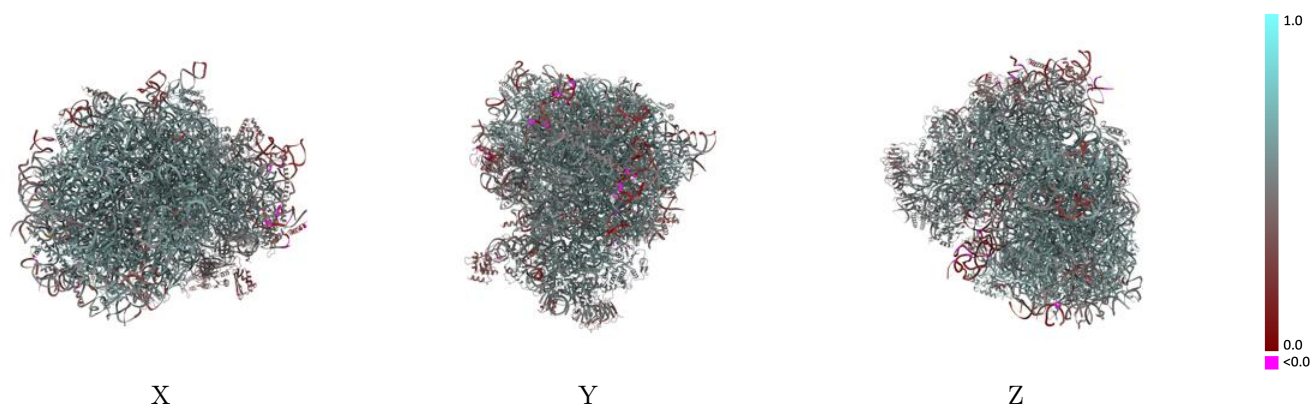
Y



Z

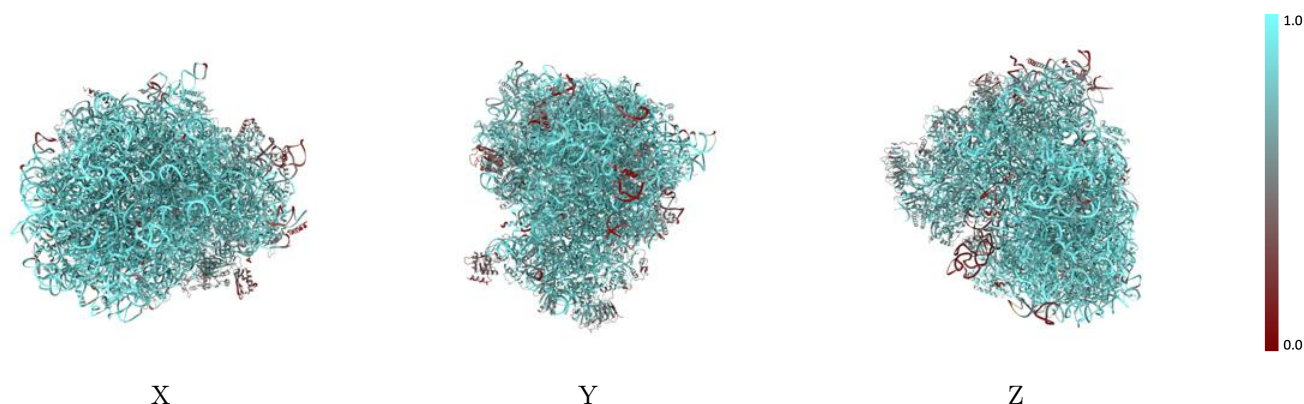
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



