



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:50 AM UTC

PDB ID : 9YPW / pdb_00009ypw
EMDB ID : EMD-73311
Title : GTPBP1*GDP*Phe-tRNA*ribosome in the post-GTP hydrolysis state,
Structure IV
Authors : Susorov, D.; Korostelev, A.A.
Deposited on : 2025-10-14
Resolution : 2.90 Å (reported)
Based on initial models : 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:

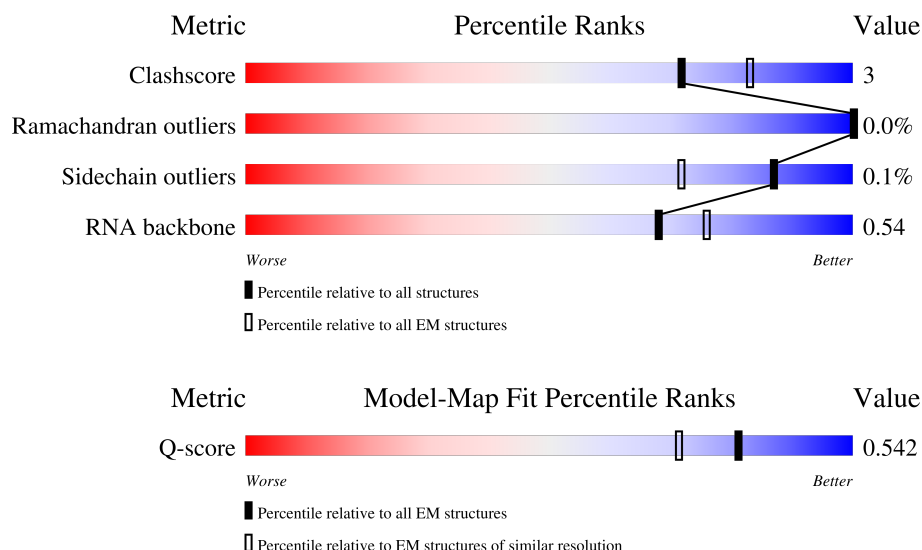
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



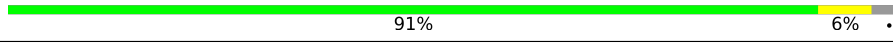
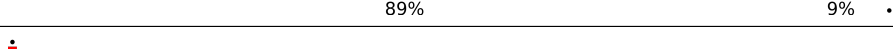
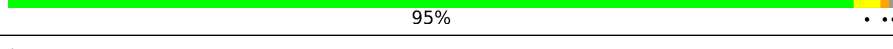
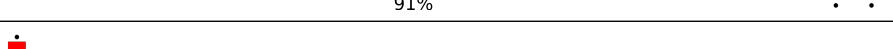
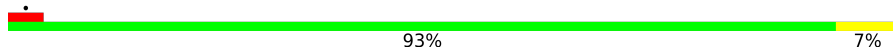
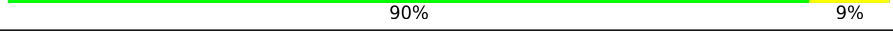
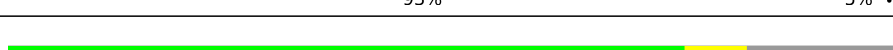
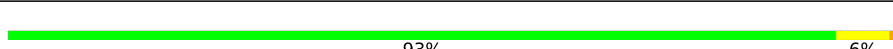
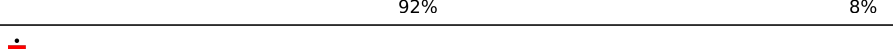
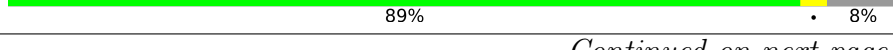
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	5	3601	
2	7	120	
3	8	156	

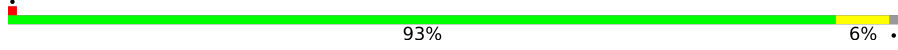
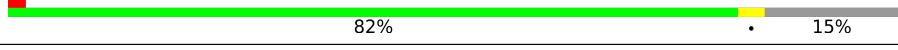
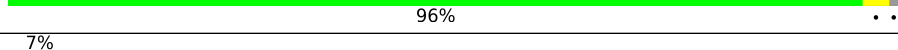
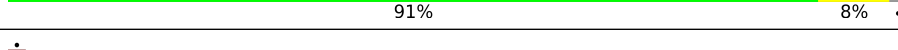
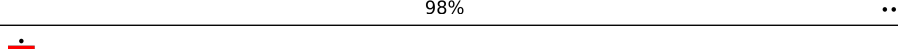
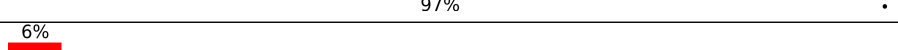
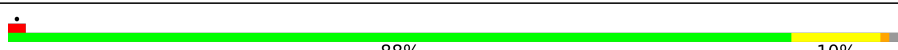
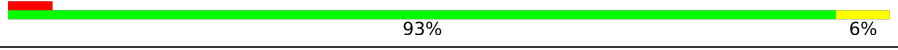
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Mol	Chain	Length	Quality of chain
4	9	1869	
5	A	257	
6	B	403	
7	C	425	
8	D	297	
9	E	291	
10	G	319	
11	H	192	
12	I	214	
13	J	178	
14	K	247	
15	L	211	
16	M	218	
17	N	204	
18	O	203	
19	P	184	
20	Q	188	
21	R	196	
22	S	176	
23	T	160	
24	U	128	
25	V	140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

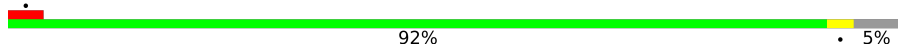
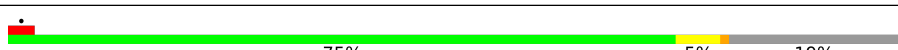
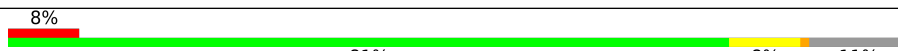
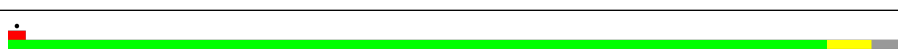
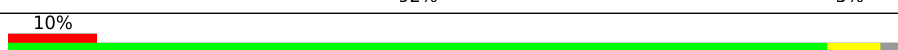
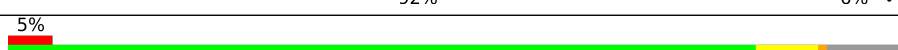
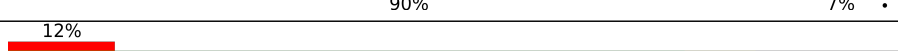
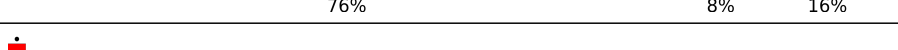
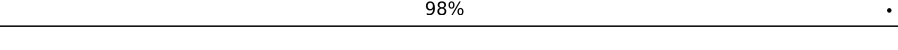
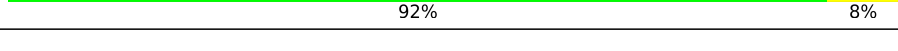
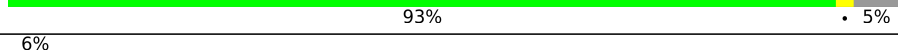
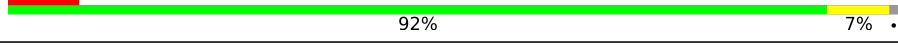
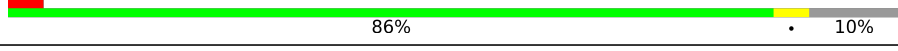
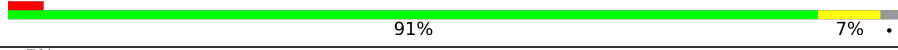
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Mol	Chain	Length	Quality of chain
29	Z	136	
30	a	148	
31	b	245	
32	c	115	
33	d	125	
34	e	135	
35	f	110	
36	g	116	
37	h	123	
38	i	105	
39	k	70	
40	l	51	
41	m	102	
42	n	25	
43	o	106	
44	p	92	
45	r	137	
46	AA	295	
47	BB	264	
48	CC	293	
49	DD	243	
50	EE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

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

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Mol	Chain	Length	Quality of chain
79	10	185	 94%
80	12	76	 47%47%
81	11	75	 73%57%41%
81	13	75	 8%59%33%7%
82	j	97	 72%16%11%
83	jj	703	 30%68%5%27%

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 219551 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	-	conflict	GB XR_011385821.1

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

- 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 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	1	MET	ILE	conflict	UNP P0DXC2
m	2	GLY	GLN	conflict	UNP P0DXC2
m	4	PRO	LYS	conflict	UNP P0DXC2
m	6	SER	-	insertion	UNP P0DXC2
m	7	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 5 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	104	ILE	CYS	conflict	UNP G1T040
o	105	GLN	TYR	conflict	UNP G1T040
o	106	PHE	ALA	conflict	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		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
OO	-16	MET	-	conflict	UNP G1T1F0
OO	-15	LYS	-	conflict	UNP G1T1F0
OO	-14	ALA	-	conflict	UNP G1T1F0
OO	-13	ARG	-	conflict	UNP G1T1F0
OO	-12	ALA	-	conflict	UNP G1T1F0
OO	-11	LEU	-	conflict	UNP G1T1F0
OO	-10	SER	-	conflict	UNP G1T1F0
OO	-9	GLY	-	conflict	UNP G1T1F0
OO	-8	SER	-	conflict	UNP G1T1F0
OO	-7	GLY	-	conflict	UNP G1T1F0
OO	-6	VAL	-	conflict	UNP G1T1F0
OO	-5	ARG	-	conflict	UNP G1T1F0
OO	-4	ARG	-	conflict	UNP G1T1F0
OO	-3	ARG	-	conflict	UNP G1T1F0
OO	-2	ARG	-	conflict	UNP G1T1F0
OO	-1	ALA	-	conflict	UNP G1T1F0
OO	0	ALA	-	conflict	UNP G1T1F0

- 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 Small ribosomal subunit protein eS24.

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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:

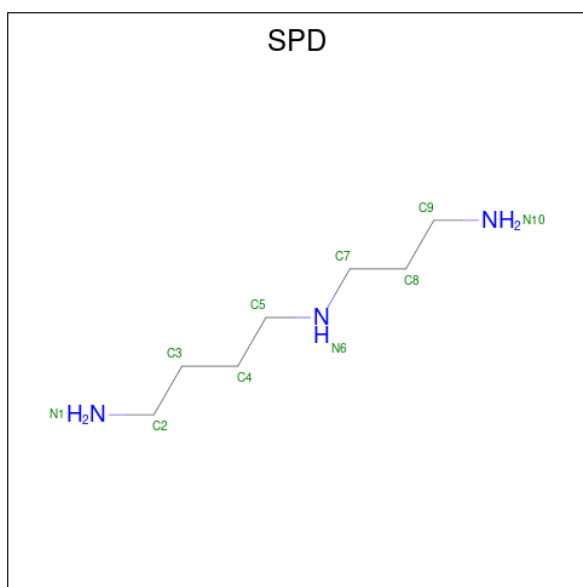
Chain	Residue	Modelled	Actual	Comment	Reference
jj	-33	MET	-	initiating methionine	UNP O00178
jj	-32	GLY	-	expression tag	UNP O00178
jj	-31	SER	-	expression tag	UNP O00178
jj	-30	SER	-	expression tag	UNP O00178
jj	-29	HIS	-	expression tag	UNP O00178

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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: C₇H₁₉N₃).

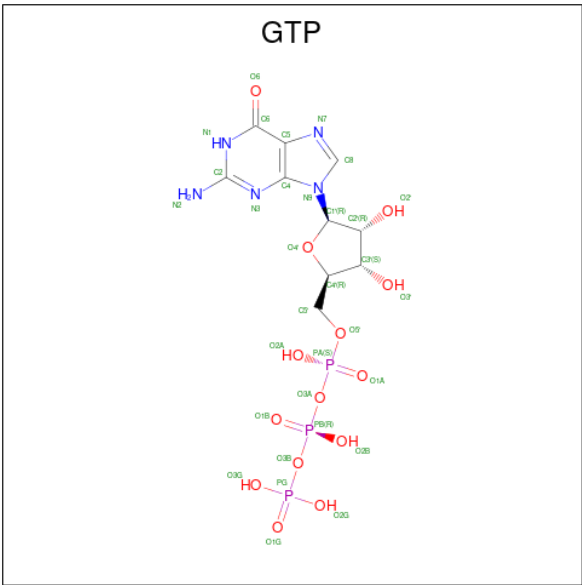


Mol	Chain	Residues	Atoms			AltConf
84	5	1	Total	C	N	0
			10	7	3	

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

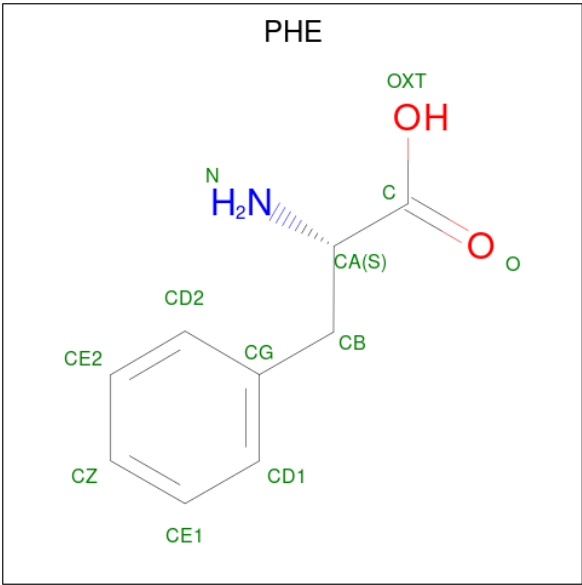
Mol	Chain	Residues	Atoms		AltConf
85	g	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	dd	1	Total	Zn	0
			1	1	
85	j	1	Total	Zn	0
			1	1	

- Molecule 86 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



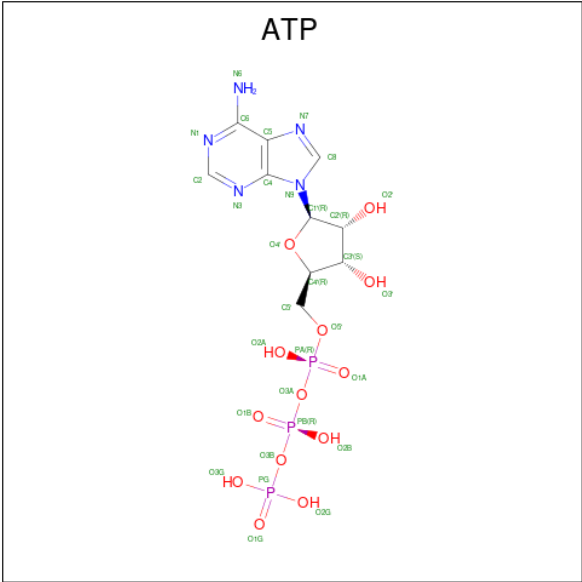
Mol	Chain	Residues	Atoms					AltConf
86	12	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 87 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



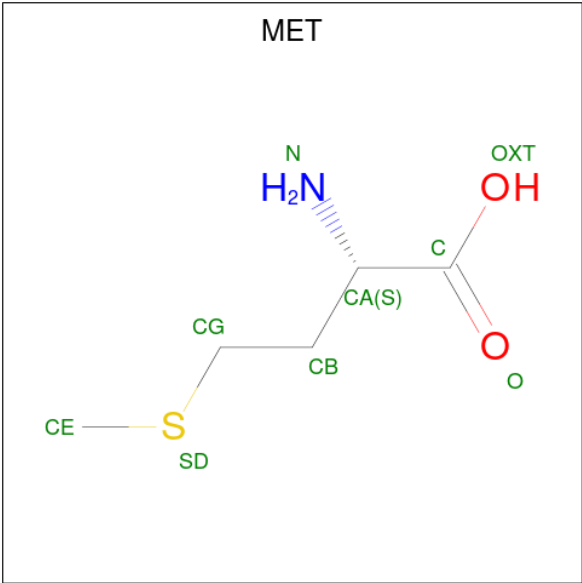
Mol	Chain	Residues	Atoms				AltConf
87	12	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 88 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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: C₅H₁₁NO₂S).



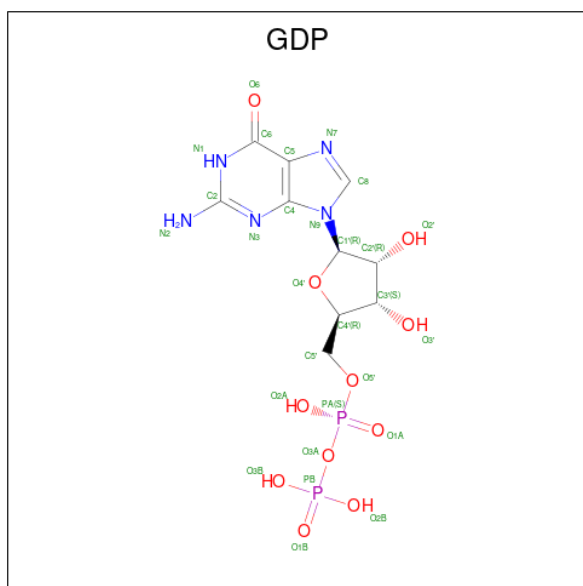
Mol	Chain	Residues	Atoms					AltConf
89	13	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 90 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest")

by depositor).

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

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
91	jj	1	Total	C	N	O	P	0
			28	10	5	11	2	

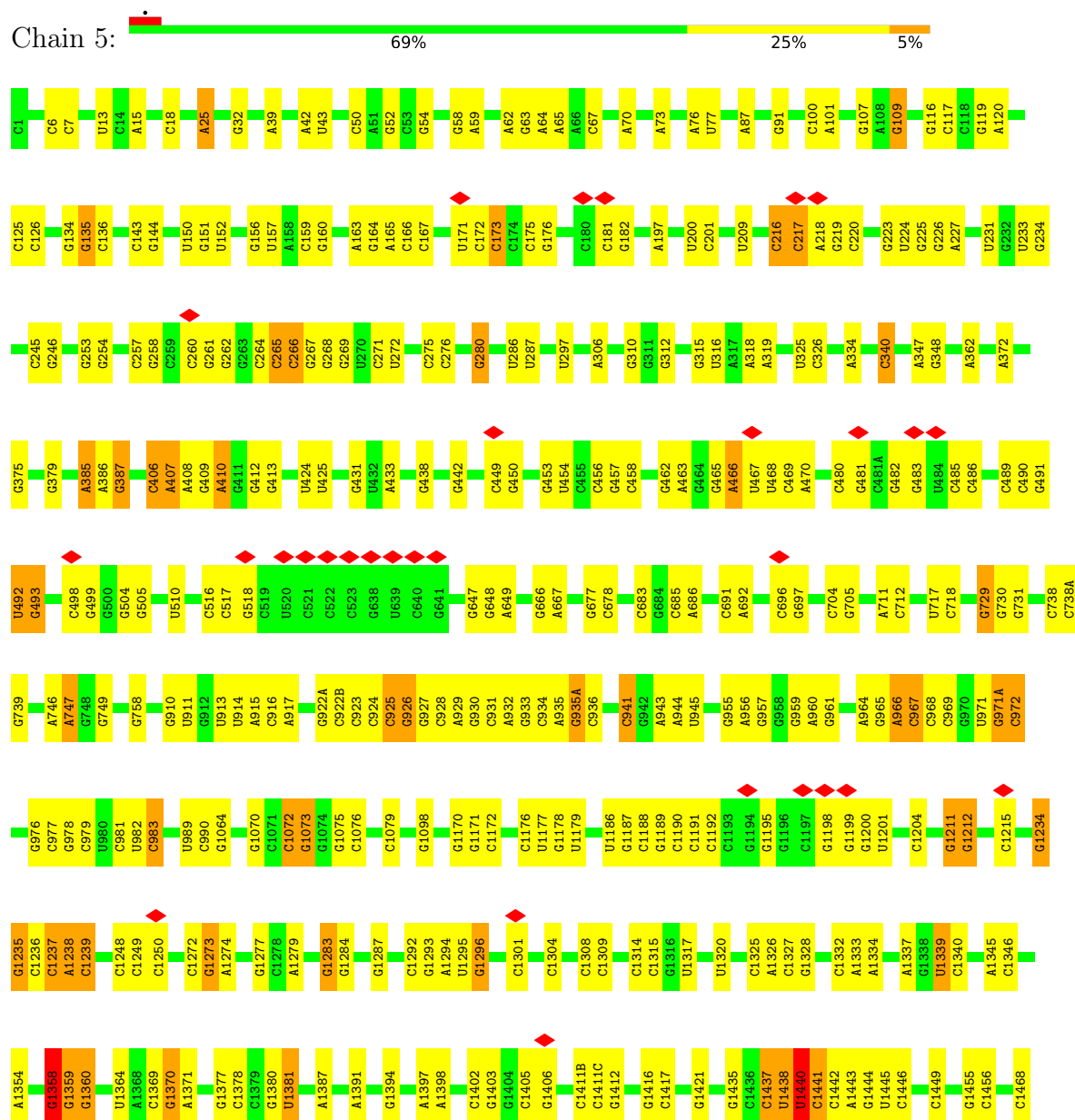
- Molecule 92 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

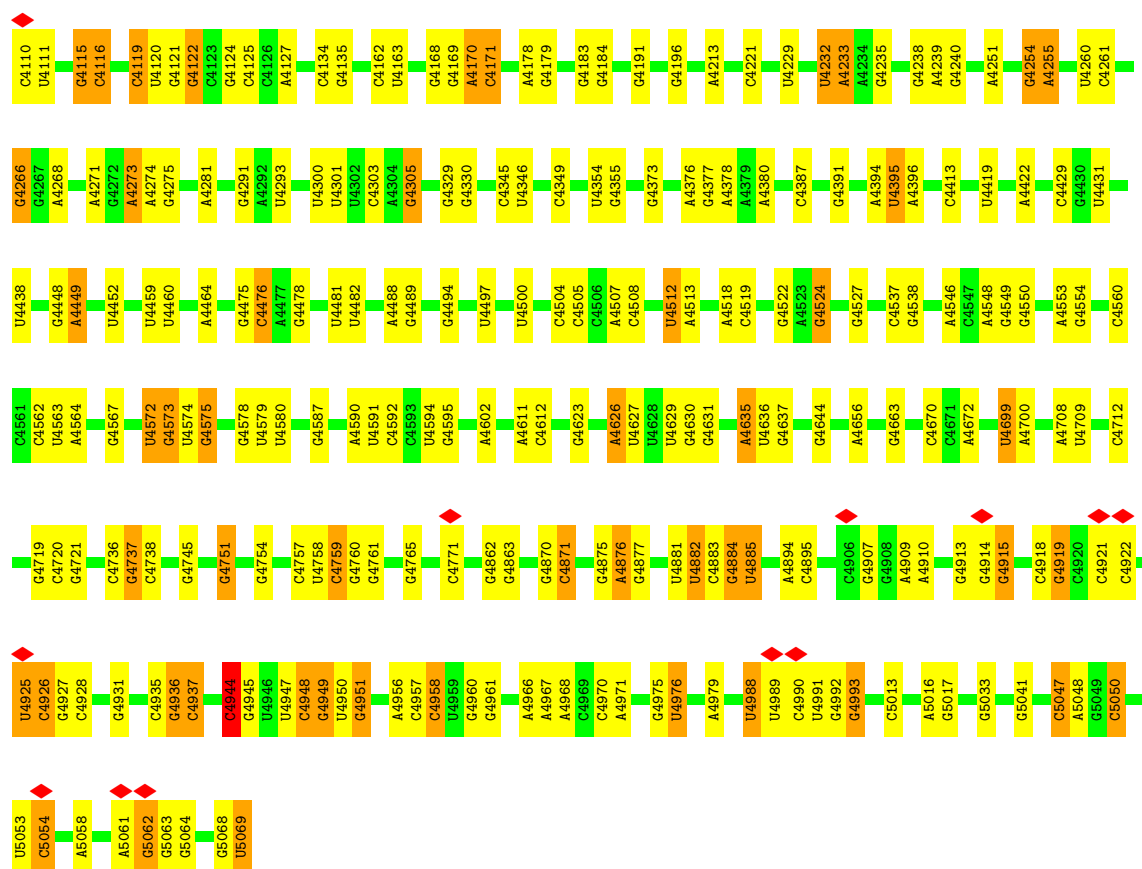
3 Residue-property plots

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

• Molecule 1: 28S ribosomal RNA

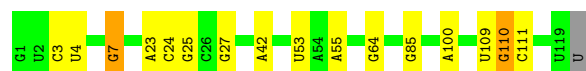






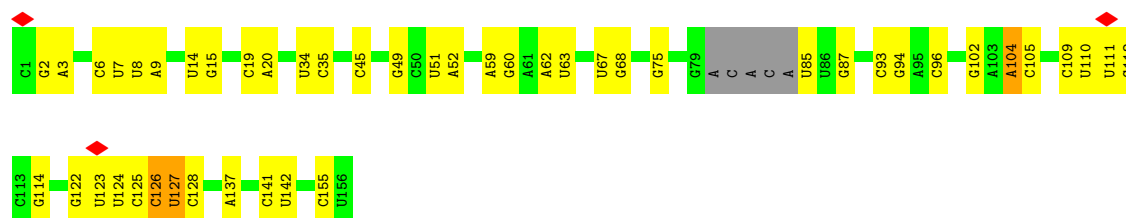
- Molecule 2: 5S ribosomal RNA

Chain 7: 86% 12% ..



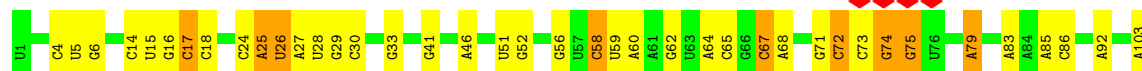
- Molecule 3: 5.8S ribosomal RNA

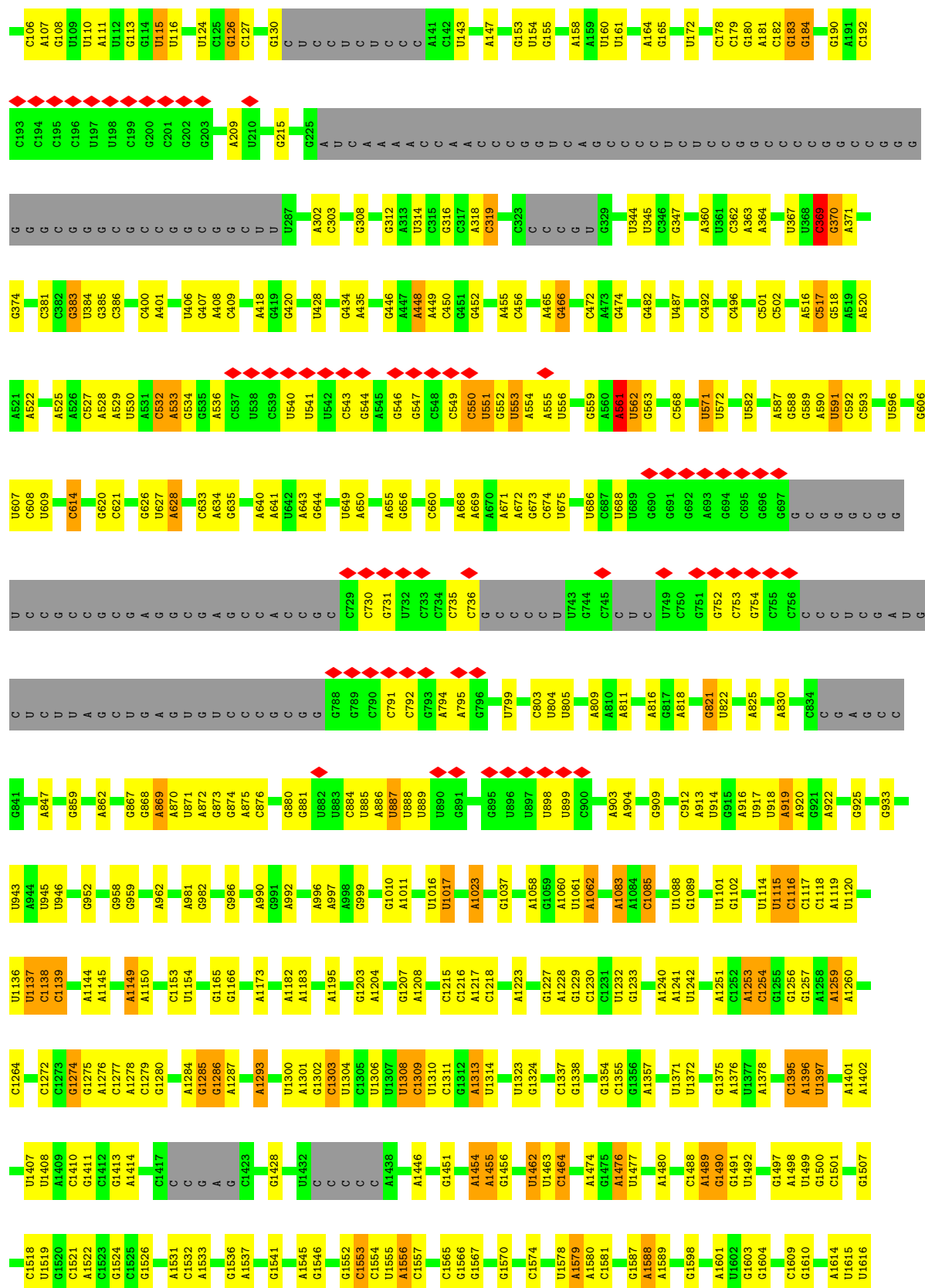
Chain 8: 67% 28% ..

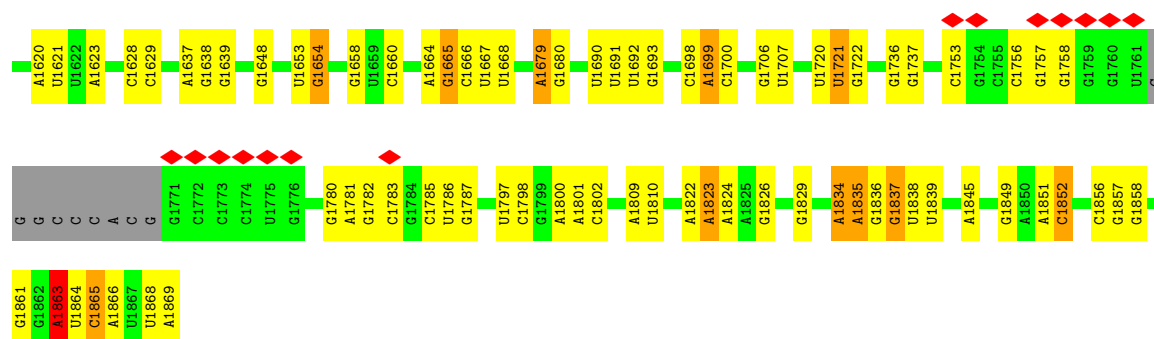


- Molecule 4: 18S ribosomal RNA

Chain 9: 62% 24% 9%







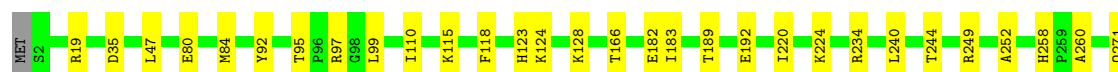
• Molecule 5: Ribosomal protein L8

Chain A: 91% 6% .



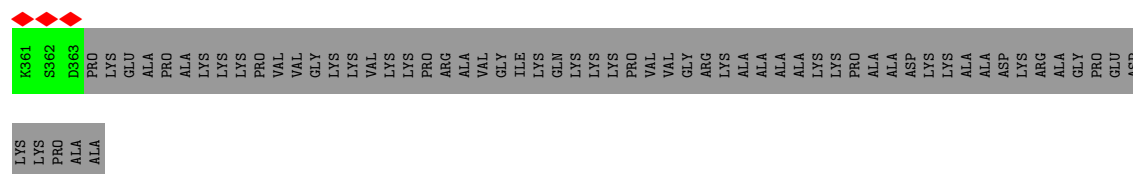
• Molecule 6: Ribosomal protein L3

Chain B: 89% 9% .



• Molecule 7: 60S ribosomal protein L4

Chain C: 79% 7% 15%



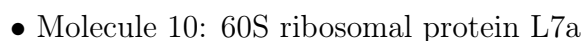
• Molecule 8: Large ribosomal subunit protein uL18

Chain D: 94% . .

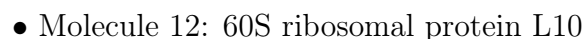
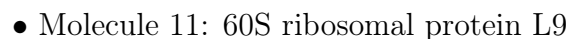


• Molecule 9: 60S ribosomal protein L6

26%



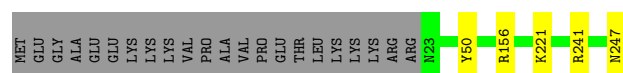
27%



8%



Chain K:  89% 9%



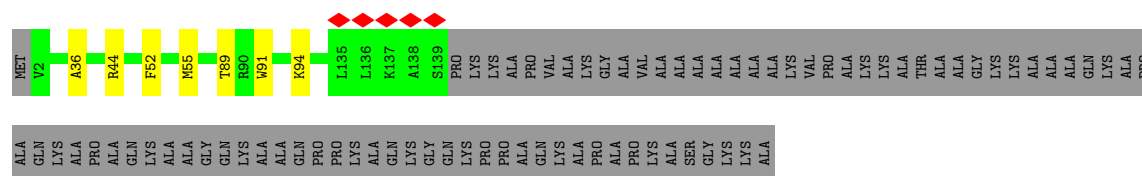
- Molecule 15: 60S ribosomal protein L13

Chain L:  93% 7%



- Molecule 16: 60S ribosomal protein L14

Chain M:  60% 37%

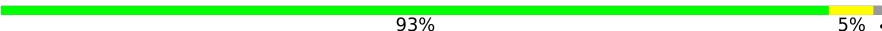


- Molecule 17: Ribosomal protein L15

Chain N:  90% 9%



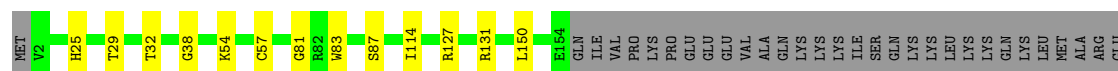
- Molecule 18: Large ribosomal subunit protein uL13

Chain O:  93% 5%



- Molecule 19: Large ribosomal subunit protein uL22

Chain P:  76% 7% 17%

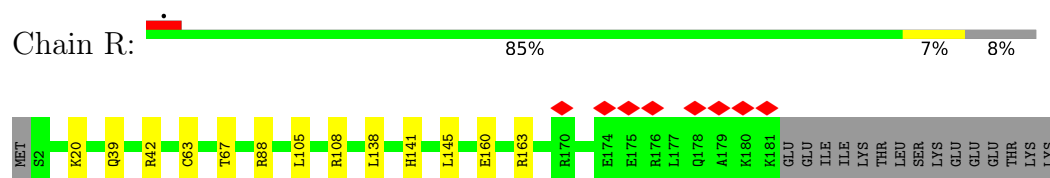


- Molecule 20: Ribosomal protein L18

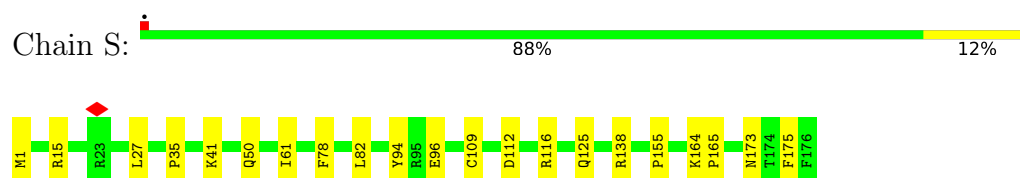
Chain Q:  93% 6%



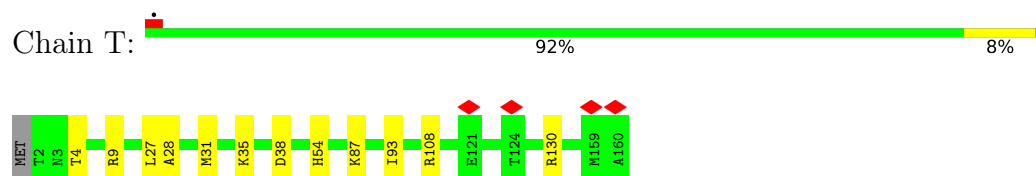
• Molecule 21: Ribosomal protein L19



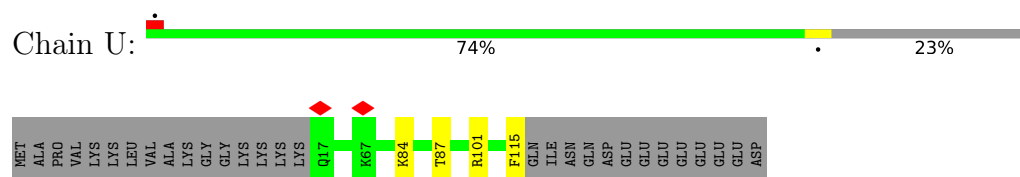
• Molecule 22: 60S ribosomal protein L18a



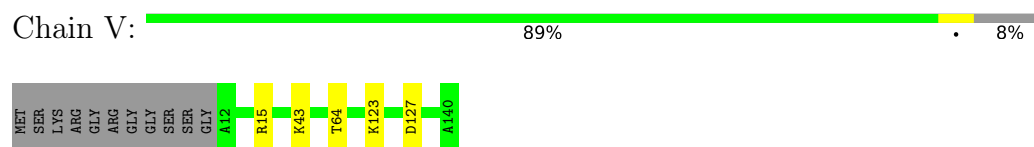
• Molecule 23: eL21



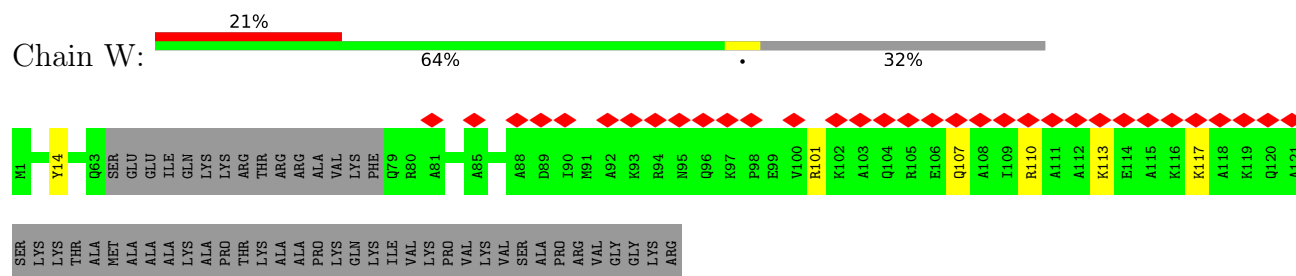
• Molecule 24: eL22



• Molecule 25: Ribosomal protein L23

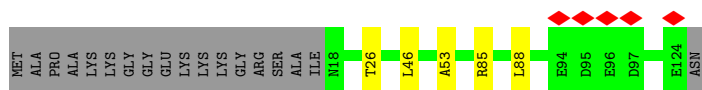


• Molecule 26: eL24



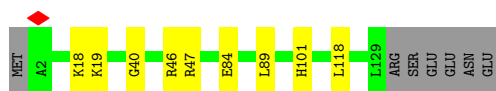
• Molecule 27: eL23





- Molecule 34: Ribosomal protein L32

Chain e: 88% 7% 5%



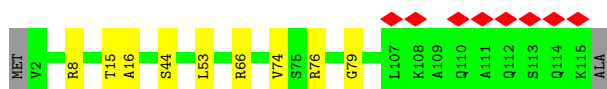
- Molecule 35: eL33

Chain f: 96% ..



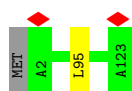
- Molecule 36: Large ribosomal subunit protein eL34

Chain g: 7% 91% 8% .



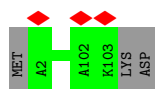
- Molecule 37: eL35

Chain h: 98% ..



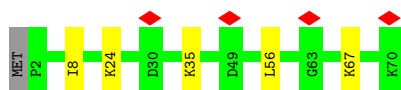
- Molecule 38: 60S ribosomal protein L36

Chain i: 97% .



- Molecule 39: eL38

Chain k: 6% 91% 7% .

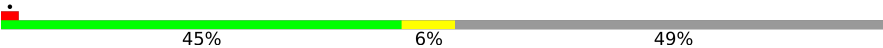


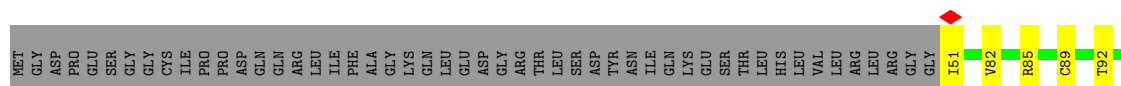
- Molecule 40: eL39

Chain l:  80% 18% .

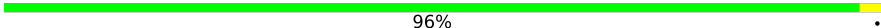


- Molecule 41: Ubiquitin-ribosomal protein eL40 fusion protein

Chain m:  45% 6% 49%



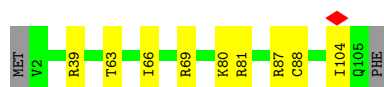
- Molecule 42: eL41

Chain n:  96% .



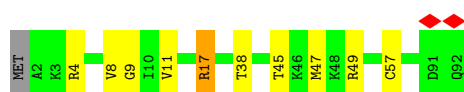
- Molecule 43: Large ribosomal subunit protein eL42

Chain o:  90% 8% .



- Molecule 44: eL43

Chain p:  88% 10% ..



- Molecule 45: eL28

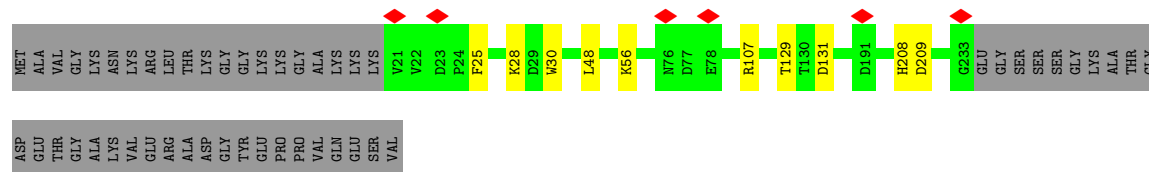
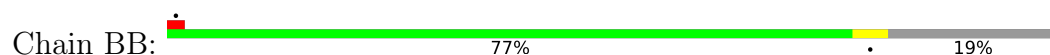
Chain r:  84% 7% 9%



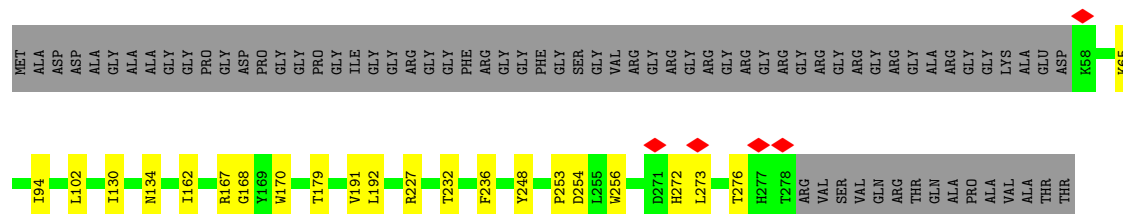
- Molecule 46: uS2 (SA)

Chain AA:  66% 8% 26%

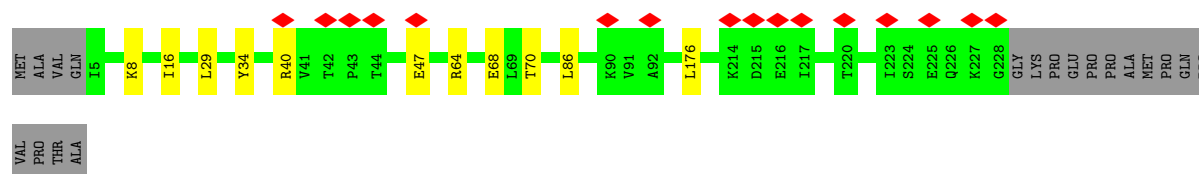
- Molecule 47: 40S ribosomal protein S3a



- Molecule 48: Small ribosomal subunit protein uS5



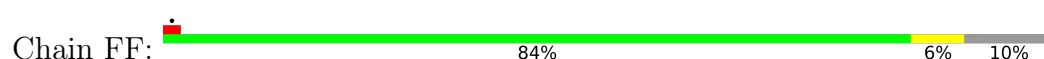
- Molecule 49: Ribosomal protein S3



- Molecule 50: eS4 (S4 X isoform)



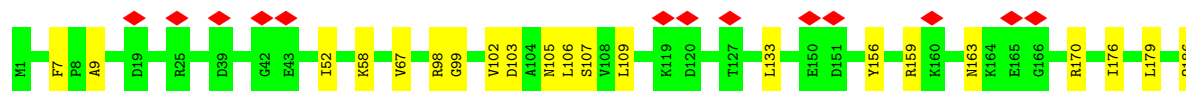
- Molecule 51: Ribosomal protein S5





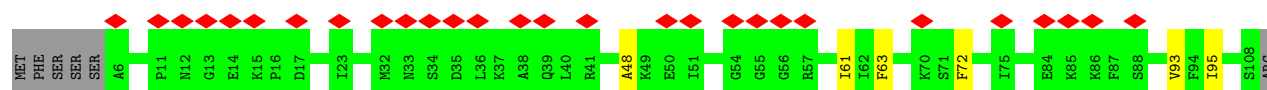
- Molecule 52: 40S ribosomal protein S6

Chain GG: 12% 84% 11% 5%



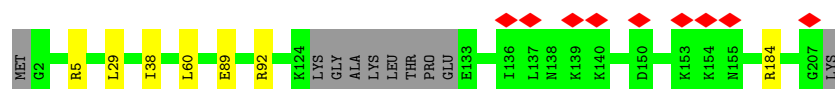
- Molecule 53: 40S ribosomal protein S7

Chain HH: 18% 88% 8% 5%



- Molecule 54: 40S ribosomal protein S8

Chain II: 92% 5% 5%



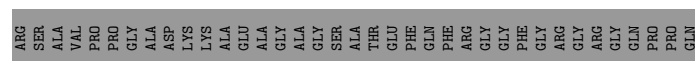
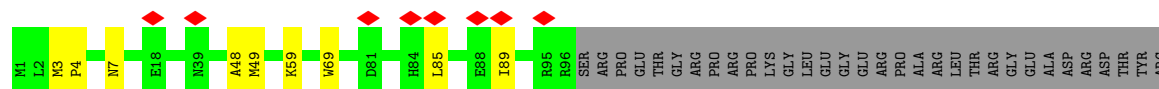
- Molecule 55: Ribosomal protein S9 (Predicted)

Chain JJ: 5% 87% 7% 7%



- Molecule 56: Small ribosomal subunit protein eS10

Chain KK: 5% 53% 5% 42%



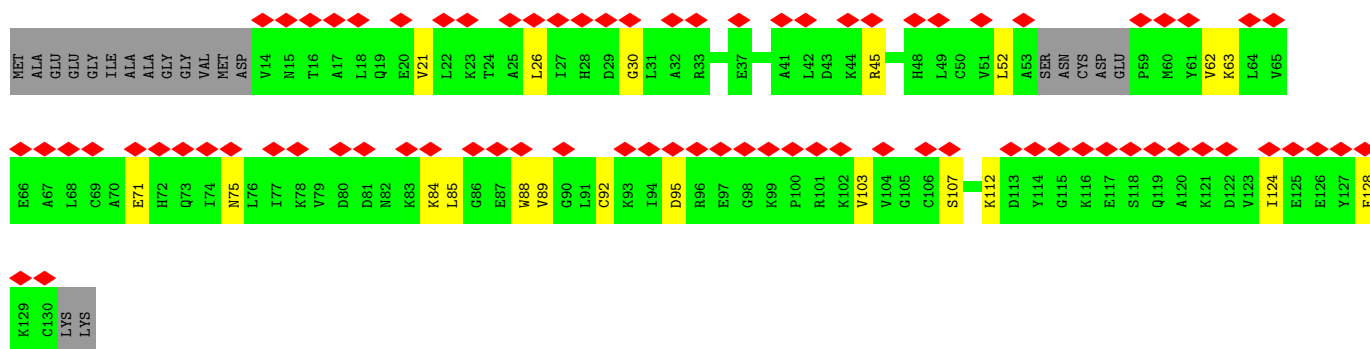
- Molecule 57: Ribosomal protein S11

Chain LL:  87% 9%

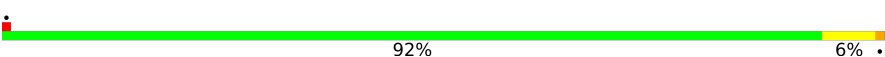


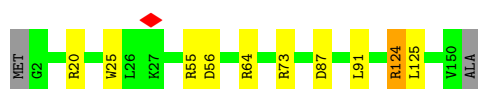
- Molecule 58: 40S ribosomal protein S12

Chain MM:  60% 70% 15% 15%



- Molecule 59: Ribosomal protein S13

Chain NN:  92% 6% ..



- Molecule 60: Small ribosomal subunit protein uS11

Chain OO:  75% 5% 19%

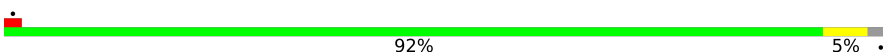


- Molecule 61: uS19

Chain PP:  8% 81% 8% 11%

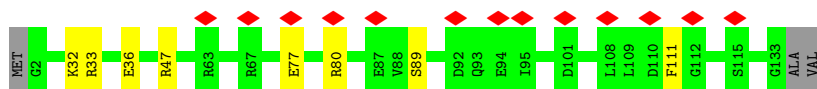


- Molecule 62: uS9

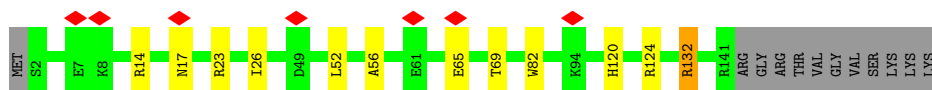
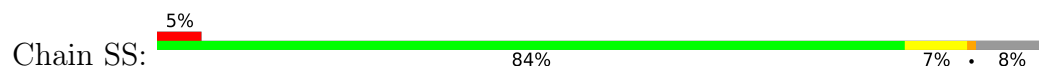
Chain QQ:  92% 5% .



• Molecule 63: eS17



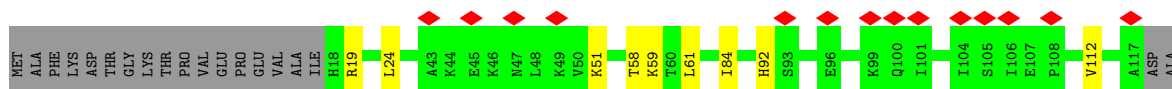
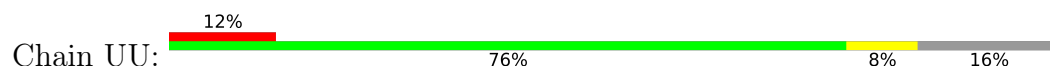
• Molecule 64: uS13



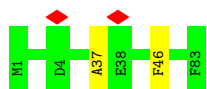
• Molecule 65: eS19



• Molecule 66: uS10



• Molecule 67: eS21

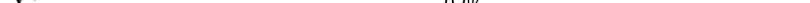


• Molecule 68: Ribosomal protein S15a

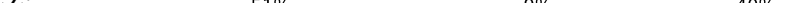


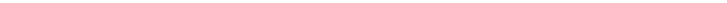
• Molecule 69: uS12

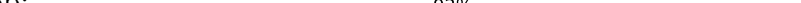
MET
G2
R5
G6
L7
L36
I50
K60
N63
K68
C69
L91
N92
F93
N97
D114
I115
R140
P141
ARG
SER

- Chain YY:  8% 93% 5%

MET ASP ASN ASP T4 R8 L17 L25 H29 K37 A45 K49 G59 D80 G95 K99 K100 G126 A127 GLY LYS LYS

- Chain ZZ: 

- Chain aa: 

- Chain bb: 

Category	Count
MET	1
P2	1
R23	1
S27	1
K36	1
C37	1
P38	1
G39	1
C40	1
Y41	1
F47	1
S48	1
H49	1
C59	1
S60	1
R72	1
K82	1
Q83	1
H84	1

- Chain cc:  86% 10%

Amino Acid	Relative Abundance (%)
MET	100
ASP	100
THR	100
SER	100
ARG	100
VAL	100
Q7	~85
T38	~75
R44	~55
D54	~45
E60	~35
L68	~85

- Chain dd:

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9969	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 ($e^-/\text{\AA}^2$)	29.7531	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	0.095	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	466.80002, 466.80002, 466.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.167, 1.167, 1.167	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.46	0/86380	0.67	15/134721 (0.0%)
2	7	0.45	0/2836	0.61	0/4421
3	8	0.45	0/3581	0.63	0/5577
4	9	0.41	0/40509	0.66	6/63128 (0.0%)
5	A	0.37	0/1936	0.52	0/2596
6	B	0.34	0/3240	0.51	0/4339
7	C	0.35	0/2937	0.51	0/3946
8	D	0.30	0/2437	0.47	0/3264
9	E	0.31	0/1762	0.53	0/2362
10	G	0.30	0/1910	0.55	0/2569
11	H	0.31	0/1535	0.48	0/2063
12	I	0.32	0/1702	0.49	0/2272
13	J	0.28	0/1385	0.46	0/1852
14	K	0.36	0/1911	0.52	0/2549
15	L	0.31	0/1733	0.51	0/2316
16	M	0.33	0/1158	0.49	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	0.37	0/1268	0.54	0/1700
20	Q	0.38	0/1539	0.55	0/2054
21	R	0.33	0/1524	0.51	0/2013
22	S	0.36	0/1501	0.50	0/2012
23	T	0.33	0/1326	0.48	0/1770
24	U	0.27	0/823	0.50	0/1104
25	V	0.35	0/983	0.50	0/1319
26	W	0.28	0/873	0.52	0/1158
27	X	0.32	0/984	0.49	0/1323
28	Y	0.32	0/1132	0.47	0/1504
29	Z	0.33	0/1130	0.48	0/1507
30	a	0.38	0/1191	0.55	0/1590
31	b	0.30	0/819	0.55	0/1081
32	c	0.34	0/771	0.45	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.36	0/903	0.52	0/1216
34	e	0.37	0/1071	0.58	0/1429
35	f	0.38	0/895	0.49	0/1198
36	g	0.36	0/916	0.56	0/1220
37	h	0.32	0/1021	0.51	0/1348
38	i	0.29	0/841	0.56	0/1112
39	k	0.28	0/575	0.48	0/761
40	l	0.36	0/459	0.52	0/608
41	m	0.31	0/435	0.44	0/575
42	n	0.39	0/241	0.54	0/305
43	o	0.33	0/864	0.49	0/1140
44	p	0.35	0/718	0.59	0/953
45	r	0.36	0/1010	0.51	0/1354
46	AA	0.29	0/1747	0.50	0/2374
47	BB	0.29	0/1756	0.49	0/2350
48	CC	0.31	0/1753	0.51	0/2369
49	DD	0.26	0/1767	0.46	0/2378
50	EE	0.25	0/2118	0.47	0/2849
51	FF	0.26	0/1481	0.51	0/1991
52	GG	0.22	0/1946	0.50	0/2590
53	HH	0.24	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	0.25	0/834	0.47	0/1125
57	LL	0.31	0/1195	0.51	0/1597
58	MM	0.18	0/880	0.50	0/1179
59	NN	0.31	0/1226	0.52	0/1649
60	OO	0.33	0/1029	0.53	0/1380
61	PP	0.23	0/1079	0.50	0/1441
62	QQ	0.28	0/1146	0.48	0/1534
63	RR	0.26	0/1082	0.54	0/1452
64	SS	0.26	0/1175	0.52	0/1575
65	TT	0.25	0/1115	0.50	0/1493
66	UU	0.25	0/805	0.45	0/1081
67	VV	0.29	0/644	0.44	0/860
68	WW	0.34	0/1051	0.47	0/1406
69	XX	0.30	0/1105	0.48	0/1476
70	YY	0.21	0/1028	0.48	0/1366
71	ZZ	0.24	0/604	0.46	0/810
72	aa	0.33	0/828	0.53	0/1109
73	bb	0.28	0/665	0.47	0/891
74	cc	0.25	0/490	0.40	0/656
75	dd	0.30	0/470	0.57	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
76	ee	0.22	0/462	0.53	0/607
77	ff	0.17	0/567	0.46	0/753
78	gg	0.22	0/2493	0.48	0/3394
79	10	0.39	0/261	0.59	0/404
80	12	0.29	0/1787	0.67	0/2783
81	11	0.26	0/1773	0.65	0/2763
81	13	0.32	0/1773	0.64	0/2763
82	j	0.37	0/720	0.58	0/952
83	jj	0.19	0/4047	0.45	0/5462
All	All	0.39	0/235774	0.61	22/346229 (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	2
8	D	0	2
9	E	0	1
11	H	0	1
12	I	0	1
20	Q	0	2
23	T	0	1
25	V	0	1
28	Y	0	1
29	Z	0	2
36	g	0	1
43	o	0	1
44	p	0	2
54	II	0	1
55	JJ	0	1
59	NN	0	1
60	OO	0	1
61	PP	0	1
64	SS	0	1
72	aa	0	1
77	ff	0	1
All	All	0	27