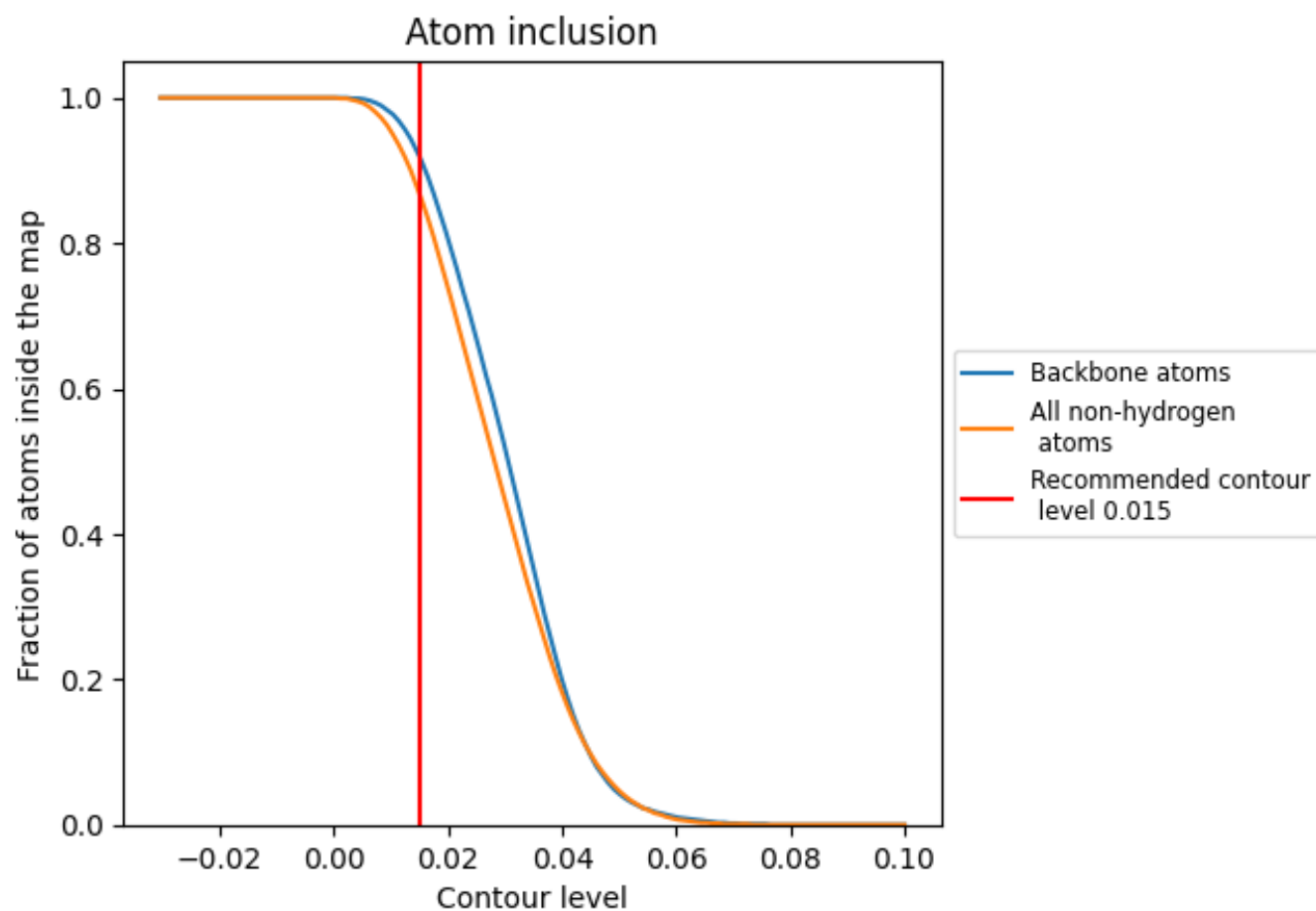
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 92% of all backbone atoms, 87% 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	 0.8680	 0.5370
10	 0.9490	 0.5630
11	 0.3330	 0.2410
12	 0.8810	 0.4700
13	 0.6800	 0.4420
5	 0.9290	 0.5490
7	 0.9910	 0.5970
8	 0.9610	 0.5760
9	 0.9110	 0.5260
A	 0.9390	 0.6060
AA	 0.7690	 0.5270
B	 0.8880	 0.5850
BB	 0.8120	 0.5460
C	 0.9050	 0.5850
CC	 0.8390	 0.5500
D	 0.8500	 0.5530
DD	 0.7450	 0.5110
E	 0.8390	 0.5490
EE	 0.7980	 0.5130
FF	 0.7760	 0.5180
G	 0.7730	 0.5250
GG	 0.6750	 0.4590
H	 0.8350	 0.5640
HH	 0.5990	 0.4650
I	 0.8790	 0.5790
II	 0.7890	 0.5230
J	 0.8050	 0.5320
JJ	 0.7690	 0.4910
K	 0.9110	 0.5900
KK	 0.7560	 0.4890
L	 0.8330	 0.5540
LL	 0.8190	 0.5520
M	 0.8710	 0.5600
MM	 0.3310	 0.3030
N	 0.9480	 0.6020



















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Chain	Atom inclusion	Q-score
NN	 0.8440	 0.5580
O	 0.9090	 0.5910
OO	 0.8490	 0.5510
P	 0.9050	 0.5930
PP	 0.7160	 0.4860
Q	 0.9050	 0.5920
QQ	 0.7890	 0.5220
R	 0.8280	 0.5460
RR	 0.6490	 0.4930
S	 0.9030	 0.5920
SS	 0.7500	 0.4980
T	 0.8610	 0.5680
TT	 0.7660	 0.5060
U	 0.7650	 0.5000
UU	 0.7160	 0.4820
V	 0.8960	 0.5910
VV	 0.7660	 0.5200
W	 0.6570	 0.4660
WW	 0.8650	 0.5700
X	 0.8610	 0.5630
XX	 0.8720	 0.5690
Y	 0.8640	 0.5700
YY	 0.7320	 0.4860
Z	 0.8580	 0.5590
ZZ	 0.6790	 0.4770
a	 0.9240	 0.5930
aa	 0.8390	 0.5530
b	 0.8160	 0.5390
bb	 0.7620	 0.5220
c	 0.8480	 0.5610
cc	 0.7550	 0.5250
d	 0.8290	 0.5600
dd	 0.8760	 0.5600
e	 0.9230	 0.5990
ee	 0.6960	 0.4700
f	 0.9330	 0.6080
ff	 0.4150	 0.3580
g	 0.8770	 0.5740
gg	 0.6100	 0.4340
h	 0.8490	 0.5530
i	 0.8430	 0.5480
j	 0.9500	 0.6030

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Chain	Atom inclusion	Q-score
jj	 0.5690	 0.3990
k	 0.7420	 0.5180
l	 0.9160	 0.5830
m	 0.8680	 0.5780
n	 0.9360	 0.5840
o	 0.8830	 0.5820
p	 0.8720	 0.5780
r	 0.9140	 0.5890