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9	1835	A	C2'-C3'-O3'	6.75	119.63	109.50
4	9	369	C	C2'-C3'-O3'	6.72	119.58	109.50
1	5	4170	A	C4'-C3'-O3'	6.36	118.93	109.40
1	5	1440	U	C2'-C3'-O3'	6.27	118.90	109.50
4	9	1863	A	C1'-O4'-C4'	-5.91	103.79	109.70
1	5	4944	C	C1'-O4'-C4'	-5.89	104.01	109.90
1	5	4119	C	C2'-C3'-O3'	5.75	118.12	109.50
18	O	110	PRO	N-CA-C	5.56	117.48	110.70
4	9	532	C	C2'-C3'-O3'	5.48	121.92	113.70
1	5	2711	G	C5'-C4'-O4'	5.42	117.23	109.10
1	5	3888	G	C2'-C3'-O3'	5.36	121.74	113.70
1	5	3876	A	C4'-C3'-O3'	5.34	117.40	109.40
1	5	2711	G	C1'-O4'-C4'	-5.32	104.38	109.70
1	5	2313	A	C2'-C3'-O3'	5.29	117.44	109.50
1	5	4170	A	C2'-C3'-O3'	5.27	117.40	109.50
1	5	4048	A	C2'-C3'-O3'	5.15	117.22	109.50
1	5	1891	A	N9-C1'-C2'	5.14	119.71	112.00
1	5	406	C	C2'-C3'-O3'	5.12	121.38	113.70
1	5	1590	C	OP1-P-O3'	-5.10	92.71	108.00
4	9	561	A	C2'-C3'-O3'	5.08	121.31	113.70
4	9	532	C	C5'-C4'-O4'	5.04	117.36	109.80
1	5	1358	G	C2'-C3'-O3'	5.02	117.03	109.50

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	5	2544	G	Sidechain
5	A	123	ARG	Sidechain
5	A	242	ARG	Sidechain
8	D	24	ARG	Sidechain
8	D	33	ARG	Sidechain
9	E	144	ARG	Sidechain
11	H	173	ARG	Sidechain
12	I	3	ARG	Sidechain
54	II	5	ARG	Sidechain
55	JJ	38	ARG	Sidechain
59	NN	124	ARG	Sidechain
60	OO	137	SER	Peptide
61	PP	13	ARG	Sidechain
20	Q	108	ARG	Sidechain

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Mol	Chain	Res	Type	Group
20	Q	181	ARG	Sidechain
64	SS	132	ARG	Sidechain
23	T	130	ARG	Sidechain
25	V	15	ARG	Sidechain
28	Y	115	ARG	Sidechain
29	Z	21	ARG	Sidechain
29	Z	65	ARG	Sidechain
72	aa	87	ARG	Sidechain
77	ff	95	ARG	Sidechain
36	g	8	ARG	Sidechain
43	o	39	ARG	Sidechain
44	p	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	536	0
2	7	2538	0	1286	9	0
3	8	3208	0	1629	21	0
4	9	36229	0	18300	279	0
5	A	1898	0	1993	9	0
6	B	3172	0	3310	26	0
7	C	2883	0	3053	21	0
8	D	2391	0	2424	8	0
9	E	1729	0	1887	16	0
10	G	1879	0	2027	10	0
11	H	1516	0	1597	4	0
12	I	1664	0	1712	7	0
13	J	1362	0	1399	10	0
14	K	1875	0	1995	4	0
15	L	1702	0	1820	12	0
16	M	1137	0	1211	5	0
17	N	1701	0	1749	20	0
18	O	1630	0	1778	7	0
19	P	1242	0	1274	11	0
20	Q	1515	0	1634	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	R	1508	0	1664	9	0
22	S	1462	0	1508	11	0
23	T	1298	0	1366	13	0
24	U	809	0	833	2	0
25	V	969	0	1031	3	0
26	W	860	0	903	4	0
27	X	967	0	1040	3	0
28	Y	1115	0	1205	3	0
29	Z	1107	0	1182	7	0
30	a	1162	0	1209	7	0
31	b	806	0	866	1	0
32	c	761	0	794	2	0
33	d	888	0	930	3	0
34	e	1053	0	1147	7	0
35	f	876	0	912	3	0
36	g	906	0	998	6	0
37	h	1013	0	1147	1	0
38	i	830	0	916	0	0
39	k	569	0	637	3	0
40	l	447	0	480	9	0
41	m	429	0	465	5	0
42	n	240	0	289	1	0
43	o	851	0	921	5	0
44	p	708	0	756	7	0
45	r	994	0	1051	7	0
46	AA	1710	0	1708	14	0
47	BB	1729	0	1803	6	0
48	CC	1716	0	1806	13	0
49	DD	1739	0	1832	7	0
50	EE	2076	0	2177	12	0
51	FF	1460	0	1509	12	0
52	GG	1923	0	2089	20	0
53	HH	1489	0	1582	9	0
54	II	1628	0	1706	5	0
55	JJ	1508	0	1626	13	0
56	KK	810	0	836	5	0
57	LL	1175	0	1249	5	0
58	MM	871	0	913	12	0
59	NN	1202	0	1289	10	0
60	OO	1016	0	1039	7	0
61	PP	1058	0	1104	7	0
62	QQ	1128	0	1195	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	RR	1068	0	1121	6	0
64	SS	1157	0	1213	11	0
65	TT	1097	0	1132	8	0
66	UU	795	0	862	7	0
67	VV	637	0	637	1	0
68	WW	1034	0	1080	7	0
69	XX	1087	0	1154	10	0
70	YY	1011	0	1083	3	0
71	ZZ	598	0	656	7	0
72	aa	814	0	867	8	0
73	bb	651	0	672	5	0
74	cc	488	0	514	2	0
75	dd	459	0	448	3	0
76	ee	457	0	502	3	0
77	ff	555	0	567	7	0
78	gg	2436	0	2393	21	0
79	10	234	0	118	2	0
80	12	1599	0	808	26	0
81	11	1585	0	804	17	0
81	13	1585	0	803	17	0
82	j	705	0	737	14	0
83	jj	3982	0	4069	19	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
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	0	0
88	13	31	0	11	1	0
89	13	8	0	8	0	0
90	jj	1	0	0	0	0
91	jj	28	0	12	2	0
92	jj	1	0	0	0	0
All	All	219551	0	163124	1275	0

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

All (1275) 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	2.13	0.96
7:C:61:GLN:OE1	82:j:55:ARG:NH2	2.10	0.84
4:9:568:C:N4	4:9:582:U:O2	2.13	0.81
4:9:1303:C:H2'	4:9:1304:U:C6	2.15	0.80
1:5:4626:A:OP2	6:B:224:LYS:NZ	2.14	0.80
74:cc:44:ARG:NH2	74:cc:60:GLU:O	2.15	0.79
1:5:4076:G:OP1	10:G:126:ARG:NH1	2.14	0.77
4:9:190:G:O2'	4:9:209:A:N6	2.18	0.77
4:9:1272:C:O2'	4:9:1274:G:N2	2.18	0.76
4:9:1308:U:H2'	4:9:1309:C:C6	2.21	0.75
1:5:2583:C:OP2	36:g:76:ARG:NH1	2.20	0.74
1:5:2758:G:O2'	1:5:2765:A:N3	2.19	0.74
4:9:448:A:N6	54:II:29:LEU:HD13	2.03	0.73
63:RR:33:ARG:NH1	78:gg:107:ASP:OD2	2.22	0.73
80:12:63:C:H2'	80:12:64:A:H8	1.54	0.72
1:5:107:G:OP1	15:L:42:ARG:NH1	2.22	0.72
1:5:2469:C:N4	1:5:2471:G:O6	2.18	0.72
7:C:14:LYS:NZ	7:C:16:GLU:OE1	2.22	0.71
1:5:3717:A:H2'	1:5:3718:A:C8	2.25	0.71
4:9:1228:A:H2'	4:9:1229:G:C8	2.26	0.71
1:5:4862:G:H2'	1:5:4863:G:C8	2.25	0.71
8:D:107:ARG:NH2	8:D:116:ASP:OD1	2.23	0.70
4:9:1834:A:H2	4:9:1837:G:H1	1.38	0.70
1:5:4635:A:H8	1:5:5048:A:H61	1.39	0.70
1:5:4751:G:H1	1:5:4948:C:H5	1.40	0.70
4:9:981:A:H2'	4:9:982:G:C8	2.27	0.70
1:5:978:G:H22	1:5:1277:G:H1	1.40	0.69
1:5:4635:A:H2	1:5:4663:G:H21	1.38	0.69
80:12:65:G:H2'	80:12:66:A:H8	1.57	0.69
57:LL:35:ARG:NH2	57:LL:55:TYR:O	2.26	0.68
1:5:2489:C:O2'	1:5:2491:C:N4	2.26	0.68
83:jj:512:MET:SD	83:jj:560:ARG:NH2	2.65	0.68
3:8:8:U:H2'	3:8:9:A:C8	2.29	0.68
4:9:303:C:O2	54:II:184:ARG:NH2	2.26	0.68
80:12:61:C:H2'	80:12:62:A:H8	1.59	0.68
1:5:1198:G:H2'	1:5:1199:G:H8	1.58	0.68
1:5:1198:G:H2'	1:5:1199:G:C8	2.30	0.67
29:Z:88:ASP:OD1	29:Z:121:ARG:NH2	2.25	0.67
1:5:3692:A:H62	1:5:3823:G:H21	1.42	0.67
3:8:8:U:H2'	3:8:9:A:H8	1.59	0.67
4:9:1541:G:N3	65:TT:12:GLN:NE2	2.42	0.67
80:12:4:G:H2'	80:12:5:A:H8	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1188:C:H2'	1:5:1189:G:H8	1.60	0.66
1:5:2477:A:H2'	1:5:2478:C:C6	2.30	0.66
1:5:4084:G:O6	5:A:72:ARG:NH2	2.25	0.66
72:aa:87:ARG:NH2	72:aa:94:ASP:O	2.23	0.66
1:5:978:G:N2	1:5:1277:G:H1	1.93	0.66
1:5:2601:A:N6	1:5:2744:A:OP2	2.29	0.66
27:X:148:ASP:OD1	27:X:152:LYS:NZ	2.26	0.66
4:9:1598:G:OP1	71:ZZ:80:ARG:NH1	2.27	0.66
49:DD:64:ARG:NH1	49:DD:68:GLU:OE2	2.29	0.66
4:9:448:A:H61	54:II:29:LEU:HD13	1.60	0.66
83:jj:520:GLN:NE2	83:jj:547:THR:OG1	2.29	0.66
1:5:910:G:H2'	1:5:911:U:H6	1.62	0.65
1:5:407:A:O2'	1:5:410:A:OP1	2.12	0.65
1:5:4303:C:H2'	1:5:4305:G:C8	2.32	0.65
47:BB:107:ARG:NH1	60:OO:133:THR:O	2.21	0.65
60:OO:95:ILE:HB	60:OO:129:ILE:HG23	1.78	0.65
4:9:1664:A:O2'	4:9:1666:C:N4	2.26	0.64
1:5:2262:G:OP2	45:r:98:ARG:NH2	2.29	0.64
1:5:2503:G:H5''	1:5:2503:G:H8	1.61	0.64
52:GG:58:LYS:HA	52:GG:107:SER:HB2	1.79	0.64
58:MM:63:LYS:HB3	77:ff:108:VAL:HG21	1.80	0.64
81:11:23:C:H2'	81:11:24:G:H8	1.61	0.64
4:9:318:A:H61	52:GG:186:GLN:HE22	1.44	0.64
1:5:1075:G:H1	1:5:1235:G:N2	1.96	0.64
81:11:23:C:H2'	81:11:24:G:C8	2.33	0.64
1:5:2395:A:O2'	1:5:2806:A:H1'	1.97	0.64
81:11:69:U:H2'	81:11:70:G:H8	1.63	0.64
62:QQ:146:ARG:NH2	81:13:33:C:OP2	2.31	0.63
80:12:43:G:H2'	80:12:44:A:H8	1.63	0.63
1:5:1836:G:O2'	23:T:108:ARG:NH1	2.32	0.63
57:LL:42:LEU:HD13	57:LL:72:ILE:HD11	1.81	0.63
80:12:23:A:H2'	80:12:24:G:C8	2.34	0.63
1:5:978:G:N2	1:5:1277:G:H22	1.97	0.63
10:G:139:VAL:HG11	10:G:238:LYS:HG3	1.80	0.63
1:5:1391:A:P	20:Q:181:ARG:HH22	2.22	0.63
1:5:1370:G:O6	7:C:239:LYS:NZ	2.26	0.62
1:5:4925:U:H4'	1:5:4926:C:C5'	2.29	0.62
4:9:367:U:H4'	4:9:371:A:C8	2.33	0.62
4:9:1488:C:O2'	4:9:1490:G:OP2	2.15	0.62
1:5:2478:C:H2'	1:5:2479:G:C8	2.34	0.62
7:C:110:ARG:O	7:C:113:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:j:20:ARG:NH2	82:j:39:TYR:OH	2.31	0.62
1:5:4925:U:H4'	1:5:4926:C:H5'	1.80	0.62
49:DD:70:THR:HG22	49:DD:86:LEU:HD13	1.82	0.62
59:NN:20:ARG:HH21	68:WW:56:HIS:CG	2.18	0.62
79:10:23:A:C8	79:10:23:A:H5''	2.34	0.62
1:5:935(A):G:OP2	16:M:44:ARG:NH1	2.32	0.62
1:5:2457:G:H21	1:5:3672:G:H21	1.47	0.62
8:D:202:GLN:NE2	8:D:237:GLU:OE1	2.30	0.62
68:WW:86:LEU:HG	68:WW:90:GLN:HE21	1.65	0.62
1:5:4039:G:N7	1:5:4041:C:N4	2.48	0.61
1:5:2407:G:O6	40:l:2:SER:N	2.33	0.61
63:RR:36:GLU:OE1	63:RR:47:ARG:NH1	2.30	0.61
1:5:173:C:OP1	15:L:129:ARG:NH1	2.27	0.61
1:5:1444:G:H21	1:5:2110:G:H1	1.48	0.61
1:5:1756:U:H2'	1:5:1757:U:C6	2.35	0.61
4:9:1480:A:O2'	75:dd:56:ASP:OD1	2.15	0.61
4:9:1565:C:OP2	65:TT:101:ARG:NH1	2.34	0.61
4:9:562:U:OP1	55:JJ:134:HIS:NE2	2.29	0.61
4:9:686:U:O2	53:HH:118:ARG:NH2	2.32	0.61
1:5:976:G:H1	1:5:1279:A:H2	1.46	0.61
1:5:2493:G:O2'	3:8:127:U:OP1	2.14	0.61
1:5:3932:U:H2'	1:5:3933:G:H8	1.66	0.61
4:9:369:C:O2'	4:9:370:G:OP1	2.18	0.61
78:gg:107:ASP:OD2	78:gg:125:ARG:NH1	2.34	0.61
1:5:4992:G:H2'	1:5:4993:G:C8	2.35	0.61
4:9:1616:U:H3	4:9:1620:A:H2	1.48	0.61
80:12:61:C:H2'	80:12:62:A:C8	2.35	0.61
1:5:910:G:H2'	1:5:911:U:C6	2.36	0.60
1:5:4572:U:H2'	1:5:4573:G:C8	2.36	0.60
4:9:546:G:H2'	4:9:547:G:C8	2.36	0.60
30:a:84:GLU:OE1	30:a:87:ARG:NH2	2.32	0.60
1:5:456:C:H2'	1:5:457:G:H8	1.66	0.60
1:5:2478:C:H2'	1:5:2479:G:H8	1.65	0.60
4:9:816:A:OP2	55:JJ:10:ARG:NH2	2.31	0.60
4:9:1834:A:H2	4:9:1837:G:N1	1.98	0.60
4:9:1395:C:O2'	4:9:1396:A:OP1	2.17	0.60
3:8:75:G:OP2	28:Y:74:TYR:OH	2.16	0.60
1:5:271:C:H2'	1:5:272:U:C6	2.36	0.60
81:11:25:U:H2'	81:11:26:G:H8	1.67	0.60
1:5:1317:U:OP1	30:a:21:ARG:NH2	2.34	0.60
7:C:335:MET:O	7:C:339:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:12:63:C:H2'	80:12:64:A:C8	2.34	0.60
9:E:191:ARG:NH1	9:E:217:ASP:OD1	2.34	0.60
1:5:3751:G:H21	1:5:3775:A:H8	1.50	0.59
4:9:455:A:H2'	4:9:456:C:C6	2.37	0.59
1:5:2313:A:O2'	1:5:2314:G:OP1	2.15	0.59
1:5:3910:C:H2'	1:5:3911:C:C6	2.38	0.59
4:9:562:U:H2'	4:9:563:G:C8	2.38	0.59
1:5:1617:G:H1'	1:5:2513:A:N6	2.18	0.59
1:5:2503:G:H5''	1:5:2503:G:C8	2.38	0.59
1:5:2546:G:O2'	1:5:2547:G:OP1	2.20	0.59
4:9:1139:C:H5	4:9:1149:A:H62	1.51	0.59
4:9:962:A:H5''	60:OO:66:ARG:HD3	1.85	0.59
4:9:730:C:H2'	4:9:731:G:C8	2.37	0.59
9:E:115:MET:O	45:r:87:ARG:NH1	2.32	0.59
1:5:2566:G:H2'	1:5:2567:G:H8	1.68	0.59
4:9:64:A:H2	4:9:83:A:H62	1.50	0.59
80:12:43:G:H2'	80:12:44:A:C8	2.38	0.59
80:12:66:A:H2'	80:12:67:A:C8	2.38	0.59
1:5:956:A:N6	1:5:1283:G:O2'	2.34	0.59
1:5:1922:G:H2'	1:5:1923:A:H5'	1.85	0.59
1:5:490:C:H2'	1:5:491:G:C8	2.38	0.58
69:XX:93:PHE:O	69:XX:140:ARG:NH1	2.36	0.58
4:9:1303:C:H2'	4:9:1304:U:H6	1.64	0.58
1:5:1405:C:H2'	1:5:1406:G:H8	1.67	0.58
4:9:536:A:H61	4:9:547:G:H1	1.51	0.58
9:E:139:HIS:O	9:E:141:ARG:NH1	2.36	0.58
1:5:4580:U:O2'	6:B:182:GLU:OE2	2.20	0.58
4:9:804:U:H2'	4:9:805:U:C6	2.39	0.58
1:5:4053:A:H2'	1:5:4054:C:C6	2.38	0.58
4:9:1667:U:H2'	4:9:1668:U:C6	2.38	0.58
1:5:4935:C:H2'	1:5:4936:G:C8	2.38	0.58
57:LL:101:ARG:NH1	69:XX:5:ARG:O	2.37	0.58
1:5:976:G:H21	7:C:323:ARG:HE	1.50	0.58
1:5:1339:U:H2'	1:5:1340:C:C6	2.39	0.58
1:5:1405:C:H2'	1:5:1406:G:C8	2.39	0.58
18:O:10:ASP:OD1	18:O:37:ARG:HD3	2.04	0.58
1:5:1771:U:H2'	1:5:1772:C:C6	2.39	0.58
1:5:3968:U:H2'	1:5:3969:G:C8	2.39	0.58
4:9:821:G:C6	55:JJ:150:ARG:HG3	2.39	0.58
4:9:1217:A:H2'	4:9:1218:C:C6	2.39	0.58
69:XX:63:ASN:HD22	69:XX:114:ASP:CG	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2755:A:P	29:Z:65:ARG:HH22	2.27	0.57
4:9:540:U:O2'	4:9:543:C:N4	2.38	0.57
80:12:50:U:H2'	80:12:51:G:H8	1.68	0.57
4:9:178:C:H2'	4:9:179:C:C6	2.39	0.57
1:5:3860:A:H61	1:5:4560:C:H5	1.50	0.57
1:5:4431:U:OP2	12:I:3:ARG:NH2	2.28	0.57
1:5:4935:C:H2'	1:5:4936:G:H8	1.69	0.57
40:l:23:ILE:HD11	40:l:28:TRP:HE1	1.70	0.57
80:12:50:U:H2'	80:12:51:G:C8	2.40	0.57
81:11:53:G:H2'	81:11:54:A:H8	1.70	0.57
3:8:102:G:OP2	3:8:104:A:O2'	2.23	0.57
49:DD:16:ILE:HD11	75:dd:36:LEU:HD23	1.87	0.57
62:QQ:102:GLU:OE2	78:gg:58:ALA:N	2.28	0.57
1:5:2570:U:H2'	1:5:2571:C:C6	2.40	0.57
1:5:32:G:H21	1:5:50:C:H5	1.52	0.57
1:5:424:U:H2'	1:5:425:U:C6	2.40	0.57
3:8:6:C:H2'	3:8:7:U:H6	1.69	0.57
1:5:3606:U:H2'	1:5:3607:U:C6	2.38	0.56
1:5:4737:G:H2'	1:5:4738:C:C6	2.40	0.56
4:9:656:G:O2'	48:CC:227:ARG:NH1	2.38	0.56
4:9:962:A:O3'	60:OO:66:ARG:NH1	2.39	0.56
17:N:178:HIS:HA	17:N:181:HIS:NE2	2.20	0.56
81:11:69:U:H2'	81:11:70:G:C8	2.39	0.56
4:9:945:U:H2'	4:9:946:U:C6	2.41	0.56
51:FF:39:ILE:HG23	51:FF:68:ILE:HG21	1.86	0.56
1:5:152:U:P	17:N:49:ARG:HH12	2.29	0.56
3:8:6:C:H2'	3:8:7:U:C6	2.41	0.56
3:8:94:G:OP2	82:j:72:ARG:NH1	2.38	0.56
4:9:5:U:H2'	4:9:6:G:H8	1.69	0.56
4:9:903:A:H2'	4:9:904:A:H8	1.71	0.56
1:5:2900:U:H2'	1:5:2901:G:C8	2.41	0.56
83:jj:173:LYS:NZ	91:jj:702:GDP:O3B	2.36	0.56
83:jj:504:THR:OG1	83:jj:531:CYS:HB3	2.05	0.56
1:5:87:A:OP2	20:Q:173:LYS:NZ	2.37	0.56
1:5:2280:G:N2	1:5:2281:U:O4	2.38	0.56
51:FF:39:ILE:HG23	51:FF:68:ILE:HD13	1.86	0.56
1:5:3911:C:H2'	1:5:3912:U:H6	1.70	0.55
1:5:4239:A:H2'	1:5:4240:G:C8	2.41	0.55
6:B:234:ARG:NH1	6:B:271:GLN:O	2.35	0.55
1:5:1378:C:N4	15:L:158:ARG:HH21	2.05	0.55
6:B:110:ILE:O	6:B:115:LYS:NZ	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:12:65:G:H2'	80:12:66:A:C8	2.40	0.55
83:jj:137:ARG:NH2	83:jj:139:GLU:OE2	2.32	0.55
1:5:2395:A:O2'	1:5:2806:A:N3	2.38	0.55
4:9:26:U:H2'	4:9:27:A:H8	1.72	0.55
5:A:137:ILE:HD11	5:A:149:LYS:HB2	1.89	0.55
80:12:4:G:H2'	80:12:5:A:C8	2.40	0.55
1:5:2664:G:H4'	1:5:2677:G:H4'	1.89	0.55
1:5:4108:G:H2'	1:5:4109:G:C8	2.42	0.55
73:bb:23:ARG:NH1	73:bb:27:SER:O	2.40	0.55
4:9:1253:A:H4'	4:9:1254:C:H5''	1.89	0.55
1:5:2639:U:O2'	1:5:2694:G:N1	2.27	0.55
4:9:1228:A:H2'	4:9:1229:G:H8	1.69	0.55
61:PP:44:ARG:NH1	61:PP:82:ASP:O	2.40	0.55
1:5:3641:U:H5	1:5:3646:A:N7	2.04	0.55
1:5:4035:G:H2'	1:5:4036:G:C8	2.42	0.55
3:8:127:U:H2'	3:8:128:C:C6	2.41	0.55
4:9:533:A:H2'	4:9:534:G:C8	2.42	0.55
4:9:886:A:H3'	4:9:887:U:H5''	1.88	0.55
4:9:903:A:H2'	4:9:904:A:C8	2.42	0.55
4:9:1693:G:H21	4:9:1834:A:H8	1.55	0.55
26:W:113:LYS:HG3	26:W:117:LYS:HD3	1.88	0.55
52:GG:67:VAL:HB	52:GG:99:GLY:HA2	1.89	0.55
1:5:1190:C:H2'	1:5:1191:C:C6	2.42	0.55
1:5:4260:U:H2'	1:5:4261:C:C6	2.42	0.55
81:13:63:A:H2'	81:13:64:U:C6	2.42	0.55
18:O:80:PHE:O	18:O:83:THR:HG22	2.07	0.55
21:R:39:GLN:OE1	21:R:42:ARG:NH1	2.40	0.55
34:e:84:GLU:CD	45:r:20:ARG:HH22	2.15	0.55
1:5:3965:A:N1	1:5:4047:A:H2'	2.23	0.54
1:5:4301:U:H4'	23:T:54:HIS:CD2	2.41	0.54
43:o:63:THR:O	43:o:87:ARG:NH1	2.40	0.54
1:5:2566:G:H2'	1:5:2567:G:C8	2.41	0.54
1:5:3635:A:N6	44:p:17:ARG:O	2.37	0.54
1:5:5053:U:H5'	1:5:5054:C:C5	2.42	0.54
1:5:2412:A:H2'	1:5:2413:U:C6	2.43	0.54
1:5:2422:C:P	19:P:127:ARG:HH22	2.30	0.54
1:5:4459:U:H2'	1:5:4460:U:C6	2.42	0.54
71:ZZ:103:HIS:HD1	71:ZZ:105:ALA:H	1.55	0.54
1:5:100:C:H2'	1:5:101:A:H8	1.71	0.54
1:5:1867:A:OP1	12:I:13:LYS:NZ	2.31	0.54
4:9:126:G:H21	4:9:180:G:H21	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1610:G:OP2	64:SS:132:ARG:NH1	2.38	0.54
4:9:1822:A:H2'	4:9:1823:A:H5''	1.89	0.54
1:5:1237:C:H4'	1:5:1238:A:O5'	2.08	0.54
1:5:2275:G:H2'	1:5:2276:A:C8	2.43	0.54
13:J:151:ILE:HD11	13:J:156:ARG:HG2	1.90	0.54
1:5:981:C:H42	1:5:1274:A:H61	1.55	0.54
1:5:1555:G:O6	44:p:4:ARG:NH2	2.41	0.54
1:5:2478:C:N4	1:5:2479:G:O6	2.41	0.54
1:5:3961:G:C6	1:5:3963:A:H2'	2.43	0.54
1:5:4572:U:H2'	1:5:4573:G:H8	1.73	0.54
4:9:1060:A:O2'	4:9:1062:A:N7	2.37	0.54
6:B:384:GLU:OE2	26:W:14:TYR:OH	2.21	0.54
4:9:72:C:H41	52:GG:170:ARG:HH12	1.56	0.54
4:9:74:G:O6	52:GG:159:ARG:NH2	2.41	0.54
15:L:62:PRO:O	15:L:63:THR:OG1	2.19	0.54
1:5:135:G:N2	37:h:95:LEU:O	2.33	0.54
1:5:691:C:H2'	1:5:692:A:C8	2.43	0.54
13:J:82:ILE:HG22	13:J:130:PHE:HE2	1.72	0.54
29:Z:41:ALA:HB2	29:Z:77:TYR:HE1	1.73	0.54
81:13:53:G:H2'	81:13:54:A:H8	1.72	0.54
1:5:175:C:H2'	1:5:176:G:C8	2.43	0.53
1:5:2088:A:H5''	1:5:2089:G:H3'	1.90	0.53
1:5:4061:G:H2'	1:5:4062:A:H8	1.73	0.53
4:9:5:U:H2'	4:9:6:G:C8	2.43	0.53
49:DD:40:ARG:NH1	49:DD:47:GLU:OE2	2.41	0.53
78:gg:101:PHE:CE2	78:gg:136:GLY:HA2	2.43	0.53
1:5:4293:U:O2'	43:o:81:ARG:NH2	2.42	0.53
4:9:115:U:H2'	4:9:116:U:C6	2.43	0.53
4:9:730:C:H2'	4:9:731:G:H8	1.73	0.53
39:k:8:ILE:HD11	39:k:56:LEU:HD13	1.91	0.53
1:5:2016:C:H2'	1:5:2017:A:H8	1.72	0.53
4:9:1144:A:H2'	4:9:1145:A:C8	2.44	0.53
30:a:90:ALA:HB3	30:a:120:GLN:HE21	1.73	0.53
48:CC:272:HIS:CE1	48:CC:276:THR:HG21	2.43	0.53
1:5:1532:G:OP2	82:j:31:LYS:NZ	2.29	0.53
1:5:5016:A:H2	1:5:5033:G:H21	1.54	0.53
48:CC:254:ASP:N	48:CC:254:ASP:OD1	2.37	0.53
1:5:956:A:H8	1:5:957:G:C8	2.26	0.53
1:5:2864:A:H2'	1:5:2865:U:C6	2.43	0.53
1:5:4546:A:N7	5:A:215:ASN:ND2	2.56	0.53
28:Y:54:GLU:OE1	28:Y:108:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1628:C:H2'	4:9:1629:C:C6	2.43	0.53
4:9:1736:G:H2'	4:9:1737:G:H8	1.74	0.53
78:gg:192:THR:OG1	78:gg:213:ASP:OD2	2.15	0.53
1:5:2490:U:H2'	1:5:2491:C:C6	2.44	0.53
1:5:966:A:H5'	1:5:967:C:H2'	1.91	0.53
1:5:979:C:OP1	9:E:49:ASN:ND2	2.42	0.53
1:5:4759:C:H2'	1:5:4760:G:C8	2.44	0.53
4:9:549:C:H5''	4:9:550:C:OP2	2.09	0.53
8:D:34:LYS:HA	23:T:27:LEU:HD11	1.90	0.53
83:jj:155:ASP:OD1	83:jj:156:ASN:N	2.41	0.53
1:5:1942:A:H2'	1:5:1943:A:C8	2.44	0.52
4:9:1451:G:OP1	63:RR:32:LYS:NZ	2.39	0.52
1:5:976:G:H21	7:C:323:ARG:NE	2.07	0.52
1:5:2029:A:H2'	1:5:2030:A:C8	2.43	0.52
1:5:2422:C:OP1	19:P:127:ARG:NH2	2.31	0.52
1:5:3707:U:H2'	1:5:3708:C:C6	2.45	0.52
4:9:107:A:H2'	4:9:108:G:C8	2.44	0.52
4:9:816:A:P	55:JJ:10:ARG:HH22	2.32	0.52
66:UU:59:LYS:HD2	66:UU:84:ILE:HD11	1.91	0.52
72:aa:59:PHE:HB2	72:aa:62:TYR:HB2	1.90	0.52
78:gg:16:GLY:N	78:gg:305:ASN:OD1	2.39	0.52
1:5:4395:U:H6	1:5:4395:U:H5'	1.75	0.52
4:9:1736:G:H2'	4:9:1737:G:C8	2.44	0.52
1:5:4038:C:H2'	1:5:4039:G:C8	2.44	0.52
1:5:4918:C:H2'	1:5:4919:G:O4'	2.09	0.52
34:e:89:LEU:HD13	34:e:118:LEU:HD22	1.90	0.52
1:5:1186:U:H2'	1:5:1187:G:N3	2.25	0.52
1:5:1835:G:O2'	1:5:1836:G:OP2	2.26	0.52
1:5:2440:U:O2'	1:5:2441:C:OP1	2.28	0.52
1:5:3692:A:H62	1:5:3823:G:N2	2.06	0.52
4:9:688:U:OP1	53:HH:116:ARG:NH2	2.36	0.52
4:9:1279:C:H2'	4:9:1280:G:H8	1.75	0.52
4:9:1293:A:H62	4:9:1306:U:H3	1.58	0.52
11:H:41:ILE:HG21	11:H:73:ILE:HD11	1.92	0.52
61:PP:17:TYR:HB3	61:PP:25:LEU:HD11	1.92	0.52
1:5:1191:C:H2'	1:5:1192:C:C6	2.44	0.52
1:5:2727:C:H2'	1:5:2728:U:C6	2.45	0.52
16:M:52:PHE:HA	16:M:55:MET:HE3	1.92	0.52
4:9:1232:U:H2'	4:9:1233:G:H8	1.75	0.52
8:D:22:ARG:NH1	8:D:28:THR:OG1	2.42	0.52
17:N:84:PRO:HA	17:N:87:HIS:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:375:G:OP2	82:j:52:LYS:NZ	2.42	0.52
1:5:3848:U:H2'	1:5:3849:A:C8	2.45	0.52
1:5:3848:U:H2'	1:5:3849:A:H8	1.75	0.52
4:9:1395:C:H1'	4:9:1474:A:C5	2.45	0.52
1:5:983:C:C5	9:E:73:ARG:HD3	2.45	0.52
1:5:3625:G:O2'	1:5:3626:G:OP1	2.27	0.52
3:8:126:C:H1'	3:8:127:U:C6	2.45	0.52
4:9:1138:C:OP1	46:AA:155:ARG:NH1	2.37	0.52
4:9:1337:C:H2'	4:9:1338:G:H8	1.75	0.52
4:9:1653:U:H2'	4:9:1654:G:C8	2.44	0.52
47:BB:25:PHE:HA	47:BB:28:LYS:HG2	1.92	0.52
1:5:3938:G:N2	1:5:4171:C:OP2	2.40	0.51
4:9:552:G:H2'	4:9:553:U:C6	2.45	0.51
4:9:1259:A:H2'	4:9:1260:A:H5''	1.92	0.51
18:O:37:ARG:HD2	18:O:108:ILE:HD11	1.91	0.51
1:5:1440:U:H2'	1:5:1441:C:C6	2.45	0.51
1:5:2092:G:OP2	45:r:101:LYS:NZ	2.42	0.51
1:5:4960:G:H2'	1:5:4961:G:H8	1.73	0.51
4:9:562:U:H2'	4:9:563:G:H8	1.73	0.51
64:SS:26:ILE:HD11	64:SS:52:LEU:HA	1.91	0.51
69:XX:68:LYS:HB3	69:XX:91:LEU:HD22	1.93	0.51
1:5:1475:G:H2'	1:5:1476:C:C6	2.45	0.51
4:9:996:A:H2'	4:9:997:A:C8	2.45	0.51
19:P:29:THR:HA	19:P:32:THR:HG22	1.91	0.51
20:Q:154:LYS:HE2	20:Q:158:THR:HG21	1.91	0.51
80:12:44:A:O2'	80:12:45:G:OP1	2.24	0.51
1:5:6:C:H2'	1:5:7:C:C6	2.45	0.51
1:5:2638:G:H22	1:5:2697:A:N6	2.06	0.51
1:5:4936:G:O2'	1:5:4937:C:OP1	2.25	0.51
4:9:1227:G:C2	4:9:1228:A:C8	2.98	0.51
1:5:2711:G:OP2	21:R:39:GLN:NE2	2.34	0.51
2:7:55:A:H4'	13:J:155:HIS:HB2	1.92	0.51
18:O:181:ALA:O	18:O:185:VAL:HG22	2.10	0.51
78:gg:87:LEU:HB3	78:gg:101:PHE:HB2	1.93	0.51
1:5:223:G:H4'	1:5:225:G:N7	2.26	0.51
1:5:457:G:H2'	1:5:458:C:C6	2.46	0.51
1:5:3717:A:H2'	1:5:3718:A:H8	1.74	0.51
4:9:1698:C:O2'	4:9:1699:A:OP1	2.29	0.51
51:FF:38:TYR:OH	74:cc:54:ASP:OD1	2.16	0.51
1:5:1327:C:H2'	1:5:1328:G:C8	2.45	0.51
1:5:1449:C:P	20:Q:134:ARG:HH12	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:44:SER:HB3	36:g:53:LEU:HD21	1.92	0.51
1:5:516:C:H2'	1:5:517:C:C6	2.45	0.51
1:5:2318:G:O6	34:e:19:LYS:NZ	2.40	0.51
81:13:4:C:H2'	81:13:5:A:H8	1.76	0.51
1:5:325:U:H2'	1:5:326:C:C6	2.46	0.51
1:5:1846:G:H2'	1:5:1847:C:C6	2.45	0.51
1:5:4239:A:H2'	1:5:4240:G:H8	1.76	0.51
1:5:4578:G:H2'	1:5:4579:U:C6	2.45	0.51
1:5:4862:G:H2'	1:5:4863:G:H8	1.76	0.51
1:5:5068:G:N2	1:5:5069:U:O4	2.30	0.51
4:9:1693:G:N2	4:9:1834:A:H8	2.08	0.51
47:BB:30:TRP:CE2	47:BB:48:LEU:HD13	2.46	0.51
56:KK:4:PRO:HG2	56:KK:7:ASN:CG	2.36	0.51
78:gg:207:CYS:HB2	78:gg:221:LEU:HD11	1.92	0.51
1:5:3799:A:OP1	25:V:64:THR:HG21	2.11	0.51
1:5:3968:U:H2'	1:5:3969:G:H8	1.76	0.51
1:5:4066:U:H2'	1:5:4067:U:C6	2.46	0.51
4:9:60:A:N3	4:9:316:G:O2'	2.34	0.51
1:5:175:C:H2'	1:5:176:G:H8	1.76	0.50
1:5:3873:G:H2'	1:5:3874:G:C8	2.45	0.50
22:S:112:ASP:OD1	22:S:116:ARG:NH1	2.41	0.50
58:MM:75:ASN:HB3	58:MM:128:PHE:CZ	2.46	0.50
59:NN:55:ARG:NH1	59:NN:56:ASP:OD1	2.44	0.50
64:SS:65:GLU:O	64:SS:69:THR:HG23	2.11	0.50
83:jj:229:ASP:OD1	83:jj:229:ASP:N	2.40	0.50
1:5:62:A:N3	1:5:77:U:O2'	2.38	0.50
1:5:4966:A:H5''	6:B:128:LYS:HG3	1.91	0.50
4:9:164:A:H3'	4:9:165:G:H21	1.77	0.50
4:9:501:C:H2'	4:9:502:C:H5''	1.93	0.50
4:9:533:A:H2'	4:9:534:G:H8	1.75	0.50
1:5:100:C:H2'	1:5:101:A:C8	2.46	0.50
1:5:362:A:N6	40:l:37:TYR:O	2.38	0.50
1:5:4305:G:H22	23:T:87:LYS:NZ	2.09	0.50
4:9:1801:A:H2'	4:9:1802:C:C6	2.47	0.50
12:I:66:GLU:OE1	12:I:69:ARG:NH1	2.43	0.50
50:EE:124:CYS:HB3	50:EE:141:THR:HB	1.93	0.50
1:5:456:C:H2'	1:5:457:G:C8	2.46	0.50
1:5:2517:A:O2'	36:g:66:ARG:NH2	2.44	0.50
4:9:1010:G:H2'	4:9:1011:A:C8	2.45	0.50
66:UU:19:ARG:HG2	66:UU:92:HIS:CD2	2.47	0.50
68:WW:11:LEU:HD22	68:WW:72:CYS:SG	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:25:A:H4'	1:5:340:C:H2'	1.93	0.50
1:5:1211:G:O2'	1:5:1212:G:OP1	2.26	0.50
1:5:3904:G:O2'	1:5:3905:A:OP1	2.28	0.50
2:7:23:A:H2'	2:7:24:C:C6	2.46	0.50
2:7:27:G:H21	2:7:55:A:N6	2.08	0.50
4:9:29:G:H2'	4:9:30:C:C6	2.46	0.50
4:9:1136:U:H2'	4:9:1137:U:C6	2.47	0.50
4:9:1489:A:H4'	4:9:1490:G:OP2	2.11	0.50
12:I:187:GLU:OE2	12:I:189:ARG:NE	2.37	0.50
13:J:111:GLU:OE1	64:SS:14:ARG:NH2	2.45	0.50
77:ff:133:ALA:N	77:ff:140:TYR:O	2.29	0.50
1:5:1903:G:OP1	35:f:87:LYS:NZ	2.38	0.50
1:5:2088:A:C5'	1:5:2089:G:H3'	2.42	0.50
1:5:2638:G:H22	1:5:2697:A:H61	1.59	0.50
4:9:880:G:H2'	4:9:881:G:H8	1.76	0.50
78:gg:68:ASP:HB3	78:gg:111:VAL:HG12	1.93	0.50
1:5:165:A:H2'	1:5:166:C:C6	2.46	0.50
1:5:1468:C:H2'	1:5:1469:C:H6	1.77	0.50
1:5:2594:C:OP1	5:A:70:LYS:NZ	2.38	0.50
4:9:126:G:H21	4:9:180:G:N2	2.10	0.50
56:KK:3:MET:HE1	56:KK:48:ALA:HB2	1.92	0.50
4:9:562:U:H5'	55:JJ:134:HIS:HE2	1.76	0.50
4:9:1023:A:OP2	59:NN:124:ARG:NH1	2.43	0.50
9:E:151:THR:HG22	9:E:203:LYS:HG2	1.92	0.50
53:HH:93:VAL:HG21	53:HH:133:LEU:HD12	1.92	0.50
1:5:1468:C:H2'	1:5:1469:C:C6	2.47	0.50
1:5:4504:C:H2'	1:5:4505:C:C6	2.47	0.50
3:8:93:C:OP1	82:j:76:HIS:HE1	1.95	0.50
19:P:57:CYS:SG	19:P:81:GLY:HA3	2.52	0.50
52:GG:7:PHE:CZ	52:GG:9:ALA:HB3	2.47	0.50
81:11:5:A:H2'	81:11:6:G:H8	1.75	0.50
1:5:717:U:H2'	1:5:718:C:C6	2.47	0.49
1:5:1693:U:OP1	20:Q:143:ARG:NH2	2.41	0.49
1:5:3732:A:H2'	1:5:3733:A:C8	2.47	0.49
1:5:4413:C:H5	1:5:4429:C:H42	1.59	0.49
4:9:179:C:H2'	4:9:180:G:H8	1.77	0.49
47:BB:208:HIS:CG	47:BB:209:ASP:H	2.30	0.49
80:12:67:A:H2'	80:12:68:U:C6	2.46	0.49
1:5:1564:A:H2'	1:5:1565:A:C8	2.46	0.49
4:9:1101:U:H2'	4:9:1102:G:C8	2.47	0.49
10:G:215:ASP:HB3	10:G:216:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:23:ILE:HG23	40:l:38:ASN:HB2	1.94	0.49
1:5:746:A:O2'	1:5:747:A:H5'	2.12	0.49
1:5:2326:G:OP2	34:e:101:HIS:ND1	2.27	0.49
3:8:19:C:H2'	3:8:20:A:C8	2.48	0.49
4:9:434:G:H2'	4:9:435:A:C8	2.47	0.49
52:GG:199:THR:O	52:GG:203:LYS:HG2	2.13	0.49
1:5:1411(B):C:H2'	1:5:1411(C):C:C6	2.48	0.49
3:8:155:C:OP2	10:G:142:ARG:NH1	2.43	0.49
4:9:821:G:C6	55:JJ:147:PHE:CZ	3.01	0.49
4:9:880:G:H2'	4:9:881:G:C8	2.47	0.49
4:9:1375:G:H2'	4:9:1376:A:C8	2.47	0.49
9:E:144:ARG:NH2	9:E:194:GLN:O	2.40	0.49
48:CC:168:GLY:N	48:CC:179:THR:O	2.31	0.49
54:II:38:ILE:HA	54:II:60:LEU:O	2.13	0.49
1:5:1976:G:H1	1:5:1990:A:H61	1.61	0.49
2:7:7:G:OP1	8:D:33:ARG:NE	2.40	0.49
4:9:1588:A:H2'	4:9:1589:A:C8	2.47	0.49
1:5:260:C:H2'	1:5:261:G:C8	2.48	0.49
1:5:424:U:H2'	1:5:425:U:H6	1.75	0.49
4:9:952:G:OP1	47:BB:56:LYS:NZ	2.34	0.49
4:9:1553:C:H2'	4:9:1554:C:C6	2.47	0.49
48:CC:191:VAL:HG11	48:CC:236:PHE:HA	1.95	0.49
80:12:11:C:H2'	80:12:12:U:C6	2.48	0.49
1:5:3948:C:H5''	1:5:3949:A:OP2	2.12	0.49
19:P:54:LYS:HA	19:P:83:TRP:CD1	2.48	0.49
1:5:489:C:H2'	1:5:490:C:C6	2.48	0.49
1:5:3947:A:H2'	1:5:3948:C:C6	2.47	0.49
3:8:45:C:OP2	40:l:15:LYS:NZ	2.33	0.49
4:9:1864:U:OP2	72:aa:4:LYS:NZ	2.36	0.49
7:C:13:GLU:OE1	7:C:161:TYR:OH	2.20	0.49
21:R:63:CYS:O	21:R:67:THR:HG23	2.13	0.49
1:5:2504:C:H2'	1:5:2505:C:H2'	1.95	0.49
1:5:2771:G:H2'	1:5:2772:C:O4'	2.12	0.49
1:5:4960:G:H2'	1:5:4961:G:C8	2.48	0.49
13:J:63:ARG:NH1	43:o:104:ILE:O	2.44	0.49
83:jj:72:SER:HA	83:jj:75:TYR:HB3	1.94	0.49
1:5:4274:A:H2'	1:5:4275:G:C8	2.47	0.49
4:9:65:C:O2'	4:9:67:C:OP2	2.29	0.49
53:HH:145:ARG:NH1	68:WW:51:GLU:OE1	2.42	0.49
1:5:1391:A:OP1	20:Q:181:ARG:NH1	2.42	0.48
4:9:26:U:H2'	4:9:27:A:C8	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1554:C:OP2	4:9:1555:U:O2'	2.29	0.48
1:5:156:G:N2	1:5:157:U:O4	2.46	0.48
1:5:3611:A:H2	1:5:5016:A:H8	1.60	0.48
4:9:898:U:H2'	4:9:899:U:H6	1.79	0.48
17:N:84:PRO:HA	17:N:87:HIS:CD2	2.48	0.48
1:5:318:A:H2'	1:5:319:A:C8	2.48	0.48
1:5:3648:A:H1'	1:5:3785:A:N6	2.28	0.48
1:5:3786:U:OP1	1:5:4550:G:O2'	2.27	0.48
59:NN:55:ARG:HG2	59:NN:55:ARG:HH11	1.78	0.48
1:5:1369:C:OP2	1:5:1370:G:O2'	2.29	0.48
1:5:1441:C:H2'	1:5:1442:C:C6	2.48	0.48
1:5:2647:A:H62	1:5:2686:G:H8	1.60	0.48
1:5:4944:C:H1'	35:f:69:VAL:HG21	1.94	0.48
1:5:4944:C:H4'	1:5:4944:C:OP1	2.12	0.48
4:9:1823:A:OP1	69:XX:60:LYS:NZ	2.46	0.48
15:L:21:ARG:HB3	17:N:197:THR:HG22	1.96	0.48
34:e:40:GLY:O	34:e:46:ARG:NH1	2.46	0.48
50:EE:212:ASP:OD1	50:EE:213:ALA:N	2.45	0.48
1:5:1188:C:H2'	1:5:1189:G:C8	2.43	0.48
4:9:179:C:H2'	4:9:180:G:C8	2.48	0.48
1:5:1308:C:H2'	1:5:1309:C:C6	2.49	0.48
1:5:1967:A:C2	1:5:2021:G:C5	3.02	0.48
1:5:4508:C:OP1	25:V:43:LYS:NZ	2.38	0.48
2:7:3:C:H2'	2:7:4:U:H6	1.78	0.48
4:9:917:U:H2'	4:9:918:U:C6	2.49	0.48
4:9:925:G:H1	4:9:1017:U:H3	1.60	0.48
10:G:139:VAL:HG11	10:G:238:LYS:CG	2.44	0.48
27:X:92:ASP:C	27:X:93:ASN:HD22	2.20	0.48
61:PP:13:ARG:NH1	61:PP:14:LYS:O	2.46	0.48
2:7:24:C:H2'	2:7:25:G:O4'	2.14	0.48
4:9:182:C:H5'	4:9:183:G:C5	2.49	0.48
4:9:1115:U:O2'	4:9:1116:C:OP2	2.30	0.48
13:J:136:ARG:HH22	13:J:161:GLU:CD	2.21	0.48
1:5:2093:G:H22	1:5:2262:G:H1	1.61	0.48
1:5:3736:A:H2'	1:5:3737:A:C8	2.48	0.48
1:5:4524:G:N3	6:B:252:ALA:HB1	2.29	0.48
1:5:4594:U:H2'	1:5:4595:G:H8	1.78	0.48
1:5:4712:C:OP1	18:O:74:ARG:NH2	2.47	0.48
4:9:986:G:C8	60:OO:137:SER:O	2.66	0.48
17:N:193:ARG:O	17:N:197:THR:HG23	2.13	0.48
46:AA:128:ARG:HH22	46:AA:151:ASP:CG	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SS:14:ARG:NH1	64:SS:17:ASN:HA	2.29	0.48
1:5:271:C:H2'	1:5:272:U:H6	1.76	0.48
1:5:2457:G:H21	1:5:3672:G:N2	2.12	0.48
1:5:5062:G:C2	1:5:5063:G:C8	3.02	0.48
4:9:1507:G:C5	77:ff:89:LYS:HB3	2.49	0.48
4:9:1570:G:N7	65:TT:97:LYS:NZ	2.54	0.48
1:5:4305:G:N2	23:T:87:LYS:HZ3	2.11	0.48
4:9:1088:U:H4'	4:9:1089:G:OP2	2.14	0.48
19:P:32:THR:HG21	19:P:87:SER:HB3	1.95	0.48
80:12:23:A:H2'	80:12:24:G:H8	1.77	0.48
81:11:5:A:H2'	81:11:6:G:C8	2.49	0.48
83:jj:429:LEU:O	83:jj:438:LEU:N	2.46	0.48
1:5:2318:G:N2	1:5:2321:G:OP2	2.37	0.47
1:5:3917:A:H2'	1:5:3918:G:H8	1.79	0.47
1:5:3932:U:H2'	1:5:3933:G:C8	2.46	0.47
4:9:1037:G:H4'	4:9:1845:A:H4'	1.95	0.47
51:FF:136:ARG:NH1	81:11:33:C:OP1	2.46	0.47
71:ZZ:79:ILE:HB	71:ZZ:83:LEU:HD23	1.95	0.47
1:5:982:U:H3	1:5:1273:G:H1	1.61	0.47
4:9:1566:G:N7	65:TT:101:ARG:NH2	2.61	0.47
9:E:185:ASN:ND2	9:E:274:LEU:O	2.47	0.47
52:GG:98:ARG:NH1	52:GG:99:GLY:O	2.48	0.47
83:jj:491:GLU:OE2	83:jj:543:ARG:NH1	2.44	0.47
1:5:372:A:OP1	82:j:36:LYS:HE2	2.14	0.47
1:5:490:C:H2'	1:5:491:G:H8	1.77	0.47
4:9:106:C:H2'	4:9:107:A:H8	1.78	0.47
4:9:640:A:H2'	4:9:641:A:C8	2.49	0.47
4:9:1507:G:C4	77:ff:89:LYS:HB3	2.49	0.47
5:A:101:VAL:HG22	5:A:165:VAL:HG22	1.97	0.47
15:L:28:GLN:OE1	17:N:202:ARG:NH1	2.41	0.47
51:FF:136:ARG:NH2	81:11:32:C:H4'	2.29	0.47
58:MM:30:GLY:O	58:MM:112:LYS:HB3	2.15	0.47
81:13:57:G:H2'	81:13:58:A:H5''	1.95	0.47
83:jj:219:ASP:OD1	83:jj:222:GLY:N	2.48	0.47
1:5:4070:U:H2'	1:5:4071:U:C6	2.50	0.47
1:5:4578:G:H2'	1:5:4579:U:H6	1.79	0.47
1:5:4988:U:OP1	6:B:123:HIS:ND1	2.43	0.47
4:9:344:U:H2'	4:9:345:U:C6	2.49	0.47
4:9:562:U:H5'	55:JJ:134:HIS:NE2	2.30	0.47
4:9:674:C:H2'	4:9:675:U:C6	2.50	0.47
4:9:1858:G:OP1	72:aa:17:HIS:HE1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:220:ILE:HG12	6:B:278:THR:HG23	1.96	0.47
7:C:76:ILE:HG12	7:C:96:CYS:SG	2.54	0.47
52:GG:102:VAL:HG13	52:GG:106:LEU:HD12	1.97	0.47
71:ZZ:100:VAL:HG21	71:ZZ:110:THR:HG23	1.96	0.47
1:5:1890:G:N2	1:5:1939:A:H61	2.13	0.47
1:5:2632:U:H2'	1:5:2633:U:C6	2.50	0.47
23:T:35:LYS:N	23:T:38:ASP:OD2	2.40	0.47
31:b:101:HIS:CD2	31:b:104:LEU:H	2.31	0.47
46:AA:198:MET:SD	63:RR:89:SER:HB2	2.55	0.47
81:13:47:U:H3'	81:13:48:C:H5'	1.97	0.47
1:5:3645:U:O2'	1:5:4553:A:O2'	2.27	0.47
1:5:4115:G:H5''	1:5:4116:C:H5'	1.95	0.47
4:9:633:C:H1'	76:ee:89:THR:HG21	1.96	0.47
4:9:1253:A:OP2	4:9:1526:G:N2	2.40	0.47
30:a:72:THR:HG22	30:a:110:LYS:HB3	1.96	0.47
56:KK:85:LEU:HD13	56:KK:89:ILE:HD11	1.96	0.47
64:SS:26:ILE:HG22	64:SS:56:ALA:HA	1.96	0.47
1:5:63:G:P	17:N:169:ARG:HH22	2.37	0.47
1:5:286:U:H2'	1:5:287:U:C6	2.49	0.47
1:5:1358:G:H2'	1:5:1360:G:O6	2.15	0.47
1:5:1772:C:H2'	1:5:1773:U:O4'	2.15	0.47
1:5:1961:G:O2'	1:5:2024:G:N2	2.48	0.47
1:5:2335:C:H2'	1:5:2336:G:H8	1.80	0.47
4:9:374:G:OP1	57:LL:59:LYS:NZ	2.43	0.47
7:C:218:VAL:HA	7:C:229:LEU:HD13	1.96	0.47
17:N:31:ARG:NH1	17:N:124:ASP:OD2	2.47	0.47
32:c:82:GLY:HA2	32:c:91:VAL:HG12	1.97	0.47
1:5:67:C:OP2	1:5:312:G:N2	2.48	0.47
1:5:1320:U:O2'	1:5:1891:A:N1	2.34	0.47
1:5:1483:C:H5''	1:5:1483:C:O2	2.14	0.47
1:5:4300:U:OP1	23:T:87:LYS:NZ	2.47	0.47
4:9:533:A:C6	4:9:552:G:C6	3.03	0.47
4:9:1144:A:H5'	4:9:1355:C:H41	1.79	0.47
4:9:1303:C:O2	4:9:1303:C:H5'	2.15	0.47
4:9:1407:U:H2'	4:9:1408:U:C6	2.50	0.47
69:XX:69:CYS:SG	69:XX:115:ILE:HD11	2.55	0.47
1:5:231:U:H4'	28:Y:100:HIS:CD2	2.49	0.47
1:5:1358:G:O2'	1:5:1359:G:O5'	2.31	0.47
1:5:3725:G:N2	1:5:3728:A:OP2	2.38	0.47
1:5:265:C:O2	1:5:266:C:N4	2.47	0.47
1:5:1234:G:HO2'	1:5:1235:G:H8	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1920:C:OP1	22:S:164:LYS:NZ	2.46	0.47
4:9:1058:A:OP1	81:13:38:A:O2'	2.26	0.47
49:DD:29:LEU:HB2	49:DD:34:TYR:HB2	1.97	0.47
1:5:2474:G:N2	1:5:2502:A:H2'	2.30	0.46
4:9:791:C:H2'	4:9:792:C:C6	2.50	0.46
4:9:919:A:OP2	59:NN:64:ARG:NH2	2.41	0.46
50:EE:95:THR:HG23	70:YY:17:LEU:HD21	1.97	0.46
65:TT:71:GLY:O	65:TT:75:MET:HG2	2.15	0.46
78:gg:294:ASP:OD1	78:gg:296:GLN:N	2.46	0.46
1:5:4563:U:H2'	1:5:4564:A:C8	2.50	0.46
4:9:1536:G:H2'	4:9:1537:A:C8	2.49	0.46
62:QQ:30:GLY:N	62:QQ:67:ASP:OD1	2.40	0.46
63:RR:77:GLU:OE1	63:RR:80:ARG:NH1	2.36	0.46
1:5:1646:A:O2'	82:j:49:TRP:O	2.27	0.46
1:5:4476:C:O2'	1:5:4478:G:OP2	2.28	0.46
3:8:141:C:H2'	3:8:142:U:C6	2.51	0.46
4:9:1293:A:N6	4:9:1306:U:H3	2.13	0.46
46:AA:38:ILE:HD11	46:AA:150:THR:HG22	1.98	0.46
51:FF:73:THR:O	51:FF:89:THR:HG21	2.14	0.46
52:GG:226:GLU:HG3	52:GG:230:LYS:HE2	1.97	0.46
59:NN:91:LEU:HD12	59:NN:125:LEU:HD12	1.96	0.46
81:11:37:A:H2'	81:11:38:A:O4'	2.16	0.46
1:5:166:C:H2'	1:5:167:C:C6	2.51	0.46
1:5:253:G:C6	1:5:254:G:C6	3.04	0.46
1:5:280:G:H5''	17:N:14:LYS:HE2	1.96	0.46
1:5:691:C:H2'	1:5:692:A:H8	1.81	0.46
1:5:1332:C:H2'	1:5:1333:A:H8	1.81	0.46
1:5:3672:G:O5'	1:5:3672:G:C8	2.69	0.46
1:5:4178:A:H2'	1:5:4179:G:C8	2.50	0.46
1:5:4927:G:H3'	1:5:4928:C:O2	2.15	0.46
4:9:30:C:O2'	4:9:596:U:OP1	2.30	0.46
4:9:1310:U:H2'	4:9:1311:C:C6	2.49	0.46
4:9:1337:C:H2'	4:9:1338:G:C8	2.50	0.46
1:5:1727:U:H2'	1:5:1728:U:C6	2.51	0.46
1:5:1883:G:OP1	34:e:47:ARG:NH1	2.38	0.46
1:5:4760:G:H2'	1:5:4761:G:O4'	2.15	0.46
4:9:67:C:H41	52:GG:163:ASN:HA	1.81	0.46
4:9:407:G:C6	69:XX:36:LEU:HD22	2.51	0.46
4:9:1397:U:H2'	4:9:1397:U:O2	2.14	0.46
4:9:1455:A:C2	4:9:1456:G:C8	3.03	0.46
4:9:1720:U:H3'	4:9:1721:U:H5''	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:89:THR:HG22	16:M:91:TRP:H	1.79	0.46
58:MM:21:VAL:HG21	58:MM:124:ILE:HD12	1.97	0.46
78:gg:218:LEU:HD12	78:gg:228:TYR:CE2	2.49	0.46
1:5:1534:A:C8	82:j:15:THR:HG23	2.51	0.46
1:5:3759:A:H5'	1:5:3765:G:H22	1.80	0.46
5:A:30:ARG:NH2	5:A:33:ASP:OD2	2.38	0.46
15:L:63:THR:HG22	15:L:64:VAL:N	2.30	0.46
22:S:173:ASN:ND2	22:S:175:PHE:O	2.47	0.46
80:12:72:C:O2	86:12:101:GTP:N2	2.29	0.46
1:5:465:G:H2'	1:5:466:A:C8	2.50	0.46
1:5:4478:G:O2'	1:5:4602:A:N1	2.47	0.46
29:Z:100:VAL:HG13	29:Z:107:LYS:HA	1.98	0.46
45:r:4:HIS:O	45:r:8:MET:HG2	2.15	0.46
50:EE:252:ARG:HG2	50:EE:252:ARG:HH11	1.81	0.46
61:PP:21:ASP:OD1	61:PP:22:LEU:N	2.49	0.46
78:gg:174:VAL:HB	78:gg:188:HIS:HB2	1.97	0.46
80:12:67:A:H2'	80:12:68:U:H6	1.80	0.46
1:5:1364:U:OP2	15:L:36:ARG:NH2	2.47	0.46
4:9:862:A:C8	68:WW:107:SER:HA	2.51	0.46
4:9:1839:U:H1'	4:9:1863:A:H2	1.80	0.46
10:G:218:GLU:OE1	17:N:26:ARG:NH2	2.49	0.46
29:Z:28:ASN:HB2	29:Z:77:TYR:OH	2.16	0.46
68:WW:30:CYS:SG	68:WW:31:SER:N	2.88	0.46
1:5:257:C:H2'	1:5:258:G:C8	2.50	0.46
1:5:2476:G:H2'	1:5:2477:A:C8	2.51	0.46
1:5:4871:C:OP1	16:M:94:LYS:NZ	2.39	0.46
4:9:1781:A:H2'	4:9:1782:G:C8	2.51	0.46
9:E:48:ARG:O	9:E:67:ARG:NH1	2.46	0.46
20:Q:43:PHE:CD1	20:Q:133:GLY:HA3	2.51	0.46
50:EE:138:HIS:CD2	50:EE:148:ARG:HB3	2.51	0.46
71:ZZ:64:ASN:O	71:ZZ:111:ARG:NH2	2.40	0.46
80:12:66:A:H2'	80:12:67:A:H8	1.81	0.46
1:5:76:A:N7	15:L:74:ARG:NH2	2.64	0.46
1:5:971(A):G:H4'	1:5:972:C:O5'	2.15	0.46
1:5:1402:C:H2'	1:5:1403:G:H8	1.81	0.46
1:5:1437:C:O2'	1:5:1438:U:O5'	2.33	0.46
1:5:2520:C:O2	1:5:2640:G:N2	2.49	0.46
1:5:3607:U:H2'	1:5:3608:A:C8	2.51	0.46
3:8:60:G:O6	3:8:96:C:O2'	2.25	0.46
4:9:735:C:H2'	4:9:736:C:C6	2.51	0.46
7:C:155:GLU:HG2	7:C:157:LYS:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:15:THR:HG22	36:g:16:ALA:H	1.81	0.46
78:gg:191:HIS:CD2	78:gg:195:LEU:HD21	2.51	0.46
78:gg:194:TYR:CZ	78:gg:212:LYS:HD3	2.50	0.46
81:13:23:C:H2'	81:13:24:G:C8	2.50	0.46
83:jj:501:HIS:H	83:jj:534:THR:HG22	1.81	0.46
1:5:1238:A:O2'	1:5:1239:C:OP1	2.29	0.45
1:5:1477:C:O2'	1:5:1478:C:OP1	2.32	0.45
1:5:4305:G:H22	23:T:87:LYS:CD	2.29	0.45
4:9:536:A:N6	4:9:547:G:H1	2.12	0.45
16:M:36:ALA:HB2	16:M:52:PHE:CZ	2.50	0.45
21:R:105:LEU:HD23	21:R:138:LEU:HD23	1.98	0.45
1:5:517:C:H2'	1:5:518:G:H8	1.81	0.45
1:5:1072:C:O2'	1:5:1073:G:O5'	2.28	0.45
1:5:4099:G:N2	1:5:4109:G:H22	2.14	0.45
1:5:4122:G:O2'	29:Z:136:PHE:OXT	2.34	0.45
1:5:4178:A:H2'	1:5:4179:G:H8	1.81	0.45
4:9:183:G:O2'	4:9:184:G:O5'	2.30	0.45
21:R:141:HIS:CE1	21:R:145:LEU:HD11	2.51	0.45
23:T:28:ALA:HA	23:T:31:MET:HG2	1.98	0.45
36:g:74:VAL:O	36:g:79:GLY:HA2	2.15	0.45
60:OO:22:ALA:N	60:OO:25:GLU:OE2	2.47	0.45
81:11:35:A:H2'	81:11:36:U:C6	2.52	0.45
1:5:1660:U:H3'	30:a:13:GLY:HA2	1.98	0.45
1:5:1920:C:H3'	1:5:1921:C:H5''	1.98	0.45
1:5:3663:A:N6	1:5:4168:G:O2'	2.48	0.45
1:5:4099:G:N2	1:5:4109:G:N2	2.64	0.45
1:5:4254:G:O2'	1:5:4255:A:OP1	2.33	0.45
4:9:1658:G:OP2	4:9:1660:C:N4	2.49	0.45
6:B:288:GLY:HA3	6:B:330:PHE:CZ	2.51	0.45
17:N:80:THR:HB	17:N:87:HIS:CB	2.45	0.45
1:5:52:G:H4'	1:5:1529:G:H4'	1.98	0.45
1:5:1984:A:C8	1:5:2011:C:OP1	2.69	0.45
4:9:571:U:OP1	70:YY:37:LYS:HE2	2.16	0.45
4:9:1229:G:H2'	4:9:1230:C:C6	2.51	0.45
4:9:1375:G:H2'	4:9:1376:A:H8	1.80	0.45
4:9:1578:U:H5'	4:9:1579:A:N3	2.30	0.45
60:OO:103:ASN:HB3	60:OO:139:SER:OG	2.17	0.45
81:11:25:U:H2'	81:11:26:G:C8	2.49	0.45
1:5:462:G:H2'	1:5:463:A:C8	2.51	0.45
1:5:1850:A:H2'	1:5:1851:G:C8	2.52	0.45
1:5:3770:U:H2'	1:5:3771:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3930:U:H2'	1:5:3931:C:C6	2.52	0.45
3:8:67:U:H2'	3:8:68:G:H8	1.81	0.45
3:8:141:C:OP1	17:N:38:ARG:NH1	2.48	0.45
4:9:1354:G:N2	4:9:1357:A:OP2	2.40	0.45
49:DD:8:LYS:HG2	66:UU:61:LEU:HD11	1.99	0.45
71:ZZ:103:HIS:CE1	71:ZZ:104:ARG:HG2	2.51	0.45
1:5:109:G:OP1	15:L:92:ARG:NH1	2.49	0.45
1:5:1558:A:H2'	1:5:1559:G:H8	1.80	0.45
1:5:2553:A:H1'	1:5:2554:U:O4'	2.17	0.45
1:5:2732:G:H2'	1:5:2733:C:C6	2.52	0.45
1:5:4481:U:H2'	1:5:4482:U:H6	1.82	0.45
1:5:4957:C:H3'	1:5:4958:C:H5''	1.99	0.45
4:9:527:C:H2'	4:9:528:A:H8	1.81	0.45
4:9:1865:C:H5	72:aa:6:ARG:H	1.64	0.45
6:B:115:LYS:HA	6:B:118:PHE:CD2	2.52	0.45
9:E:164:ARG:HG2	9:E:164:ARG:HH11	1.82	0.45
83:jj:186:ASP:OD2	91:jj:702:GDP:O2'	2.26	0.45
1:5:3653:A:H4'	5:A:179:ILE:O	2.16	0.45
1:5:4907:G:N2	1:5:4915:G:C4	2.85	0.45
11:H:141:LYS:NZ	11:H:142:ASP:OD2	2.38	0.45
13:J:28:GLU:OE2	13:J:32:ARG:NH1	2.41	0.45
58:MM:92:CYS:HB3	58:MM:103:VAL:HG22	1.99	0.45
1:5:1170:G:H2'	1:5:1171:G:C8	2.51	0.45
1:5:1381:U:H5''	1:5:1381:U:O2	2.16	0.45
1:5:1804:A:H5''	1:5:1805:A:H2'	1.99	0.45
1:5:3606:U:H2'	1:5:3607:U:H6	1.82	0.45
1:5:4051:C:H2'	1:5:4052:C:C6	2.52	0.45
1:5:4591:U:H2'	1:5:4592:C:C6	2.52	0.45
4:9:65:C:N4	52:GG:133:LEU:HB3	2.31	0.45
4:9:1173:A:OP2	42:n:14:LYS:NZ	2.47	0.45
4:9:1679:A:C2	51:FF:60:ARG:HA	2.52	0.45
4:9:1856:C:H2'	4:9:1857:G:C8	2.52	0.45
57:LL:101:ARG:HB2	69:XX:7:LEU:O	2.17	0.45
1:5:4611:A:H2'	1:5:4612:C:C6	2.52	0.45
4:9:1101:U:H2'	4:9:1102:G:H8	1.80	0.45
4:9:1285:G:OP1	58:MM:107:SER:OG	2.33	0.45
4:9:1287:A:C2	4:9:1313:A:H1'	2.52	0.45
4:9:1690:U:H2'	4:9:1691:U:C6	2.51	0.45
13:J:94:LEU:O	13:J:174:ILE:HA	2.17	0.45
64:SS:14:ARG:HH12	64:SS:17:ASN:HA	1.82	0.45
78:gg:25:PRO:HA	78:gg:293:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:13:23:C:H2'	81:13:24:G:H8	1.82	0.45
1:5:385:A:N3	1:5:387:G:H5''	2.32	0.45
1:5:1961:G:O2'	1:5:2025:A:N6	2.49	0.45
1:5:2837:U:OP1	6:B:249:ARG:NH1	2.40	0.45
1:5:4563:U:H2'	1:5:4564:A:H8	1.81	0.45
1:5:4948:C:O2	1:5:4949:G:H2'	2.16	0.45
4:9:28:U:H2'	4:9:29:G:H8	1.82	0.45
11:H:173:ARG:HD2	41:m:101:VAL:HB	1.99	0.45
54:II:89:GLU:OE2	54:II:92:ARG:NH2	2.42	0.45
81:13:3:G:C8	88:13:101:ATP:H2'	2.52	0.45
1:5:2083:C:OP2	20:Q:14:ARG:NH2	2.49	0.44
1:5:4273:A:H2'	1:5:4274:A:C8	2.52	0.44
1:5:4413:C:H5	1:5:4429:C:N4	2.14	0.44
1:5:4881:U:H4'	1:5:4882:U:C5	2.52	0.44
53:HH:48:ALA:HA	53:HH:61:ILE:O	2.16	0.44
81:11:66:C:H2'	81:11:67:U:H6	1.82	0.44
1:5:469:C:H2'	1:5:470:A:H8	1.82	0.44
1:5:983:C:C6	9:E:73:ARG:HD3	2.52	0.44
1:5:3859:G:OP2	19:P:25:HIS:HE1	2.00	0.44
1:5:5047:C:O2'	1:5:5050:C:OP2	2.31	0.44
4:9:626:G:H3'	4:9:627:U:C5'	2.48	0.44
81:13:25:U:C2	81:13:26:G:C8	3.06	0.44
1:5:1171:G:H2'	1:5:1172:C:C6	2.52	0.44
1:5:1976:G:H1	1:5:1990:A:N6	2.16	0.44
1:5:3926:C:O2'	17:N:87:HIS:HE1	1.99	0.44
1:5:4395:U:H5'	1:5:4395:U:C6	2.53	0.44
4:9:106:C:H2'	4:9:107:A:C8	2.51	0.44
4:9:869:A:N6	53:HH:115:LYS:O	2.40	0.44
6:B:381:THR:HG23	6:B:384:GLU:H	1.82	0.44
7:C:339:THR:HG22	7:C:342:ARG:HH22	1.83	0.44
83:jj:200:LYS:NZ	83:jj:204:GLU:OE2	2.34	0.44
1:5:54:G:OP1	82:j:43:ARG:NH1	2.49	0.44
1:5:150:U:H4'	1:5:151:G:OP2	2.18	0.44
1:5:3770:U:H2'	1:5:3771:C:H6	1.82	0.44
4:9:25:A:HO2'	4:9:26:U:H6	1.62	0.44
4:9:1863:A:H8	72:aa:79:ILE:HG21	1.83	0.44
6:B:95:THR:C	6:B:97:ARG:H	2.25	0.44
23:T:4:THR:OG1	23:T:9:ARG:HD3	2.17	0.44
36:g:15:THR:HG22	36:g:16:ALA:N	2.33	0.44
46:AA:205:ARG:HH22	46:AA:213:GLU:CD	2.24	0.44
1:5:1177:U:H2'	1:5:1178:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1332:C:H2'	1:5:1333:A:C8	2.52	0.44
4:9:1286:G:OP1	77:f:99:LYS:NZ	2.39	0.44
6:B:240:LEU:HB3	6:B:244:THR:HG21	1.99	0.44
56:KK:49:MET:HG3	56:KK:69:TRP:CE3	2.53	0.44
62:QQ:86:GLN:HE22	62:QQ:122:ALA:HA	1.81	0.44
64:SS:120:HIS:CE1	64:SS:124:ARG:HD2	2.53	0.44
66:UU:19:ARG:HG2	66:UU:92:HIS:NE2	2.33	0.44
81:13:58:A:H1'	81:13:60:A:N7	2.33	0.44
1:5:1098:G:C2	1:5:1198:G:N2	2.86	0.44
1:5:2673:G:N3	1:5:2673:G:H5'	2.32	0.44
1:5:4303:C:H2'	1:5:4305:G:H8	1.79	0.44
1:5:4623:G:OP1	6:B:19:ARG:NH2	2.48	0.44
4:9:614:C:H2'	4:9:626:G:C4	2.53	0.44
4:9:1116:C:O2	4:9:1116:C:H2'	2.17	0.44
7:C:140:LYS:O	7:C:204:ARG:NH2	2.50	0.44
7:C:339:THR:HG22	7:C:342:ARG:NH2	2.33	0.44
58:MM:45:ARG:HH22	58:MM:71:GLU:CD	2.25	0.44
1:5:2089:G:H1'	1:5:2090:U:OP2	2.18	0.44
1:5:2372:U:O2'	33:d:46:LEU:HD13	2.18	0.44
1:5:2758:G:H2'	1:5:2759:G:C8	2.53	0.44
1:5:3607:U:H2'	1:5:3608:A:H8	1.83	0.44
1:5:4629:U:C2	1:5:4630:G:C8	3.05	0.44
4:9:1229:G:H2'	4:9:1230:C:O4'	2.18	0.44
58:MM:26:LEU:HD11	58:MM:89:VAL:HA	2.00	0.44
69:XX:50:ILE:HG23	69:XX:97:ASN:HA	1.98	0.44
81:13:4:C:H2'	81:13:5:A:C8	2.53	0.44
1:5:18:C:H4'	17:N:138:PHE:CE1	2.52	0.44
1:5:2809:G:O2'	1:5:4644:G:OP1	2.32	0.44
1:5:4524:G:H4'	1:5:4524:G:OP2	2.17	0.44
13:J:112:HIS:CE1	13:J:125:ILE:HA	2.53	0.44
26:W:101:ARG:HD2	52:GG:156:TYR:OH	2.17	0.44
29:Z:28:ASN:ND2	29:Z:30:ASP:OD1	2.48	0.44
41:m:89:CYS:O	41:m:92:THR:HG23	2.18	0.44
58:MM:84:LYS:HB3	58:MM:88:TRP:CZ2	2.53	0.44
67:VV:37:ALA:HB1	67:VV:46:PHE:CD1	2.53	0.44
1:5:4039:G:H4'	1:5:4049:U:H2'	1.99	0.44
4:9:164:A:H3'	4:9:165:G:N2	2.32	0.44
4:9:884:C:H2'	4:9:885:U:C6	2.53	0.44
22:S:41:LYS:HG2	22:S:61:ILE:HD13	2.00	0.44
27:X:72:ASP:OD1	27:X:73:HIS:N	2.45	0.44
44:p:38:THR:HA	44:p:45:THR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AA:2:SER:O	46:AA:8:LEU:HB2	2.18	0.44
80:12:43:G:C2	80:12:44:A:C5	3.06	0.44
1:5:1295:U:H4'	1:5:1296:G:O5'	2.18	0.43
1:5:1502:G:C8	1:5:1502:G:H5''	2.53	0.43
1:5:2478:C:N3	1:5:2479:G:C5	2.86	0.43
1:5:2725:A:N6	21:R:88:ARG:O	2.51	0.43
1:5:3642:A:C4	82:j:3:LYS:HB3	2.52	0.43
1:5:4064:C:H2'	1:5:4065:G:C8	2.53	0.43
4:9:1010:G:H2'	4:9:1011:A:H8	1.83	0.43
4:9:1556:A:H2'	4:9:1556:A:N3	2.33	0.43
6:B:47:LEU:HD23	6:B:166:THR:HG23	1.99	0.43
8:D:62:CYS:HB3	8:D:105:LEU:HD22	2.00	0.43
46:AA:15:VAL:HG21	63:RR:111:PHE:CD2	2.53	0.43
53:HH:192:PHE:O	53:HH:194:LEU:N	2.51	0.43
62:QQ:89:SER:OG	62:QQ:112:LEU:HD13	2.18	0.43
1:5:1662:C:H2'	1:5:1663:C:C6	2.53	0.43
1:5:3868:G:H22	1:5:3900:G:H1'	1.82	0.43
1:5:4238:G:H2'	1:5:4239:A:C8	2.53	0.43
4:9:561:A:H2'	4:9:562:U:C6	2.53	0.43
4:9:818:A:H4'	55:JJ:72:PHE:CE2	2.53	0.43
6:B:35:ASP:N	6:B:35:ASP:OD1	2.51	0.43
10:G:218:GLU:CD	17:N:26:ARG:HH21	2.26	0.43
46:AA:200:ASP:OD1	46:AA:200:ASP:N	2.50	0.43
1:5:1345:A:H2'	1:5:1346:C:C6	2.53	0.43
1:5:1973:G:H2'	1:5:1974:U:C5	2.52	0.43
1:5:2409:U:H5	1:5:2783:A:N1	2.16	0.43
4:9:809:A:OP1	50:EE:186:GLY:HA3	2.18	0.43
4:9:1692:U:H2'	4:9:1693:G:C8	2.52	0.43
9:E:216:THR:H	9:E:219:TYR:HB3	1.82	0.43
18:O:16:LEU:HD11	18:O:83:THR:HG21	2.00	0.43
21:R:160:GLU:OE1	21:R:163:ARG:NH2	2.35	0.43
50:EE:19:MET:HE2	50:EE:19:MET:HA	2.01	0.43
69:XX:91:LEU:HD23	76:ee:82:VAL:HG21	2.00	0.43
1:5:261:G:H2'	1:5:262:G:O4'	2.18	0.43
1:5:1333:A:H2'	1:5:1334:A:C8	2.52	0.43
1:5:2683:C:H2'	1:5:2684:C:C6	2.54	0.43
2:7:3:C:H2'	2:7:4:U:C6	2.52	0.43
4:9:1567:G:C6	64:SS:82:TRP:CD1	3.06	0.43
19:P:114:ILE:HA	19:P:150:LEU:HD23	2.01	0.43
22:S:1:MET:HE1	22:S:35:PRO:HD3	2.00	0.43
48:CC:94:ILE:HD12	48:CC:162:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1558:A:H2'	1:5:1559:G:C8	2.53	0.43
1:5:4266:G:N3	1:5:4266:G:H2'	2.33	0.43
1:5:4345:C:H2'	1:5:4346:U:C6	2.54	0.43
1:5:4574:U:H3'	1:5:4575:G:H5''	2.01	0.43
1:5:5064:G:O6	6:B:124:LYS:NZ	2.51	0.43
4:9:958:G:H2'	4:9:959:G:C8	2.54	0.43
4:9:1260:A:C2	4:9:1620:A:C8	3.06	0.43
4:9:1786:U:H2'	4:9:1787:G:H8	1.83	0.43
77:ff:83:LYS:HD2	77:ff:85:TYR:OH	2.19	0.43
82:j:21:ARG:NH2	82:j:41:ALA:O	2.47	0.43
1:5:216:C:H2'	1:5:217:C:H3'	2.01	0.43
1:5:971:U:H2'	1:5:971(A):G:C8	2.53	0.43
1:5:1064:G:C8	1:5:1064:G:O5'	2.71	0.43
1:5:2001:G:O5'	1:5:2001:G:C8	2.72	0.43
1:5:2567:G:H2'	1:5:2568:C:C6	2.52	0.43
1:5:2814:C:O2	1:5:2814:C:H2'	2.18	0.43
1:5:4950:U:O2'	1:5:4951:G:OP1	2.34	0.43
4:9:534:G:N2	4:9:551:U:O2	2.51	0.43
4:9:1797:U:H2'	4:9:1798:C:C6	2.54	0.43
50:EE:54:TYR:OH	50:EE:97:GLU:OE1	2.22	0.43
66:UU:24:LEU:HD22	66:UU:112:VAL:HG22	2.01	0.43
75:dd:3:HIS:CE1	75:dd:7:TYR:HB2	2.53	0.43
1:5:469:C:H2'	1:5:470:A:C8	2.53	0.43
1:5:711:A:H2'	1:5:712:C:C6	2.54	0.43
1:5:1358:G:H4'	1:5:1359:G:OP1	2.18	0.43
1:5:1402:C:H2'	1:5:1403:G:C8	2.54	0.43
1:5:2293:U:H2'	1:5:2294:G:C8	2.53	0.43
1:5:2711:G:O2'	1:5:2712:G:OP1	2.33	0.43
1:5:3876:A:H5''	1:5:3877:A:H5'	2.01	0.43
1:5:4169:G:H4'	1:5:4171:C:C2	2.52	0.43
4:9:1446:A:OP1	66:UU:58:THR:HG22	2.19	0.43
4:9:1462:U:H2'	4:9:1464:C:C5	2.53	0.43
4:9:1518:C:OP1	4:9:1519:U:H2'	2.19	0.43
20:Q:42:THR:O	20:Q:46:VAL:HG23	2.19	0.43
45:r:97:ILE:HD13	45:r:107:ARG:HA	2.00	0.43
48:CC:65:LYS:HD3	48:CC:273:LEU:HD13	2.00	0.43
59:NN:25:TRP:CG	73:bb:82:LYS:HE2	2.53	0.43
1:5:1739:G:N3	1:5:1742:A:N6	2.67	0.43
1:5:2409:U:H4'	1:5:2428:A:H4'	2.01	0.43
1:5:2431:A:P	40:l:41:ARG:HH12	2.42	0.43
1:5:2491:C:H2'	1:5:2492:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2730:U:H2'	1:5:2731:C:C6	2.54	0.43
39:k:24:LYS:HB3	39:k:67:LYS:HB3	2.01	0.43
46:AA:120:ARG:HH11	46:AA:120:ARG:HG2	1.84	0.43
46:AA:123:VAL:HG12	46:AA:145:ILE:HB	1.99	0.43
80:12:3:G:C6	80:12:71:G:C6	3.07	0.43
80:12:18:G:C4	80:12:57:G:C6	3.07	0.43
81:11:25:U:C2	81:11:26:G:C8	3.07	0.43
1:5:1075:G:N1	1:5:1235:G:N2	2.63	0.43
1:5:1637:A:N3	82:j:11:ARG:NH2	2.66	0.43
1:5:3949:A:H2'	1:5:3950:U:C6	2.54	0.43
1:5:4233:A:C8	1:5:4235:G:C8	3.06	0.43
4:9:15:U:H2'	4:9:16:G:O4'	2.19	0.43
4:9:153:G:H2'	4:9:154:U:C6	2.53	0.43
4:9:1780:G:H2'	4:9:1781:A:C8	2.54	0.43
6:B:80:GLU:OE1	6:B:323:TYR:OH	2.18	0.43
59:NN:25:TRP:CD2	73:bb:82:LYS:HE2	2.54	0.43
1:5:925:C:H3'	1:5:926:G:H5'	2.01	0.43
1:5:982:U:H2'	9:E:75:TYR:CE1	2.54	0.43
1:5:4090:G:OP1	10:G:305:LYS:NZ	2.30	0.43
1:5:4970:C:H2'	1:5:4971:A:H8	1.83	0.43
4:9:17:C:H2'	4:9:18:C:C6	2.53	0.43
19:P:114:ILE:HG23	19:P:114:ILE:O	2.19	0.43
22:S:15:ARG:HB3	22:S:27:LEU:HD23	2.01	0.43
51:FF:41:VAL:HG23	51:FF:42:LYS:N	2.33	0.43
3:8:14:U:C4	3:8:15:G:C6	3.07	0.42
4:9:51:U:H2'	4:9:52:G:C8	2.54	0.42
4:9:546:G:H2'	4:9:547:G:H8	1.84	0.42
10:G:119:GLN:HG3	17:N:28:TRP:CH2	2.54	0.42
22:S:50:GLN:HE22	22:S:125:GLN:HE22	1.67	0.42
32:c:18:LEU:O	32:c:22:MET:HG2	2.19	0.42
65:TT:27:LYS:HG3	65:TT:110:LEU:HD21	2.00	0.42
78:gg:11:LEU:HB3	78:gg:43:TRP:CZ3	2.54	0.42
1:5:181:C:N4	1:5:182:G:O6	2.52	0.42
1:5:1884:C:H4'	1:5:2070:U:C4	2.54	0.42
1:5:2065:G:H2'	1:5:2066:C:O4'	2.19	0.42
1:5:2376:A:H2'	1:5:2377:C:C6	2.54	0.42
1:5:4110:C:C2	1:5:4111:U:C5	3.07	0.42
4:9:58:C:H1'	4:9:59:U:C5	2.54	0.42
4:9:115:U:O2'	4:9:381:C:O2	2.26	0.42
4:9:124:U:OP1	50:EE:148:ARG:NH2	2.52	0.42
4:9:126:G:N2	4:9:180:G:H21	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1223:A:OP1	51:FF:79:HIS:HA	2.19	0.42
46:AA:23:THR:HG22	46:AA:170:SER:HB2	2.02	0.42
1:5:1786:A:H2'	1:5:1789:C:C5	2.54	0.42
4:9:383:G:H5'	4:9:383:G:H8	1.83	0.42
4:9:1114:U:H5''	4:9:1115:U:OP2	2.19	0.42
26:W:107:GLN:OE1	26:W:110:ARG:NH1	2.53	0.42
44:p:47:MET:HE2	44:p:57:CYS:HB2	2.01	0.42
48:CC:102:LEU:HG	48:CC:130:ILE:HG12	2.01	0.42
1:5:4068:U:H2'	1:5:4069:U:O4'	2.20	0.42
1:5:4238:G:H2'	1:5:4239:A:H8	1.83	0.42
1:5:4751:G:N1	1:5:4948:C:H5	2.14	0.42
4:9:916:A:C5	59:NN:73:ARG:HD3	2.55	0.42
6:B:92:TYR:HB3	6:B:99:LEU:HD22	2.00	0.42
1:5:264:C:H5''	1:5:265:C:OP2	2.19	0.42
1:5:1875:C:H2'	1:5:1876:U:C6	2.54	0.42
1:5:2276:A:H2'	1:5:2277:C:O4'	2.19	0.42
1:5:2562:G:N2	1:5:2565:A:OP2	2.44	0.42
1:5:2706:G:H3'	1:5:2707:U:H5''	2.01	0.42
4:9:406:U:O3'	4:9:407:G:H3'	2.19	0.42
4:9:552:G:H5'	76:ee:116:VAL:HG11	2.00	0.42
4:9:1665:G:OP2	65:TT:91:HIS:NE2	2.39	0.42
17:N:26:ARG:HH11	17:N:26:ARG:HG2	1.84	0.42
20:Q:154:LYS:HE2	20:Q:158:THR:CG2	2.50	0.42
46:AA:189:ILE:HD13	46:AA:195:TRP:CD1	2.55	0.42
1:5:70:A:OP2	30:a:67:GLN:NE2	2.47	0.42
1:5:1416:G:H2'	1:5:1417:C:C6	2.54	0.42
1:5:1494:U:H2'	1:5:1495:G:H8	1.84	0.42
2:7:85:G:OP1	14:K:221:LYS:NZ	2.40	0.42
4:9:318:A:N6	52:GG:186:GLN:HE22	2.11	0.42
4:9:804:U:H2'	4:9:805:U:H6	1.82	0.42
4:9:1120:U:H5''	73:bb:72:ARG:NH2	2.34	0.42
4:9:1491:G:H2'	4:9:1492:U:C6	2.54	0.42
48:CC:192:LEU:HB3	48:CC:227:ARG:HB3	2.01	0.42
1:5:4587:G:H5''	18:O:61:ARG:HH21	1.84	0.42
4:9:1402:A:H4'	66:UU:51:LYS:HE2	2.02	0.42
22:S:94:TYR:CE2	22:S:138:ARG:HD3	2.54	0.42
1:5:677:G:H2'	1:5:678:C:C6	2.55	0.42
1:5:927:G:C6	1:5:928:C:C4	3.08	0.42
1:5:966:A:H5''	1:5:967:C:C6	2.55	0.42
1:5:1947:U:C4	41:m:82:VAL:HG21	2.55	0.42
1:5:2844:A:O2'	1:5:4631:G:H4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3911:C:H2'	1:5:3912:U:C6	2.52	0.42
1:5:4037:C:H2'	1:5:4038:C:C6	2.55	0.42
3:8:52:A:H62	40:l:27:ILE:HD13	1.84	0.42
4:9:319:C:H4'	4:9:319:C:OP1	2.19	0.42
4:9:1786:U:H2'	4:9:1787:G:C8	2.54	0.42
6:B:189:THR:HG23	6:B:192:GLU:H	1.83	0.42
7:C:218:VAL:HA	7:C:229:LEU:CD1	2.50	0.42
7:C:283:LYS:HE3	7:C:283:LYS:HB2	1.88	0.42
24:U:101:ARG:HG2	24:U:115:PHE:CZ	2.54	0.42
33:d:53:ALA:HA	33:d:88:LEU:HD21	2.01	0.42
48:CC:134:ASN:OD1	48:CC:167:ARG:NH2	2.53	0.42
61:PP:13:ARG:NH2	61:PP:16:THR:OG1	2.48	0.42
1:5:1198:G:N2	1:5:1199:G:C6	2.88	0.42
1:5:1211:G:HO2'	1:5:1212:G:P	2.40	0.42
1:5:2705:G:N2	1:5:2712:G:H1'	2.34	0.42
1:5:3926:C:O2'	17:N:87:HIS:CE1	2.73	0.42
1:5:4047:A:O2'	1:5:4048:A:OP1	2.30	0.42
1:5:4876:A:OP2	22:S:165:PRO:HG3	2.20	0.42
4:9:1203:G:H2'	4:9:1204:A:C8	2.55	0.42
4:9:1531:A:H2'	4:9:1532:C:C6	2.54	0.42
10:G:140:LEU:HG	10:G:144:THR:HB	2.01	0.42
40:l:51:LEU:OXT	82:j:14:LYS:NZ	2.48	0.42
41:m:51:ILE:HD12	41:m:51:ILE:HA	1.88	0.42
55:JJ:178:ALA:O	55:JJ:182:GLN:HG2	2.20	0.42
78:gg:80:SER:O	78:gg:87:LEU:HD12	2.19	0.42
1:5:1510:G:H2'	1:5:1511:U:C6	2.56	0.41
1:5:4975:G:H4'	1:5:4976:U:O5'	2.19	0.41
4:9:1706:G:H2'	4:9:1707:U:C6	2.54	0.41
4:9:1865:C:OP2	72:aa:5:ARG:NH1	2.53	0.41
15:L:61:CYS:SG	15:L:71:ARG:HG3	2.60	0.41
33:d:26:THR:OG1	33:d:85:ARG:NH1	2.48	0.41
52:GG:103:ASP:CG	52:GG:105:ASN:HD22	2.27	0.41
58:MM:52:LEU:HD21	58:MM:62:VAL:HG13	2.01	0.41
78:gg:153:CYS:HB3	78:gg:198:VAL:HG12	2.02	0.41
1:5:465:G:H2'	1:5:466:A:H8	1.85	0.41
1:5:1435:G:O2'	1:5:2105:A:N1	2.48	0.41
1:5:1494:U:H2'	1:5:1495:G:C8	2.55	0.41
1:5:1960:A:H4'	1:5:1961:G:OP2	2.20	0.41
1:5:2712:G:C8	1:5:2712:G:H5'	2.56	0.41
1:5:2743:A:H2'	1:5:2744:A:C8	2.55	0.41
1:5:4507:A:H2'	1:5:4508:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4967:A:H2'	1:5:4968:A:C8	2.55	0.41
4:9:74:G:H2'	4:9:75:G:O4'	2.20	0.41
4:9:1115:U:O2'	4:9:1116:C:P	2.78	0.41
4:9:1454:A:C2	4:9:1476:A:H1'	2.55	0.41
6:B:288:GLY:HA3	6:B:330:PHE:CE2	2.55	0.41
81:11:66:C:H2'	81:11:67:U:C6	2.55	0.41
1:5:1590:C:H5''	1:5:1591:U:O5'	2.20	0.41
1:5:2465:C:H1'	1:5:3672:G:H22	1.85	0.41
1:5:3959:U:H1'	1:5:3960:A:O5'	2.20	0.41
1:5:4537:C:H2'	1:5:4538:G:C8	2.55	0.41
4:9:85:A:H2'	4:9:86:C:C6	2.55	0.41
4:9:1410:C:H2'	4:9:1411:G:H8	1.85	0.41
4:9:1500:G:H2'	4:9:1501:C:C6	2.56	0.41
9:E:206:ILE:O	9:E:206:ILE:HG22	2.21	0.41
52:GG:176:ILE:HG22	52:GG:179:LEU:HB2	2.02	0.41
1:5:922(A):G:H2'	1:5:922(B):C:C6	2.56	0.41
1:5:1237:C:H2'	14:K:50:TYR:CE1	2.56	0.41
1:5:4431:U:P	12:I:3:ARG:HH22	2.42	0.41
1:5:4508:C:N3	1:5:4512:U:H5	2.18	0.41
4:9:92:A:C6	4:9:446:G:C6	3.09	0.41
4:9:649:U:H2'	4:9:650:A:C8	2.55	0.41
4:9:1232:U:H2'	4:9:1233:G:C8	2.54	0.41
6:B:84:MET:HE1	6:B:183:ILE:HD11	2.03	0.41
43:o:66:ILE:HD12	43:o:88:CYS:SG	2.60	0.41
55:JJ:155:LYS:HG3	55:JJ:156:HIS:CD2	2.55	0.41
78:gg:8:ARG:N	78:gg:309:VAL:O	2.47	0.41
1:5:3917:A:H2'	1:5:3918:G:C8	2.54	0.41
1:5:4699:U:OP2	41:m:85:ARG:NH1	2.45	0.41
4:9:520:A:O2'	4:9:825:A:N3	2.40	0.41
4:9:1545:A:H2'	4:9:1546:G:C8	2.56	0.41
4:9:1851:A:H5'	4:9:1852:C:OP2	2.20	0.41
9:E:69:ALA:HA	9:E:71:TYR:CE2	2.55	0.41
19:P:38:GLY:H	19:P:114:ILE:HG23	1.86	0.41
53:HH:135:PHE:CG	53:HH:136:PRO:HA	2.55	0.41
58:MM:71:GLU:HG3	77:ff:114:ILE:HD11	2.03	0.41
81:13:74:C:HO2'	81:13:75:C:P	2.42	0.41
1:5:433:A:C2	1:5:3867:A:H4'	2.55	0.41
1:5:442:G:OP1	35:f:68:ARG:NH1	2.44	0.41
1:5:941:C:OP2	14:K:241:ARG:NE	2.37	0.41
1:5:1973:G:H2'	1:5:1974:U:C6	2.55	0.41
1:5:3801:U:O2	1:5:4497:U:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4232:U:H4'	1:5:4233:A:O5'	2.21	0.41
1:5:4305:G:N2	23:T:87:LYS:NZ	2.69	0.41
1:5:4970:C:H2'	1:5:4971:A:C8	2.55	0.41
4:9:517:C:H2'	4:9:518:G:O4'	2.20	0.41
4:9:1706:G:H2'	4:9:1707:U:H6	1.85	0.41
14:K:156:ARG:NH1	14:K:247:ASN:OXT	2.52	0.41
43:o:69:ARG:NH2	43:o:80:LYS:HE2	2.35	0.41
45:r:105:ASP:N	45:r:105:ASP:OD1	2.52	0.41
65:TT:75:MET:HA	65:TT:78:ILE:HG22	2.03	0.41
81:13:74:C:O2'	81:13:75:C:OP1	2.29	0.41
83:jj:500:HIS:HA	83:jj:534:THR:HG22	2.02	0.41
1:5:1442:C:H2'	1:5:1443:A:H8	1.86	0.41
1:5:1554:A:H5'	44:p:9:GLY:C	2.46	0.41
1:5:2559:G:C6	1:5:2569:G:C6	3.08	0.41
1:5:3816:A:OP1	1:5:3818:U:H5	2.04	0.41
1:5:3942:A:H2'	1:5:3943:A:C8	2.56	0.41
1:5:4305:G:H22	23:T:87:LYS:HD3	1.85	0.41
1:5:4518:A:N7	6:B:258:HIS:HE1	2.19	0.41
4:9:126:G:OP1	52:GG:198:ARG:NH1	2.38	0.41
4:9:420:G:H2'	4:9:660:C:H42	1.85	0.41
4:9:1182:A:C5	4:9:1183:A:H1'	2.56	0.41
4:9:1264:C:N3	4:9:1518:C:H5	2.18	0.41
4:9:1609:C:OP2	64:SS:132:ARG:HD3	2.21	0.41
53:HH:63:PHE:HA	53:HH:95:ILE:O	2.21	0.41
78:gg:64:HIS:CG	78:gg:65:PHE:H	2.39	0.41
1:5:318:A:H2'	1:5:319:A:H8	1.86	0.41
1:5:1200:G:H2'	1:5:1201:U:C6	2.56	0.41
1:5:1411(C):C:H2'	1:5:1412:G:C8	2.56	0.41
1:5:2097:A:OP1	1:5:2107:A:N6	2.54	0.41
1:5:2477:A:C6	1:5:2478:C:N4	2.88	0.41
1:5:2539:C:H2'	1:5:2540:C:C6	2.54	0.41
1:5:2822:G:N7	21:R:20:LYS:NZ	2.67	0.41
4:9:628:A:N6	4:9:1500:G:O2'	2.54	0.41
4:9:1277:C:H2'	4:9:1278:A:H8	1.86	0.41
4:9:1524:G:O2'	81:13:30:G:OP1	2.35	0.41
50:EE:104:ASP:OD1	50:EE:107:GLY:N	2.54	0.41
83:jj:150:ARG:NH2	83:jj:381:ASN:OD1	2.41	0.41
1:5:70:A:P	30:a:67:GLN:HE21	2.44	0.41
1:5:116:G:H2'	1:5:117:C:C6	2.56	0.41
1:5:268:G:H2'	1:5:269:G:C8	2.56	0.41
1:5:347:A:H2'	1:5:348:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:438:G:OP2	34:e:18:LYS:NZ	2.51	0.41
1:5:964:A:H2'	1:5:965:G:C8	2.56	0.41
1:5:977:C:N4	1:5:978:G:O6	2.54	0.41
1:5:1176:C:H2'	1:5:1177:U:C6	2.56	0.41
1:5:1314:C:C2	1:5:1315:C:C5	3.08	0.41
1:5:1836:G:H4'	1:5:1837:A:O5'	2.20	0.41
1:5:1964:A:H3'	1:5:1965:G:H8	1.86	0.41
1:5:2404:A:OP2	40:l:2:SER:OG	2.28	0.41
1:5:2421:G:N3	1:5:2421:G:H5'	2.36	0.41
1:5:2602:G:H2'	1:5:2603:C:C6	2.56	0.41
1:5:2696:A:H62	39:k:35:LYS:NZ	2.19	0.41
1:5:3652:A:H2'	1:5:3653:A:C8	2.55	0.41
1:5:3657:U:OP1	5:A:245:ARG:NH1	2.53	0.41
1:5:3751:G:N2	1:5:3775:A:H8	2.16	0.41
1:5:3860:A:N3	19:P:131:ARG:NH1	2.56	0.41
1:5:4884:G:H2'	1:5:4885:U:O4'	2.21	0.41
4:9:158:A:N6	4:9:466:G:C6	2.89	0.41
4:9:572:U:OP1	70:YY:59:GLY:N	2.54	0.41
4:9:1413:G:H2'	4:9:1414:A:H8	1.85	0.41
4:9:1700:C:C2	4:9:1834:A:N6	2.89	0.41
47:BB:129:THR:OG1	47:BB:131:ASP:OD1	2.37	0.41
51:FF:76:MET:HB2	51:FF:89:THR:CG2	2.51	0.41
55:JJ:50:LEU:HD13	55:JJ:105:PHE:CE1	2.56	0.41
83:jj:572:LYS:HE2	83:jj:574:LEU:HD21	2.02	0.41
1:5:647:G:C5	1:5:648:G:C8	3.09	0.41
1:5:989:U:H2'	1:5:990:C:C6	2.55	0.41
1:5:1757:U:H2'	1:5:1758:G:H8	1.86	0.41
1:5:2306:G:H1'	1:5:2332:A:N6	2.35	0.41
1:5:2787:A:N3	1:5:2787:A:H2'	2.36	0.41
1:5:2899:C:OP1	21:R:108:ARG:NH2	2.37	0.41
1:5:3827:G:O2'	1:5:3829:G:OP2	2.34	0.41
1:5:3953:G:H2'	1:5:3954:A:H8	1.85	0.41
4:9:85:A:H2'	4:9:86:C:H6	1.86	0.41
4:9:502:C:C5	50:EE:66:MET:HB3	2.56	0.41
4:9:1615:U:C2	4:9:1616:U:C5	3.09	0.41
4:9:1664:A:H4'	4:9:1665:G:OP1	2.21	0.41
4:9:1679:A:OP1	51:FF:60:ARG:NH2	2.53	0.41
11:H:36:ARG:HD3	11:H:38:PHE:CZ	2.56	0.41
48:CC:253:PRO:HA	48:CC:256:TRP:CE2	2.55	0.41
51:FF:80:GLY:HA2	51:FF:83:ASN:ND2	2.36	0.41
59:NN:87:ASP:OD1	59:NN:87:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:12:54:U:H5''	80:12:55:U:OP2	2.21	0.41
81:13:62:C:H2'	81:13:63:A:C8	2.56	0.41
1:5:1234:G:C6	1:5:1235:G:C6	3.09	0.40
1:5:3644:U:O2	1:5:4554:G:O2'	2.39	0.40
1:5:4594:U:H2'	1:5:4595:G:C8	2.55	0.40
2:7:110:G:H2'	2:7:111:C:C6	2.56	0.40
4:9:14:C:OP2	48:CC:232:THR:HG21	2.22	0.40
4:9:62:G:H4'	4:9:172:U:C5	2.55	0.40
4:9:181:A:H3'	4:9:182:C:H2'	2.03	0.40
4:9:529:A:H2'	4:9:530:U:H6	1.86	0.40
4:9:634:A:H2'	4:9:635:G:H8	1.86	0.40
4:9:1413:G:H2'	4:9:1414:A:C8	2.56	0.40
6:B:258:HIS:HA	6:B:260:ALA:N	2.36	0.40
7:C:189:MET:HE1	7:C:200:ARG:HG3	2.03	0.40
8:D:41:LYS:HG3	23:T:93:ILE:HG13	2.02	0.40
8:D:68:ARG:HD3	8:D:68:ARG:HA	1.91	0.40
9:E:186:ARG:HD2	9:E:186:ARG:HA	1.97	0.40
12:I:152:LEU:O	12:I:156:LYS:HG3	2.21	0.40
17:N:155:VAL:O	17:N:162:ARG:NH2	2.54	0.40
44:p:8:VAL:O	44:p:11:VAL:HG22	2.21	0.40
58:MM:85:LEU:O	58:MM:89:VAL:HG22	2.21	0.40
78:gg:29:ASP:HA	78:gg:47:ARG:HH22	1.85	0.40
1:5:76:A:OP2	15:L:74:ARG:NH1	2.53	0.40
1:5:492:U:H4'	1:5:493:G:OP2	2.20	0.40
1:5:729:G:H5'	1:5:729:G:N3	2.36	0.40
1:5:1279:A:O2'	7:C:323:ARG:NH2	2.54	0.40
1:5:1633:G:H5'	1:5:1634:A:OP1	2.21	0.40
1:5:1812:C:H2'	1:5:1813:U:H6	1.85	0.40
1:5:2340:C:H5'	7:C:42:THR:HG21	2.03	0.40
1:5:2544:G:C8	3:8:126:C:C2	3.10	0.40
1:5:3907:G:H5'	1:5:4449:A:C2	2.56	0.40
1:5:4134:C:H2'	1:5:4135:G:H8	1.86	0.40
4:9:360:A:C2	4:9:363:A:C8	3.08	0.40
4:9:589:G:C4	4:9:591:U:C5	3.09	0.40
4:9:1614:A:H2'	4:9:1615:U:H6	1.87	0.40
4:9:1866:A:N1	72:aa:87:ARG:HD2	2.36	0.40
7:C:29:LYS:HB2	7:C:267:TRP:HH2	1.85	0.40
7:C:147:VAL:HG13	7:C:148:PRO:HD2	2.03	0.40
12:I:38:ARG:HH22	12:I:45:GLU:CD	2.29	0.40
46:AA:32:PHE:CE1	46:AA:33:GLN:HG3	2.57	0.40
50:EE:45:ILE:HD12	50:EE:80:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:KK:59:LYS:HE3	56:KK:59:LYS:HB3	1.93	0.40
61:PP:37:TYR:HB3	61:PP:41:GLN:HB2	2.03	0.40
83:jj:164:ALA:HA	83:jj:251:ILE:HB	2.02	0.40
1:5:966:A:H1'	1:5:968:C:N4	2.37	0.40
1:5:4562:C:H2'	1:5:4563:U:C6	2.56	0.40
4:9:71:G:C6	4:9:79:A:C8	3.10	0.40
4:9:182:C:H4'	4:9:183:G:O5'	2.21	0.40
4:9:794:A:H2'	4:9:795:A:C8	2.56	0.40
4:9:803:C:H2'	4:9:804:U:C6	2.56	0.40
4:9:1083:A:H4'	4:9:1085:C:C4	2.56	0.40
4:9:1323:U:H2'	4:9:1324:G:C8	2.56	0.40
4:9:1401:A:H2'	4:9:1402:A:C8	2.55	0.40
4:9:1499:U:H5''	49:DD:176:LEU:HD21	2.04	0.40
4:9:1809:A:H2'	4:9:1810:U:C6	2.57	0.40
5:A:226:ARG:NE	5:A:228:ASP:OD1	2.48	0.40
48:CC:170:TRP:CE2	68:WW:97:ARG:HD2	2.55	0.40
52:GG:52:ILE:HG23	52:GG:52:ILE:O	2.21	0.40
73:bb:47:PHE:CE2	73:bb:49:HIS:HB2	2.57	0.40
83:jj:311:ASP:OD1	83:jj:366:SER:OG	2.32	0.40
1:5:163:A:H2'	1:5:164:G:H8	1.86	0.40
1:5:517:C:H2'	1:5:518:G:C8	2.55	0.40
1:5:1189:G:C6	1:5:1190:C:C4	3.08	0.40
1:5:1440:U:H2'	1:5:1441:C:C5	2.57	0.40
1:5:1554:A:OP2	44:p:4:ARG:NH1	2.44	0.40
1:5:1985:G:H1'	1:5:2003:G:H2'	2.02	0.40
1:5:4494:G:C6	1:5:4507:A:N1	2.89	0.40
4:9:522:A:H5''	55:JJ:145:PRO:HD2	2.02	0.40
24:U:84:LYS:HA	24:U:87:THR:HG22	2.03	0.40
25:V:123:LYS:NZ	25:V:127:ASP:OD2	2.48	0.40
46:AA:58:LEU:HD21	46:AA:177:MET:HB3	2.04	0.40
55:JJ:155:LYS:HE3	55:JJ:156:HIS:CE1	2.56	0.40
61:PP:41:GLN:NE2	61:PP:113:GLY:O	2.53	0.40
80:12:37:C:H2'	80:12:38:A:O4'	2.22	0.40
1:5:2093:G:N2	1:5:2262:G:H1	2.20	0.40
1:5:2299:G:H5''	1:5:2300:A:OP2	2.20	0.40
1:5:3748:A:H2'	1:5:3749:C:C6	2.57	0.40
13:J:112:HIS:HE1	13:J:125:ILE:HA	1.85	0.40
22:S:78:PHE:O	22:S:96:GLU:HA	2.21	0.40
22:S:82:LEU:HD21	22:S:109:CYS:SG	2.61	0.40
52:GG:102:VAL:HG11	52:GG:109:LEU:HD11	2.04	0.40
52:GG:232:ARG:HA	52:GG:235:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SS:23:ARG:HB3	71:ZZ:48:VAL:HG11	2.04	0.40
79:10:22:U:O2'	79:10:23:A:OP1	2.34	0.40
81:11:11:G:C2	81:11:26:G:H1'	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	246/257 (96%)	239 (97%)	7 (3%)	0	100	100
6	B	392/403 (97%)	375 (96%)	17 (4%)	0	100	100
7	C	360/425 (85%)	350 (97%)	10 (3%)	0	100	100
8	D	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
9	E	208/291 (72%)	200 (96%)	8 (4%)	0	100	100
10	G	229/319 (72%)	221 (96%)	8 (4%)	0	100	100
11	H	188/192 (98%)	179 (95%)	9 (5%)	0	100	100
12	I	201/214 (94%)	198 (98%)	3 (2%)	0	100	100
13	J	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
14	K	223/247 (90%)	217 (97%)	6 (3%)	0	100	100
15	L	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
16	M	136/218 (62%)	135 (99%)	1 (1%)	0	100	100
17	N	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
18	O	197/203 (97%)	192 (98%)	5 (2%)	0	100	100
19	P	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
20	Q	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
21	R	178/196 (91%)	178 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	S	174/176 (99%)	171 (98%)	2 (1%)	1 (1%)	21	51
23	T	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
24	U	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
25	V	127/140 (91%)	124 (98%)	3 (2%)	0	100	100
26	W	102/157 (65%)	101 (99%)	1 (1%)	0	100	100
27	X	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
28	Y	132/145 (91%)	127 (96%)	5 (4%)	0	100	100
29	Z	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
30	a	145/148 (98%)	138 (95%)	7 (5%)	0	100	100
31	b	94/245 (38%)	91 (97%)	3 (3%)	0	100	100
32	c	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
33	d	105/125 (84%)	99 (94%)	6 (6%)	0	100	100
34	e	126/135 (93%)	125 (99%)	1 (1%)	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%)	115 (96%)	5 (4%)	0	100	100
38	i	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
39	k	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
40	l	48/51 (94%)	48 (100%)	0	0	100	100
41	m	50/102 (49%)	47 (94%)	3 (6%)	0	100	100
42	n	23/25 (92%)	23 (100%)	0	0	100	100
43	o	102/106 (96%)	97 (95%)	5 (5%)	0	100	100
44	p	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
45	r	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
46	AA	215/295 (73%)	211 (98%)	4 (2%)	0	100	100
47	BB	211/264 (80%)	203 (96%)	8 (4%)	0	100	100
48	CC	219/293 (75%)	215 (98%)	4 (2%)	0	100	100
49	DD	222/243 (91%)	220 (99%)	2 (1%)	0	100	100
50	EE	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
51	FF	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
52	GG	235/249 (94%)	232 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	HH	181/194 (93%)	173 (96%)	8 (4%)	0	100	100
54	II	194/208 (93%)	191 (98%)	3 (2%)	0	100	100
55	JJ	179/194 (92%)	177 (99%)	2 (1%)	0	100	100
56	KK	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
57	LL	139/158 (88%)	136 (98%)	3 (2%)	0	100	100
58	MM	108/132 (82%)	105 (97%)	3 (3%)	0	100	100
59	NN	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
60	OO	134/168 (80%)	131 (98%)	3 (2%)	0	100	100
61	PP	127/145 (88%)	123 (97%)	4 (3%)	0	100	100
62	QQ	140/146 (96%)	137 (98%)	3 (2%)	0	100	100
63	RR	130/135 (96%)	124 (95%)	6 (5%)	0	100	100
64	SS	138/152 (91%)	135 (98%)	3 (2%)	0	100	100
65	TT	139/145 (96%)	138 (99%)	1 (1%)	0	100	100
66	UU	98/119 (82%)	97 (99%)	1 (1%)	0	100	100
67	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
68	WW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
69	XX	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
70	YY	122/130 (94%)	121 (99%)	1 (1%)	0	100	100
71	ZZ	73/125 (58%)	72 (99%)	1 (1%)	0	100	100
72	aa	99/115 (86%)	95 (96%)	4 (4%)	0	100	100
73	bb	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
74	cc	60/69 (87%)	59 (98%)	1 (2%)	0	100	100
75	dd	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
76	ee	55/133 (41%)	55 (100%)	0	0	100	100
77	ff	66/156 (42%)	62 (94%)	4 (6%)	0	100	100
78	gg	311/317 (98%)	296 (95%)	15 (5%)	0	100	100
82	j	84/97 (87%)	80 (95%)	4 (5%)	0	100	100
83	jj	511/703 (73%)	486 (95%)	25 (5%)	0	100	100
All	All	11657/13594 (86%)	11331 (97%)	325 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	S	155	PRO

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%)	174 (99%)	1 (1%)	78	93
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%)	157 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	Y	124/135 (92%)	124 (100%)	0	100	100
29	Z	117/118 (99%)	117 (100%)	0	100	100
30	a	119/120 (99%)	119 (100%)	0	100	100
31	b	80/184 (44%)	80 (100%)	0	100	100
32	c	84/98 (86%)	84 (100%)	0	100	100
33	d	98/110 (89%)	98 (100%)	0	100	100
34	e	114/121 (94%)	114 (100%)	0	100	100
35	f	88/89 (99%)	88 (100%)	0	100	100
36	g	98/99 (99%)	98 (100%)	0	100	100
37	h	109/110 (99%)	109 (100%)	0	100	100
38	i	86/89 (97%)	86 (100%)	0	100	100
39	k	64/65 (98%)	64 (100%)	0	100	100
40	l	47/48 (98%)	47 (100%)	0	100	100
41	m	48/90 (53%)	48 (100%)	0	100	100
42	n	24/24 (100%)	24 (100%)	0	100	100
43	o	92/94 (98%)	92 (100%)	0	100	100
44	p	74/75 (99%)	74 (100%)	0	100	100
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%)	81	93
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%)	164 (99%)	1 (1%)	78	93
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%)	93 (99%)	1 (1%)	65	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	NN	130/131 (99%)	130 (100%)	0	100	100
60	OO	106/130 (82%)	105 (99%)	1 (1%)	70	90
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%)	110 (99%)	1 (1%)	70	90
66	UU	92/107 (86%)	92 (100%)	0	100	100
67	VV	67/67 (100%)	67 (100%)	0	100	100
68	WW	112/113 (99%)	112 (100%)	0	100	100
69	XX	112/115 (97%)	112 (100%)	0	100	100
70	YY	107/112 (96%)	107 (100%)	0	100	100
71	ZZ	66/103 (64%)	66 (100%)	0	100	100
72	aa	88/98 (90%)	88 (100%)	0	100	100
73	bb	75/76 (99%)	75 (100%)	0	100	100
74	cc	55/62 (89%)	55 (100%)	0	100	100
75	dd	48/49 (98%)	48 (100%)	0	100	100
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%)	10175 (100%)	6 (0%)	87	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	L	67	HIS
48	CC	248	TYR
53	HH	72	PHE
58	MM	95	ASP
60	OO	46	ASP
65	TT	33	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	97	ASN
5	A	216	HIS
6	B	167	GLN
6	B	184	GLN
6	B	186	ASN
6	B	204	GLN
6	B	276	HIS
6	B	301	ASN
6	B	315	ASN
6	B	376	HIS
7	C	21	ASN
7	C	38	ASN
8	D	225	GLN
8	D	282	GLN
9	E	170	GLN
9	E	185	ASN
9	E	253	GLN
10	G	99	GLN
10	G	134	ASN
10	G	202	ASN
12	I	59	GLN
12	I	100	ASN
12	I	213	HIS
13	J	71	HIS
13	J	104	ASN
14	K	79	ASN
14	K	162	ASN
14	K	199	HIS
14	K	204	ASN
15	L	104	ASN
16	M	20	HIS
17	N	8	GLN
17	N	29	GLN
17	N	87	HIS
18	O	50	ASN
18	O	167	HIS
19	P	25	HIS
20	Q	7	HIS
20	Q	57	ASN
21	R	141	HIS
21	R	143	HIS

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Mol	Chain	Res	Type
22	S	50	GLN
23	T	66	ASN
23	T	98	HIS
24	U	94	ASN
25	V	36	ASN
25	V	77	HIS
26	W	59	HIS
26	W	104	GLN
27	X	93	ASN
27	X	107	HIS
27	X	151	ASN
28	Y	20	ASN
28	Y	72	GLN
29	Z	78	ASN
30	a	14	HIS
30	a	120	GLN
31	b	101	HIS
32	c	40	GLN
32	c	72	HIS
33	d	79	ASN
33	d	100	ASN
33	d	116	ASN
35	f	21	GLN
37	h	20	GLN
38	i	20	ASN
41	m	61	GLN
41	m	94	ASN
44	p	92	GLN
45	r	45	HIS
45	r	70	GLN
46	AA	169	HIS
47	BB	95	ASN
47	BB	163	GLN
47	BB	208	HIS
49	DD	159	HIS
49	DD	226	GLN
51	FF	137	GLN
51	FF	203	ASN
52	GG	105	ASN
52	GG	163	ASN
52	GG	186	GLN
53	HH	25	GLN

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Mol	Chain	Res	Type
53	HH	44	ASN
53	HH	73	GLN
53	HH	186	ASN
55	JJ	111	GLN
55	JJ	113	GLN
55	JJ	124	HIS
57	LL	94	HIS
57	LL	112	HIS
60	OO	32	HIS
60	OO	79	GLN
61	PP	79	HIS
61	PP	114	HIS
61	PP	128	HIS
62	QQ	29	ASN
62	QQ	80	GLN
62	QQ	86	GLN
65	TT	12	GLN
66	UU	92	HIS
68	WW	90	GLN
69	XX	16	HIS
69	XX	73	GLN
69	XX	87	ASN
70	YY	19	GLN
71	ZZ	89	GLN
72	aa	17	HIS
72	aa	43	ASN
75	dd	3	HIS
75	dd	4	GLN
75	dd	37	ASN
78	gg	64	HIS
78	gg	133	ASN
78	gg	143	GLN
78	gg	222	ASN
82	j	76	HIS
83	jj	126	GLN
83	jj	436	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3579/3601 (99%)	541 (15%)	170 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	7	118/120 (98%)	6 (5%)	1 (0%)
3	8	150/156 (96%)	23 (15%)	5 (3%)
4	9	1685/1869 (90%)	243 (14%)	64 (3%)
79	10	10/185 (5%)	2 (20%)	1 (10%)
80	12	74/76 (97%)	12 (16%)	4 (5%)
81	11	73/75 (97%)	9 (12%)	4 (5%)
81	13	73/75 (97%)	10 (13%)	4 (5%)
All	All	5762/6157 (93%)	846 (14%)	253 (4%)

All (846) 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	58	G
1	5	59	A
1	5	65	A
1	5	73	A
1	5	91	G
1	5	109	G
1	5	119	G
1	5	120	A
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	173	C
1	5	197	A
1	5	200	U
1	5	201	C
1	5	209	U
1	5	217	C

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Mol	Chain	Res	Type
1	5	218	A
1	5	219	G
1	5	220	C
1	5	224	U
1	5	226	G
1	5	227	A
1	5	233	U
1	5	234	G
1	5	246	G
1	5	265	C
1	5	266	C
1	5	267	G
1	5	275	C
1	5	276	C
1	5	280	G
1	5	297	U
1	5	306	A
1	5	310	G
1	5	315	G
1	5	316	U
1	5	334	A
1	5	340	C
1	5	379	G
1	5	386	A
1	5	387	G
1	5	407	A
1	5	409	G
1	5	410	A
1	5	412	G
1	5	413	G
1	5	431	G
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	482	G
1	5	483	G
1	5	486	C

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Mol	Chain	Res	Type
1	5	493	G
1	5	498	C
1	5	499	G
1	5	505	G
1	5	510	U
1	5	666	G
1	5	683	C
1	5	685	C
1	5	686	A
1	5	696	C
1	5	697	G
1	5	704	C
1	5	705	G
1	5	730	G
1	5	731	G
1	5	738	C
1	5	738(A)	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	916	C
1	5	917	A
1	5	923	C
1	5	924	C
1	5	925	C
1	5	926	G
1	5	929	A
1	5	931	C
1	5	932	A
1	5	933	G
1	5	934	C
1	5	935	A
1	5	935(A)	G
1	5	936	C
1	5	941	C
1	5	943	A
1	5	944	A
1	5	945	U

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Mol	Chain	Res	Type
1	5	959	G
1	5	960	A
1	5	961	G
1	5	967	C
1	5	969	C
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	1195	G
1	5	1204	C
1	5	1211	G
1	5	1212	G
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	1248	C
1	5	1249	C
1	5	1250	C
1	5	1272	C
1	5	1273	G
1	5	1283	G
1	5	1284	G
1	5	1287	G
1	5	1292	C
1	5	1293	G
1	5	1294	A
1	5	1296	G
1	5	1301	C
1	5	1304	C
1	5	1326	A
1	5	1337	A
1	5	1339	U
1	5	1354	A

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Mol	Chain	Res	Type
1	5	1359	G
1	5	1360	G
1	5	1370	G
1	5	1371	A
1	5	1377	G
1	5	1381	U
1	5	1387	A
1	5	1394	G
1	5	1397	A
1	5	1398	A
1	5	1421	G
1	5	1437	C
1	5	1438	U
1	5	1441	C
1	5	1445	U
1	5	1446	C
1	5	1455	G
1	5	1456	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

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Mol	Chain	Res	Type
1	5	1654	G
1	5	1661	C
1	5	1676	C
1	5	1677	U
1	5	1691	G
1	5	1742	A
1	5	1750	G
1	5	1755	C
1	5	1756	U
1	5	1761	G
1	5	1764	G
1	5	1766	A
1	5	1768	C
1	5	1769	G
1	5	1773	U
1	5	1774	C
1	5	1787	A
1	5	1805	A
1	5	1821	G
1	5	1822	U
1	5	1836	G
1	5	1837	A
1	5	1842	G
1	5	1855	G
1	5	1869	G
1	5	1897	A
1	5	1899	G
1	5	1918	U
1	5	1919	G
1	5	1920	C
1	5	1921	C
1	5	1922	G
1	5	1923	A
1	5	1940	G
1	5	1948	G
1	5	1958	A
1	5	1962	A
1	5	1964	A
1	5	1978	C
1	5	1980	U
1	5	1981	G
1	5	1984	A

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Mol	Chain	Res	Type
1	5	1987	C
1	5	1991	A
1	5	1992	U
1	5	1993	C
1	5	2001	G
1	5	2002	A
1	5	2005	G
1	5	2008	U
1	5	2011	C
1	5	2026	A
1	5	2042	A
1	5	2043	A
1	5	2044	U
1	5	2048	U
1	5	2052	G
1	5	2055	G
1	5	2056	G
1	5	2064	G
1	5	2069	A
1	5	2084	U
1	5	2089	G
1	5	2090	U
1	5	2092	G
1	5	2093	G
1	5	2094	C
1	5	2097	A
1	5	2098	G
1	5	2100	G
1	5	2101	A
1	5	2102	G
1	5	2104	A
1	5	2106	G
1	5	2107	A
1	5	2108	G
1	5	2110	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

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Mol	Chain	Res	Type
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	2447	U
1	5	2471	G
1	5	2475	G
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2503	G
1	5	2504	C
1	5	2513	A
1	5	2520	C
1	5	2546	G
1	5	2547	G
1	5	2553	A
1	5	2554	U
1	5	2555	G
1	5	2587	A
1	5	2601	A
1	5	2627	C
1	5	2669	C
1	5	2686	G
1	5	2687	U
1	5	2695	A
1	5	2696	A
1	5	2705	G
1	5	2708	U
1	5	2710	C
1	5	2711	G
1	5	2712	G
1	5	2719	C
1	5	2726	G

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Mol	Chain	Res	Type
1	5	2740	U
1	5	2743	A
1	5	2760	G
1	5	2761	U
1	5	2763	U
1	5	2764	A
1	5	2772	C
1	5	2787	A
1	5	2788	U
1	5	2789	A
1	5	2790	U
1	5	2794	C
1	5	2795	A
1	5	2796	G
1	5	2806	A
1	5	2807	A
1	5	2826	U
1	5	2827	G
1	5	2842	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	3662	A
1	5	3672	G
1	5	3673	C
1	5	3674	G
1	5	3711	A
1	5	3712	A
1	5	3748	A
1	5	3753	G
1	5	3759	A
1	5	3760	A
1	5	3777	G
1	5	3783	A
1	5	3784	A

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Mol	Chain	Res	Type
1	5	3811	G
1	5	3812	C
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3838	U
1	5	3839	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
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	4041	C
1	5	4042	G
1	5	4046	A
1	5	4047	A
1	5	4048	A
1	5	4049	U
1	5	4069	U
1	5	4076	G
1	5	4084	G
1	5	4097	G

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Mol	Chain	Res	Type
1	5	4115	G
1	5	4116	C
1	5	4119	C
1	5	4120	U
1	5	4121	G
1	5	4122	G
1	5	4125	C
1	5	4127	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	4196	G
1	5	4213	A
1	5	4229	U
1	5	4233	A
1	5	4251	A
1	5	4255	A
1	5	4266	G
1	5	4268	A
1	5	4271	A
1	5	4273	A
1	5	4281	A
1	5	4291	G
1	5	4305	G
1	5	4329	G
1	5	4330	G
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	4391	G
1	5	4394	A
1	5	4395	U
1	5	4396	A

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Mol	Chain	Res	Type
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	4464	A
1	5	4475	G
1	5	4476	C
1	5	4488	A
1	5	4489	G
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	4567	G
1	5	4572	U
1	5	4573	G
1	5	4575	G
1	5	4590	A
1	5	4627	U
1	5	4635	A
1	5	4636	U
1	5	4637	G
1	5	4656	A
1	5	4670	C
1	5	4672	A
1	5	4700	A
1	5	4708	A
1	5	4709	U
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

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Mol	Chain	Res	Type
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	4876	A
1	5	4877	G
1	5	4882	U
1	5	4883	C
1	5	4885	U
1	5	4894	A
1	5	4895	C
1	5	4909	A
1	5	4910	A
1	5	4913	G
1	5	4914	G
1	5	4915	G
1	5	4919	G
1	5	4921	C
1	5	4922	C
1	5	4925	U
1	5	4926	C
1	5	4931	G
1	5	4937	C
1	5	4944	C
1	5	4945	G
1	5	4948	C
1	5	4949	G
1	5	4951	G
1	5	4956	A
1	5	4958	C
1	5	4976	U
1	5	4979	A
1	5	4988	U
1	5	4989	U
1	5	4990	C
1	5	4991	U
1	5	4993	G
1	5	5017	G
1	5	5041	G

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Mol	Chain	Res	Type
1	5	5047	C
1	5	5050	C
1	5	5054	C
1	5	5058	A
1	5	5061	A
1	5	5062	G
1	5	5069	U
2	7	7	G
2	7	42	A
2	7	53	U
2	7	64	G
2	7	100	A
2	7	110	G
3	8	2	G
3	8	3	A
3	8	34	U
3	8	35	C
3	8	49	G
3	8	59	A
3	8	62	A
3	8	63	U
3	8	87	G
3	8	104	A
3	8	105	C
3	8	109	C
3	8	110	U
3	8	111	U
3	8	112	G
3	8	114	G
3	8	122	G
3	8	123	U
3	8	124	U
3	8	125	C
3	8	126	C
3	8	127	U
3	8	137	A
4	9	4	C
4	9	17	C
4	9	25	A
4	9	26	U
4	9	33	G
4	9	41	G

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Mol	Chain	Res	Type
4	9	46	A
4	9	56	G
4	9	67	C
4	9	68	A
4	9	73	C
4	9	74	G
4	9	75	G
4	9	79	A
4	9	103	A
4	9	111	A
4	9	113	G
4	9	115	U
4	9	126	G
4	9	127	C
4	9	130	G
4	9	143	U
4	9	147	A
4	9	155	G
4	9	161	U
4	9	183	G
4	9	184	G
4	9	192	C
4	9	215	G
4	9	302	A
4	9	308	G
4	9	312	G
4	9	314	U
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	383	G
4	9	384	U
4	9	385	G
4	9	386	C
4	9	400	C
4	9	401	A
4	9	408	A
4	9	409	C
4	9	418	A

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Mol	Chain	Res	Type
4	9	428	U
4	9	448	A
4	9	449	A
4	9	450	C
4	9	452	G
4	9	465	A
4	9	466	G
4	9	472	C
4	9	474	G
4	9	482	G
4	9	487	U
4	9	492	C
4	9	496	C
4	9	516	A
4	9	517	C
4	9	525	A
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
4	9	555	A
4	9	556	U
4	9	559	G
4	9	561	A
4	9	562	U
4	9	571	U
4	9	587	A
4	9	588	G
4	9	590	A
4	9	591	U
4	9	592	C
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

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Mol	Chain	Res	Type
4	9	643	A
4	9	644	G
4	9	655	A
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	847	A
4	9	859	G
4	9	867	G
4	9	868	G
4	9	869	A
4	9	870	A
4	9	871	U
4	9	872	A
4	9	873	G
4	9	874	G
4	9	875	A
4	9	876	C
4	9	887	U
4	9	888	U
4	9	889	U
4	9	909	G
4	9	912	C
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

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Mol	Chain	Res	Type
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	1119	A
4	9	1138	C
4	9	1139	C
4	9	1149	A
4	9	1150	A
4	9	1153	C
4	9	1154	U
4	9	1165	G
4	9	1166	G
4	9	1195	A
4	9	1207	G
4	9	1208	A
4	9	1215	C
4	9	1216	C
4	9	1240	A
4	9	1241	A
4	9	1242	U
4	9	1251	A
4	9	1253	A
4	9	1254	C
4	9	1256	G
4	9	1257	G
4	9	1259	A
4	9	1274	G
4	9	1275	G
4	9	1276	A
4	9	1284	A
4	9	1285	G
4	9	1286	G
4	9	1293	A
4	9	1300	U
4	9	1301	A
4	9	1302	G

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Mol	Chain	Res	Type
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	1454	A
4	9	1455	A
4	9	1462	U
4	9	1463	U
4	9	1464	C
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	1552	G
4	9	1553	C
4	9	1556	A
4	9	1557	C
4	9	1574	C
4	9	1579	A
4	9	1580	A
4	9	1581	C
4	9	1587	G
4	9	1588	A
4	9	1601	A
4	9	1603	G
4	9	1604	G
4	9	1621	U
4	9	1623	A
4	9	1637	A
4	9	1638	G
4	9	1639	G
4	9	1648	G
4	9	1654	G

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Mol	Chain	Res	Type
4	9	1665	G
4	9	1680	G
4	9	1699	A
4	9	1721	U
4	9	1722	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	1800	A
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	1852	C
4	9	1861	G
4	9	1863	A
4	9	1865	C
4	9	1869	A
79	10	19	U
79	10	23	A
80	12	10	G
80	12	13	C
80	12	19	G
80	12	20	G
80	12	21	A
80	12	45	G
80	12	46	G
80	12	47	U
80	12	48	C
80	12	55	U
80	12	75	C
80	12	76	A
81	13	17	C

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Mol	Chain	Res	Type
81	13	18	G
81	13	20	A
81	13	22	G
81	13	47	U
81	13	48	C
81	13	58	A
81	13	59	A
81	13	75	C
81	13	76	A
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 (253) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	42	A
1	5	64	A
1	5	65	A
1	5	119	G
1	5	125	C
1	5	134	G
1	5	143	C
1	5	172	C
1	5	216	C
1	5	217	C
1	5	218	A
1	5	219	G
1	5	226	G
1	5	245	C
1	5	265	C
1	5	266	C
1	5	275	C
1	5	315	G
1	5	385	A
1	5	406	C

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Mol	Chain	Res	Type
1	5	408	A
1	5	449	C
1	5	466	A
1	5	480	C
1	5	482	G
1	5	485	C
1	5	492	U
1	5	504	G
1	5	649	A
1	5	667	A
1	5	696	C
1	5	729	G
1	5	738(A)	C
1	5	749	G
1	5	913	U
1	5	914	U
1	5	915	A
1	5	916	C
1	5	924	C
1	5	930	G
1	5	935(A)	G
1	5	955	G
1	5	959	G
1	5	960	A
1	5	966	A
1	5	971(A)	G
1	5	972	C
1	5	1072	C
1	5	1211	G
1	5	1237	C
1	5	1238	A
1	5	1249	C
1	5	1283	G
1	5	1292	C
1	5	1293	G
1	5	1301	C
1	5	1325	C
1	5	1358	G
1	5	1359	G
1	5	1370	G
1	5	1380	G
1	5	1387	A

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Mol	Chain	Res	Type
1	5	1440	U
1	5	1445	U
1	5	1455	G
1	5	1477	C
1	5	1483	C
1	5	1484	G
1	5	1485	C
1	5	1502	G
1	5	1533	A
1	5	1534	A
1	5	1590	C
1	5	1613	A
1	5	1633	G
1	5	1773	U
1	5	1804	A
1	5	1835	G
1	5	1836	G
1	5	1898	C
1	5	1918	U
1	5	1921	C
1	5	1979	A
1	5	1986	U
1	5	1992	U
1	5	2001	G
1	5	2010	A
1	5	2023	C
1	5	2042	A
1	5	2088	A
1	5	2089	G
1	5	2093	G
1	5	2100	G
1	5	2106	G
1	5	2266	C
1	5	2267	U
1	5	2278	G
1	5	2313	A
1	5	2421	G
1	5	2428	A
1	5	2474	G
1	5	2490	U
1	5	2502	A
1	5	2503	G

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Mol	Chain	Res	Type
1	5	2546	G
1	5	2553	A
1	5	2587	A
1	5	2696	A
1	5	2710	C
1	5	2711	G
1	5	2790	U
1	5	2794	C
1	5	2806	A
1	5	3603	G
1	5	3614	G
1	5	3625	G
1	5	3672	G
1	5	3673	C
1	5	3710	G
1	5	3759	A
1	5	3810	C
1	5	3876	A
1	5	3878	C
1	5	3888	G
1	5	3904	G
1	5	3907	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	4069	U
1	5	4115	G
1	5	4119	C
1	5	4121	G
1	5	4124	G
1	5	4162	C
1	5	4170	A
1	5	4221	C
1	5	4232	U
1	5	4233	A
1	5	4254	G
1	5	4281	A

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Mol	Chain	Res	Type
1	5	4395	U
1	5	4448	G
1	5	4475	G
1	5	4488	A
1	5	4527	G
1	5	4572	U
1	5	4626	A
1	5	4635	A
1	5	4699	U
1	5	4719	G
1	5	4736	C
1	5	4871	C
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	4947	U
1	5	4949	G
1	5	5013	C
1	5	5047	C
1	5	5061	A
2	7	109	U
3	8	2	G
3	8	51	U
3	8	85	U
3	8	104	A
3	8	124	U
4	9	24	C
4	9	58	C
4	9	72	C
4	9	110	U
4	9	126	G
4	9	160	U
4	9	319	C
4	9	369	C
4	9	400	C
4	9	465	A
4	9	516	A
4	9	532	C

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Mol	Chain	Res	Type
4	9	553	U
4	9	555	A
4	9	561	A
4	9	591	U
4	9	593	C
4	9	606	G
4	9	608	C
4	9	620	G
4	9	752	G
4	9	821	G
4	9	867	G
4	9	869	A
4	9	870	A
4	9	872	A
4	9	874	G
4	9	875	A
4	9	912	C
4	9	919	A
4	9	1016	U
4	9	1061	U
4	9	1117	C
4	9	1118	C
4	9	1137	U
4	9	1138	C
4	9	1165	G
4	9	1215	C
4	9	1240	A
4	9	1253	A
4	9	1275	G
4	9	1284	A
4	9	1300	U
4	9	1303	C
4	9	1308	U
4	9	1313	A
4	9	1395	C
4	9	1396	A
4	9	1454	A
4	9	1463	U
4	9	1476	A
4	9	1489	A
4	9	1556	A
4	9	1580	A

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Mol	Chain	Res	Type
4	9	1581	C
4	9	1603	G
4	9	1637	A
4	9	1638	G
4	9	1679	A
4	9	1757	G
4	9	1835	A
4	9	1837	G
4	9	1863	A
4	9	1868	U
79	10	22	U
80	12	44	A
80	12	45	G
80	12	47	U
80	12	74	C
81	13	16	G
81	13	19	G
81	13	58	A
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	0.38	0	8,13,15	0.19	0
86	GTP	12	101	80	33,34,34	0.85	0	50,54,54	1.61	8 (16%)
89	MET	13	102	81	6,7,8	0.50	0	2,7,9	0.07	0
84	SPD	5	5101	-	9,9,9	0.26	0	8,8,8	0.48	0
88	ATP	13	101	81	32,33,33	0.34	0	48,52,52	0.43	0
91	GDP	jj	702	92	29,30,30	1.17	3 (10%)	45,47,47	1.67	5 (11%)
88	ATP	11	101	81	32,33,33	0.31	0	48,52,52	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	PHE	12	102	80	-	2/5/6/8	0/1/1/1
86	GTP	12	101	80	-	4/22/38/38	0/3/3/3
89	MET	13	102	81	-	0/5/6/8	-
84	SPD	5	5101	-	-	1/7/7/7	-
88	ATP	13	101	81	-	2/22/38/38	0/3/3/3
91	GDP	jj	702	92	-	0/16/32/32	0/3/3/3
88	ATP	11	101	81	-	0/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	jj	702	GDP	C5-C4	3.09	1.47	1.38
91	jj	702	GDP	C6-N1	-2.63	1.33	1.38
91	jj	702	GDP	C5-N7	-2.10	1.34	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	jj	702	GDP	C5-C4-N3	-6.05	118.76	128.39
86	12	101	GTP	C5-C4-N3	-4.85	120.68	128.39
91	jj	702	GDP	C2-N3-C4	4.83	120.61	112.30
86	12	101	GTP	C2-N3-C4	4.64	120.30	112.30
91	jj	702	GDP	N9-C4-N3	4.42	134.79	125.95
91	jj	702	GDP	C6-C5-N7	3.25	136.21	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	12	101	GTP	C2-N1-C6	-3.11	119.48	125.11
86	12	101	GTP	N9-C4-N3	2.96	131.88	125.95
86	12	101	GTP	N9-C8-N7	-2.90	108.02	113.40
86	12	101	GTP	C5-C6-N1	2.68	120.07	113.25
91	jj	702	GDP	C4-C5-N7	-2.67	106.44	110.67
86	12	101	GTP	C8-N7-C5	2.58	108.86	104.26
86	12	101	GTP	O6-C6-C5	-2.38	120.24	126.53

There are no chirality outliers.

All (9) torsion outliers are listed below:

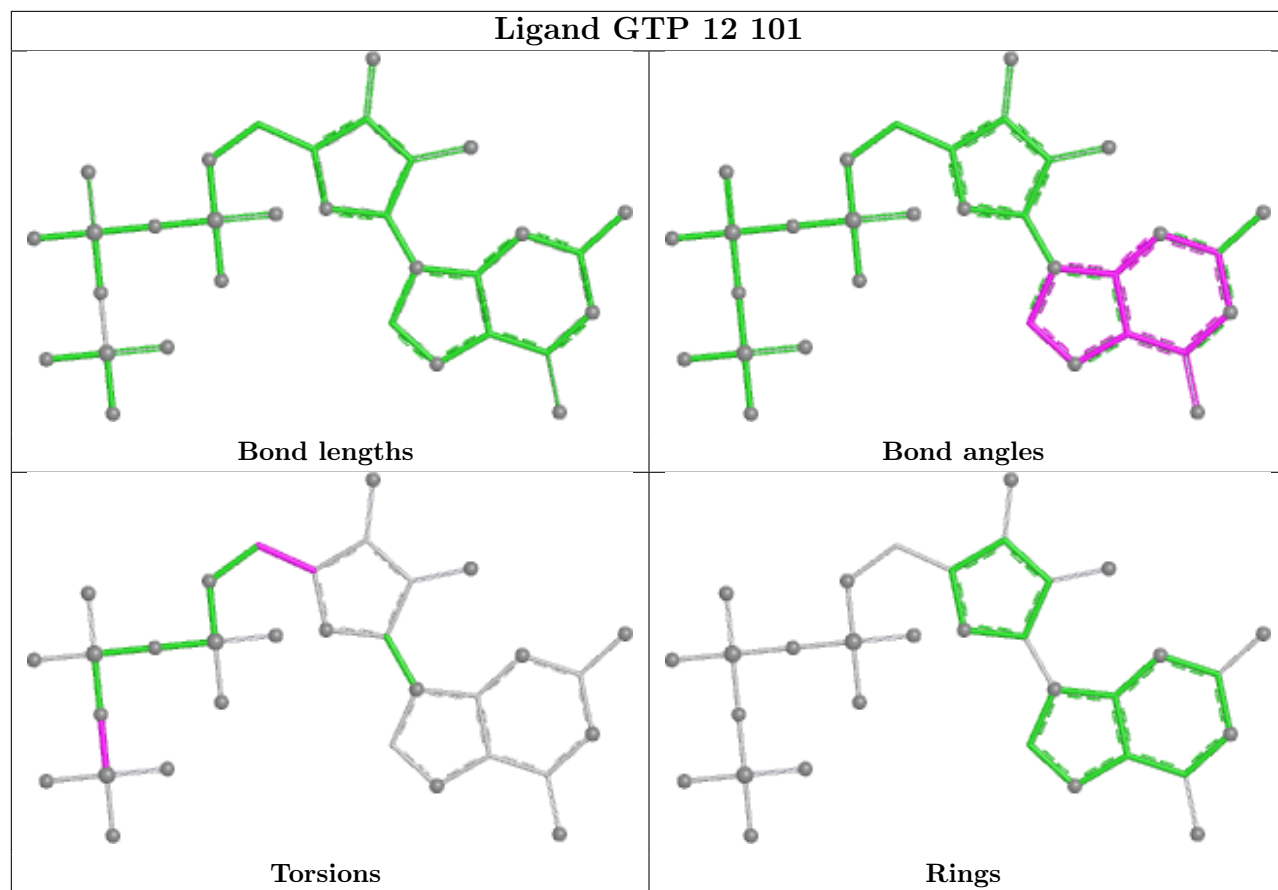
Mol	Chain	Res	Type	Atoms
86	12	101	GTP	PB-O3B-PG-O2G
87	12	102	PHE	C-CA-CB-CG
86	12	101	GTP	O4'-C4'-C5'-O5'
86	12	101	GTP	C3'-C4'-C5'-O5'
87	12	102	PHE	N-CA-CB-CG
84	5	5101	SPD	C2-C3-C4-C5
86	12	101	GTP	PB-O3B-PG-O1G
88	13	101	ATP	O4'-C4'-C5'-O5'
88	13	101	ATP	C4'-C5'-O5'-PA

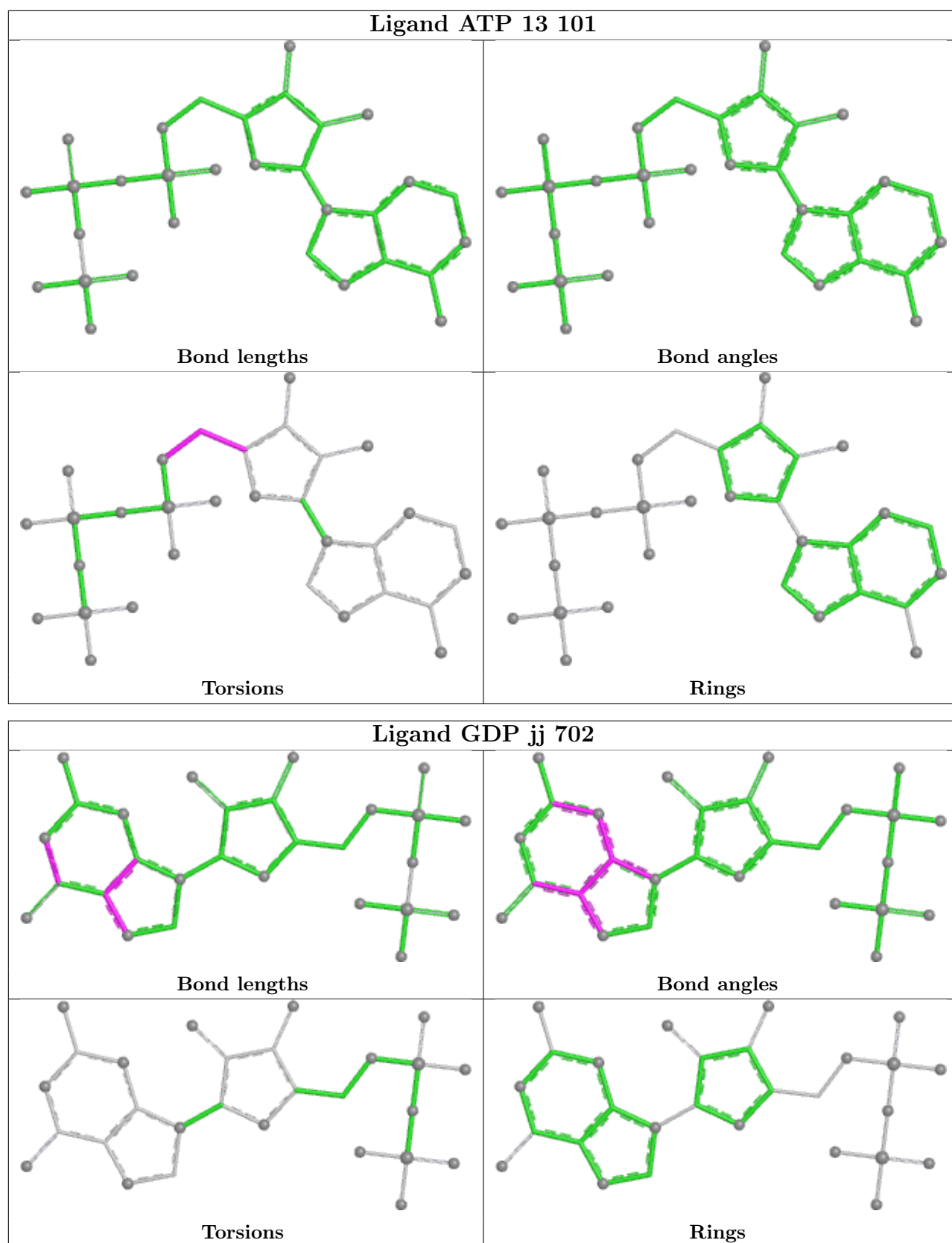
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	12	101	GTP	1	0
88	13	101	ATP	1	0
91	jj	702	GDP	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	40.72
1	5	1252:C	O3'	1271:G	P	35.27
1	5	1219:G	O3'	1233:G	P	20.32
1	5	523:C	O3'	638:G	P	18.25
1	5	3976:C	O3'	4035:G	P	17.79
1	5	4101:C	O3'	4107:G	P	17.61
1	5	1406(C):G	O3'	1411:C	P	17.25
1	5	4138:C	O3'	4146:G	P	17.00
1	5	4777:C	O3'	4859:C	P	16.90
1	5	990:C	O3'	1064:G	P	16.35
1	5	1696:C	O3'	1720:C	P	15.49
1	5	5022:U	O3'	5028:G	P	14.99
1	5	760:G	O3'	904:C	P	14.72
1	5	1364:U	O3'	1368:A	P	14.59
1	5	2901:G	O3'	3597:G	P	12.70
1	5	182:G	O3'	189:G	P	12.15
1	5	1180:C	O3'	1183:C	P	9.18
1	5	512:U	O3'	515:C	P	9.02
1	5	4729:A	O3'	4735:G	P	8.77
1	5	500:G	O3'	504:G	P	5.67
1	5	1100:U	O3'	1168:G	P	5.51
1	5	4740:G	O3'	4743:G	P	5.38
1	5	4899:G	O3'	4902:C	P	3.09

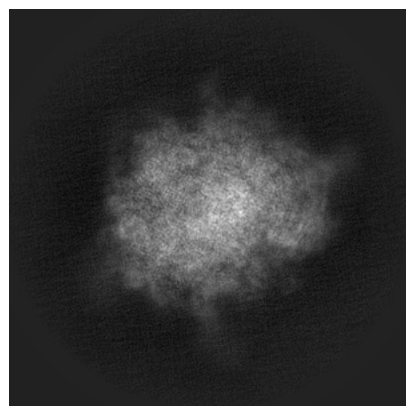
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73311. These allow visual inspection of the internal detail of the map and identification of artifacts.

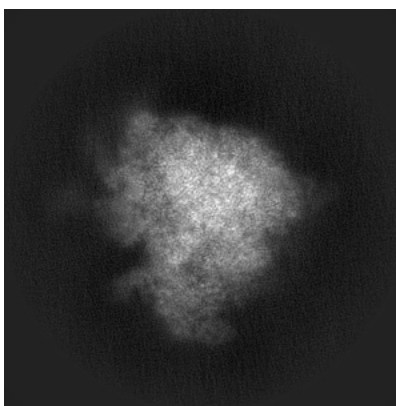
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

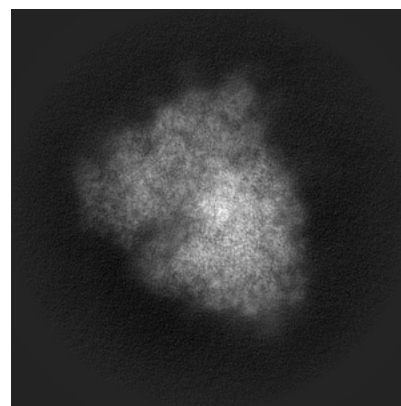
6.1.1 Primary map



X

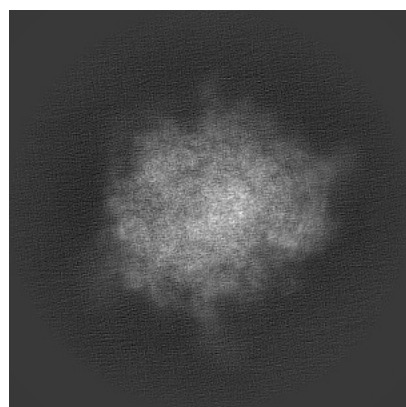


Y

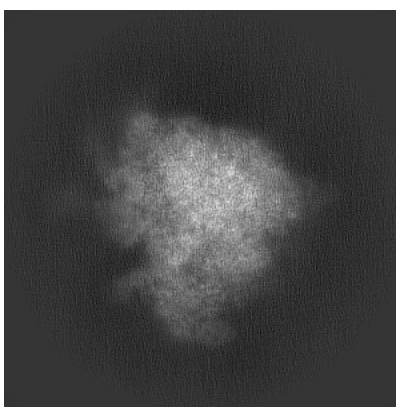


Z

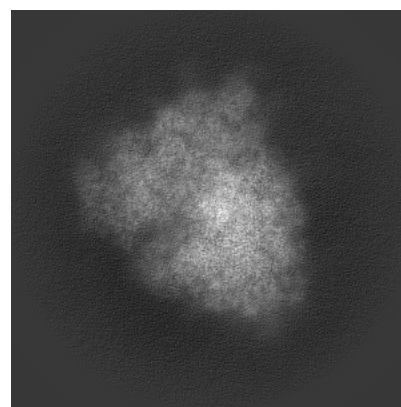
6.1.2 Raw map



X



Y

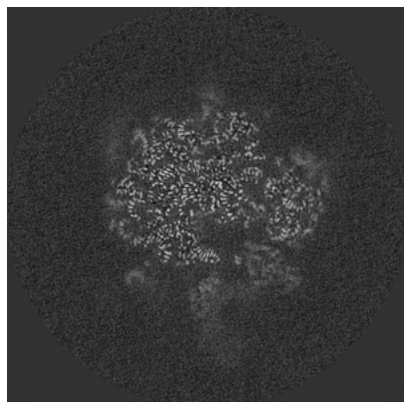


Z

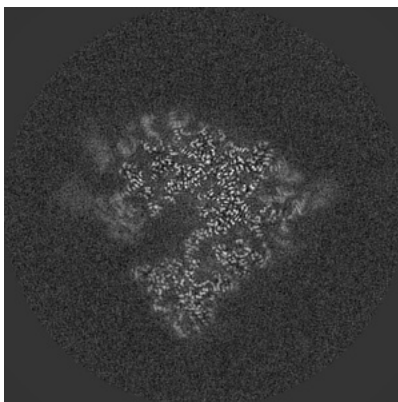
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

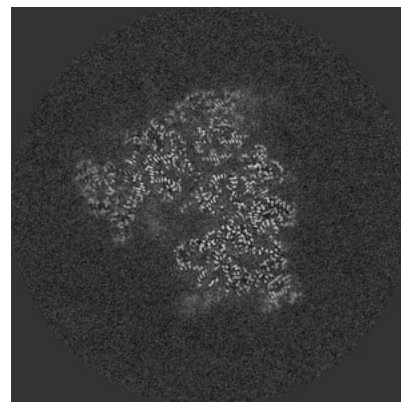
6.2.1 Primary map



X Index: 200

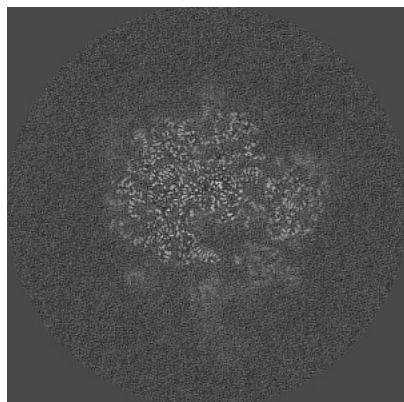


Y Index: 200

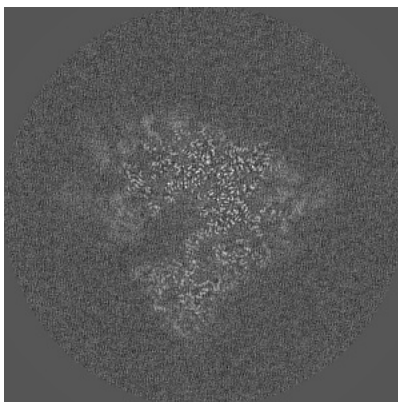


Z Index: 200

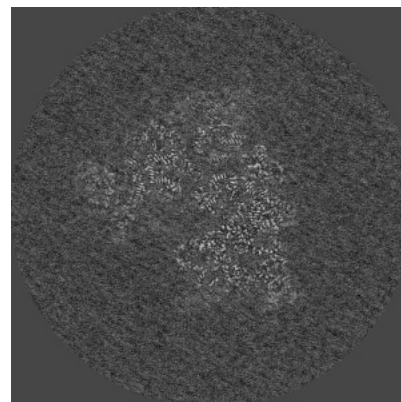
6.2.2 Raw map



X Index: 200



Y Index: 200

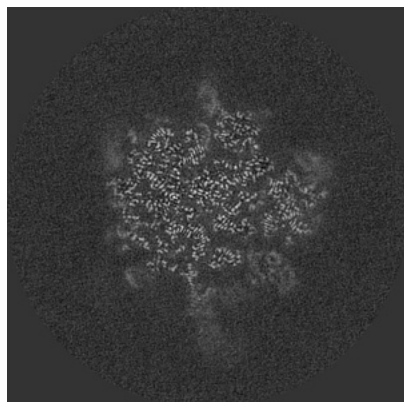


Z Index: 200

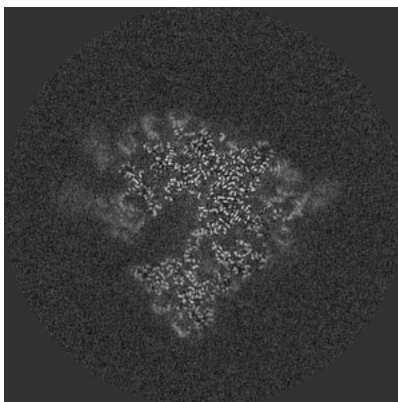
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

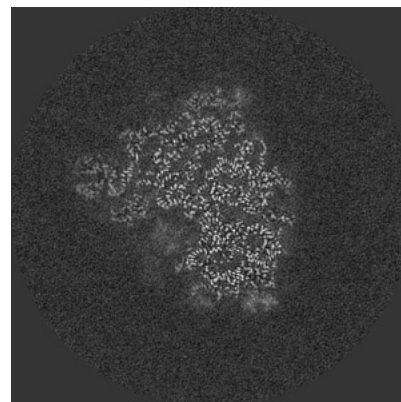
6.3.1 Primary map



X Index: 207

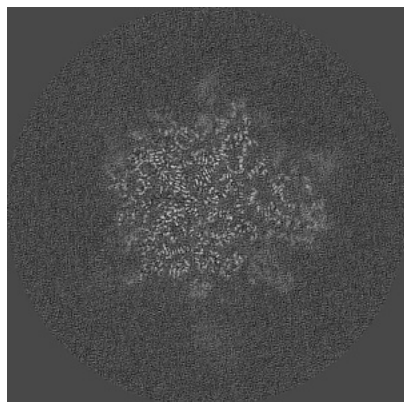


Y Index: 201

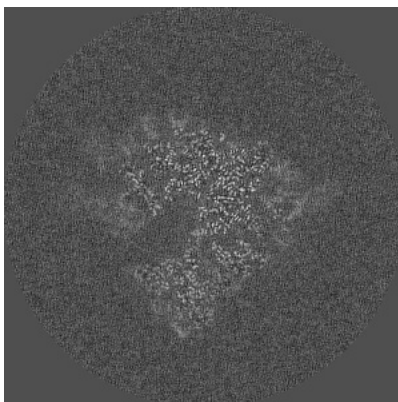


Z Index: 212

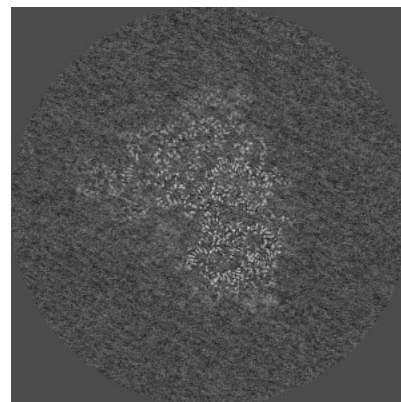
6.3.2 Raw map



X Index: 214



Y Index: 201

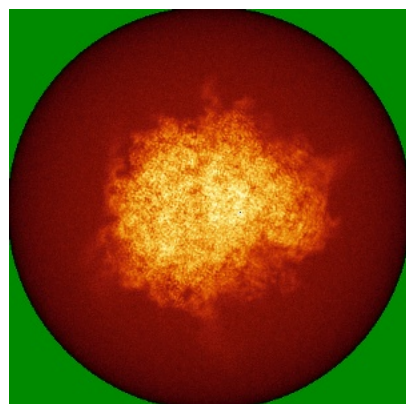


Z Index: 212

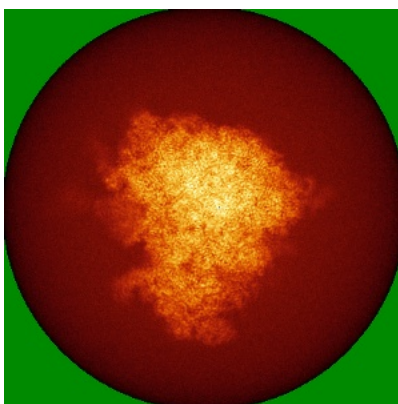
The images above show the largest variance slices of the map in three orthogonal directions.

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

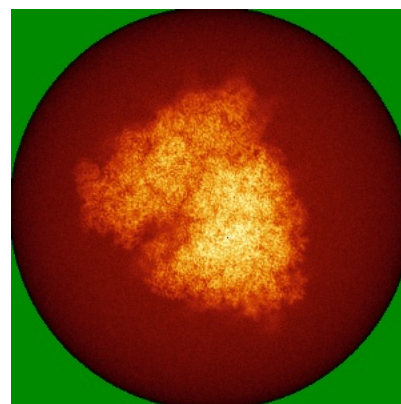
6.4.1 Primary map



X

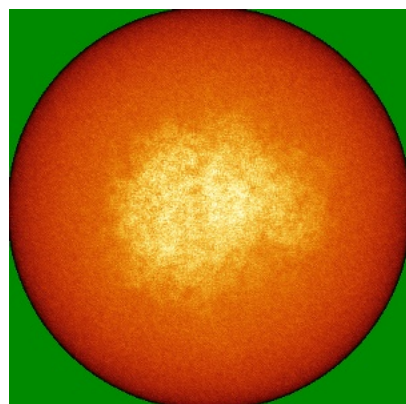


Y

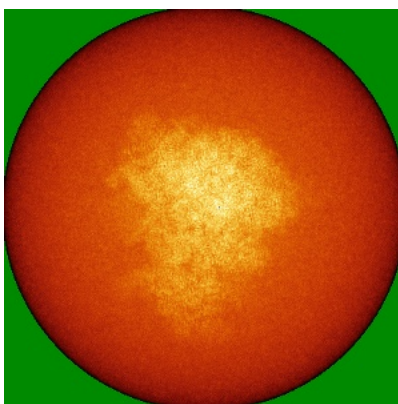


Z

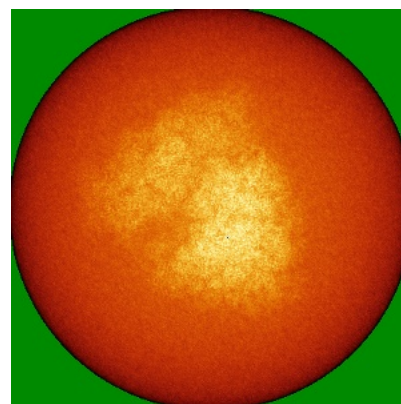
6.4.2 Raw map



X



Y

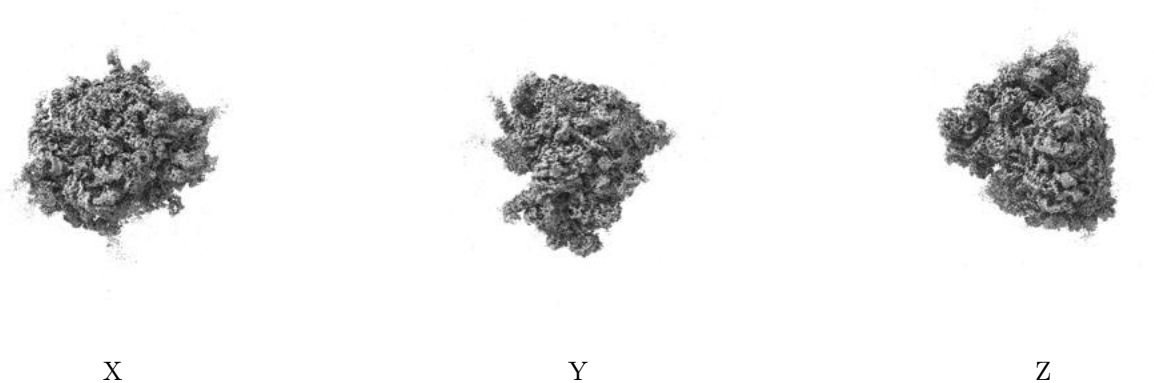


Z

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

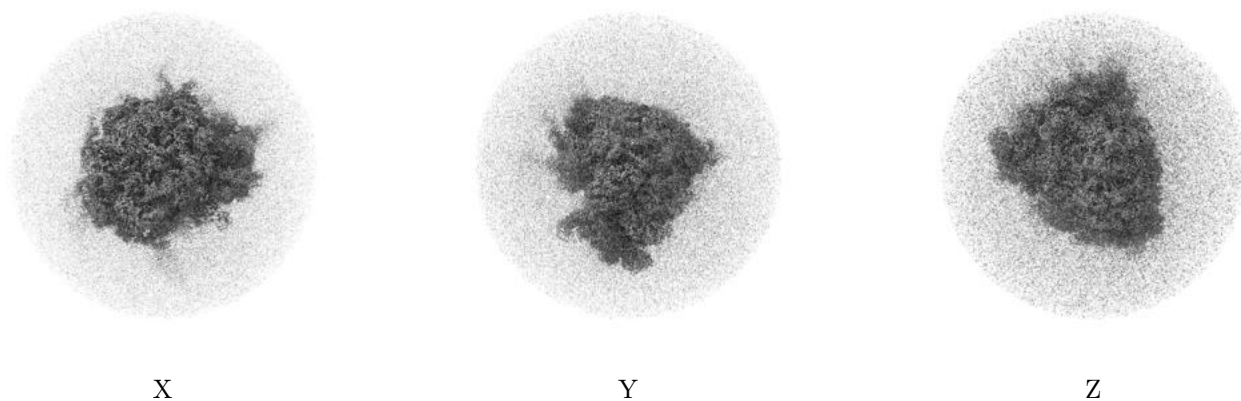
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

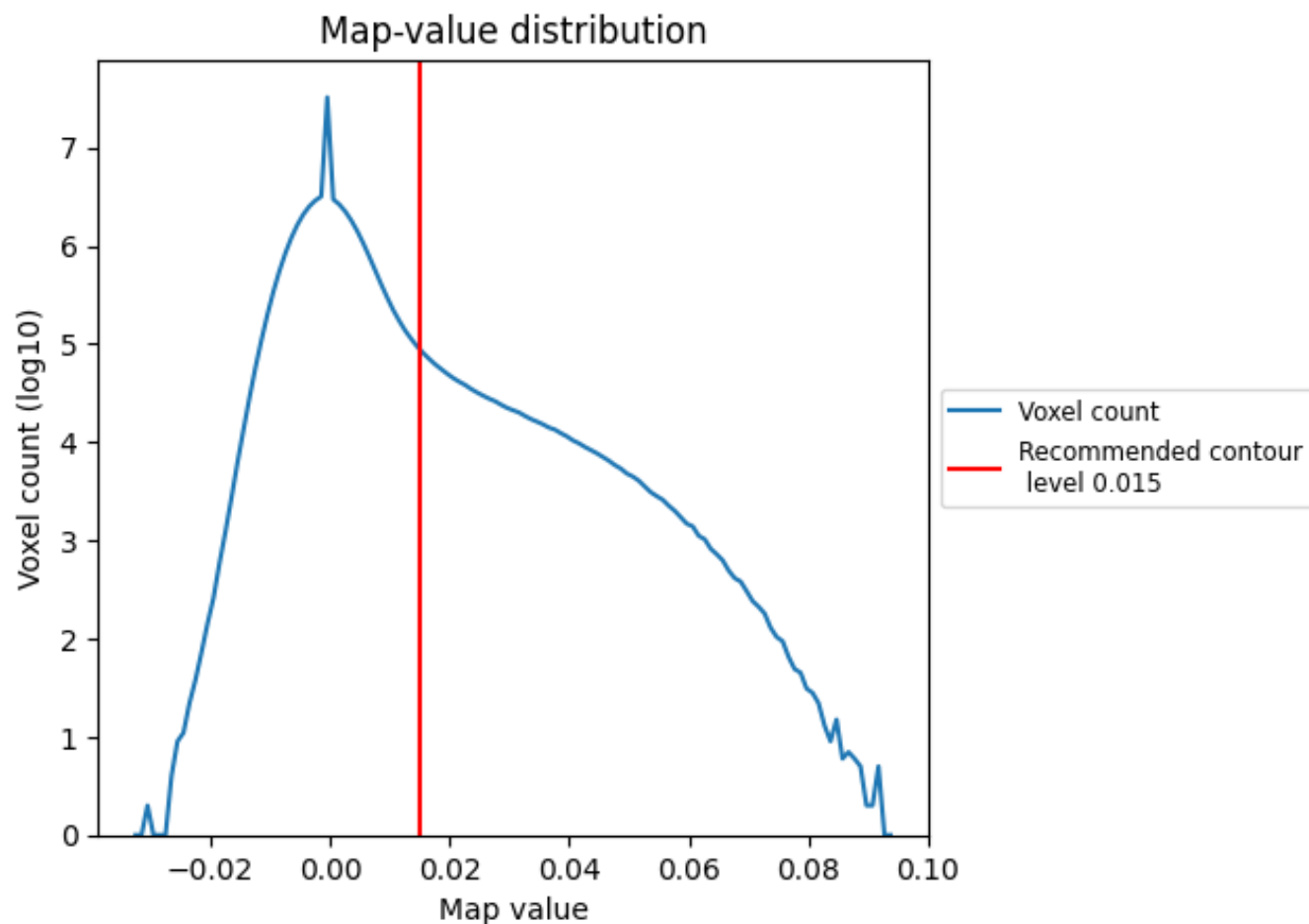
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

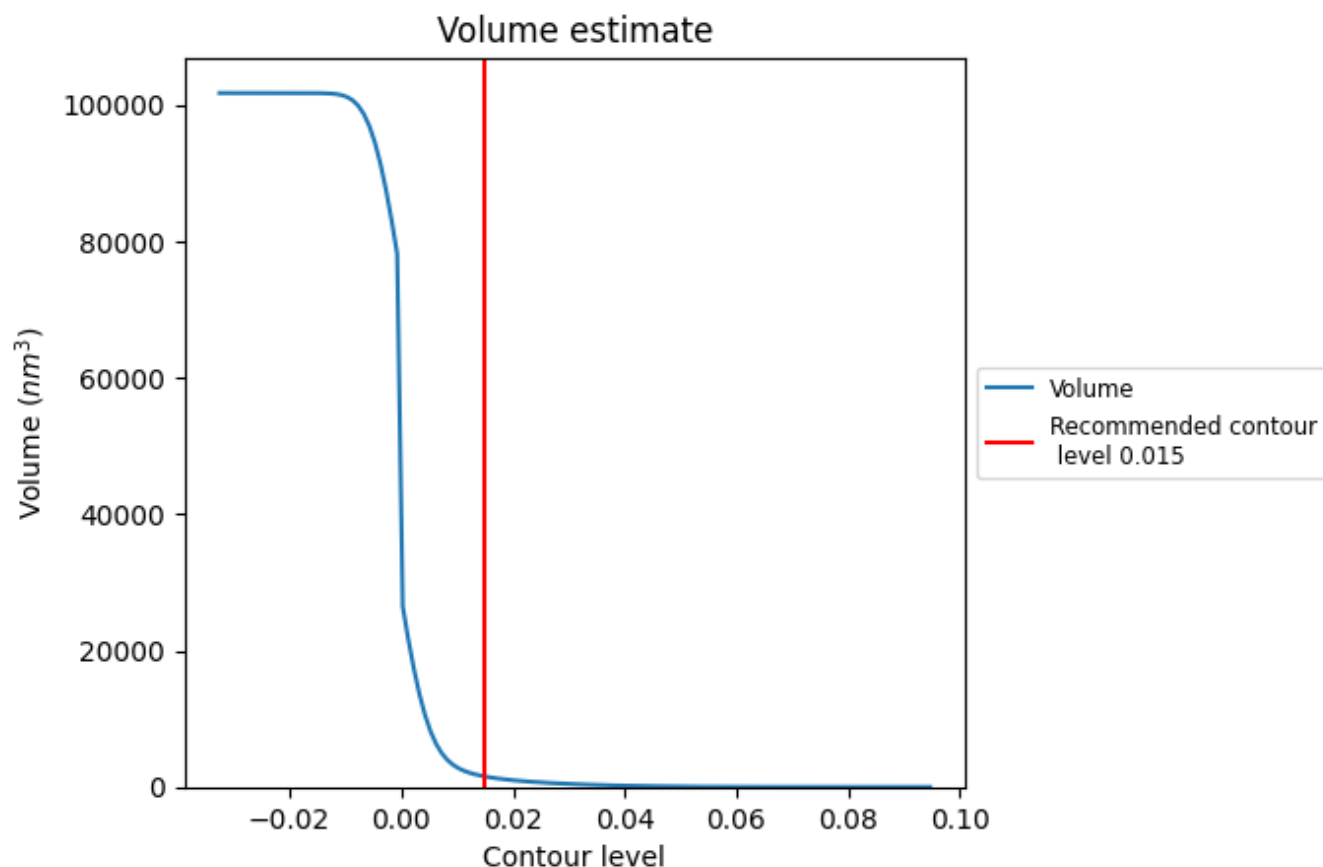
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

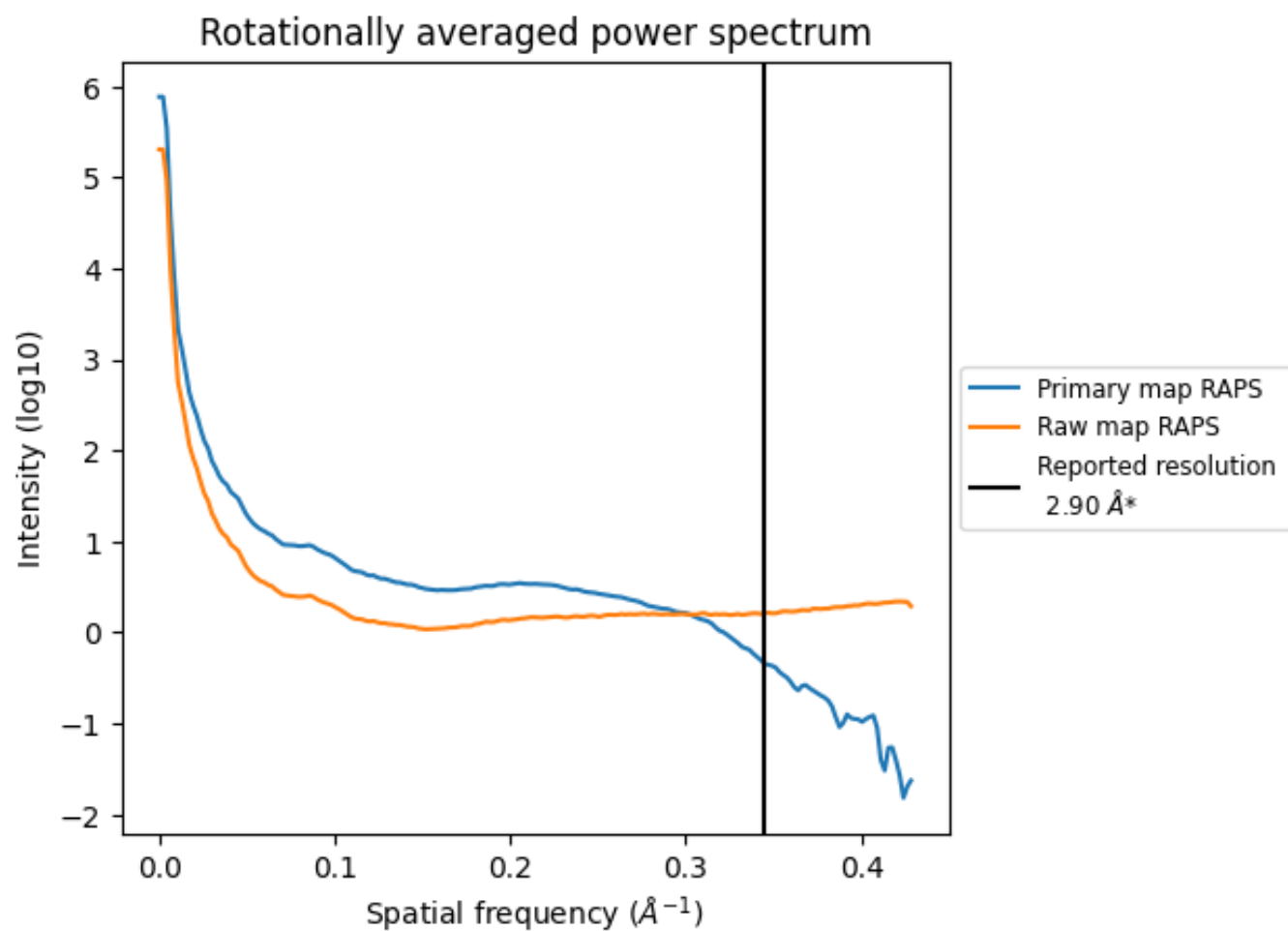
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1529 nm^3 ; this corresponds to an approximate mass of 1381 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

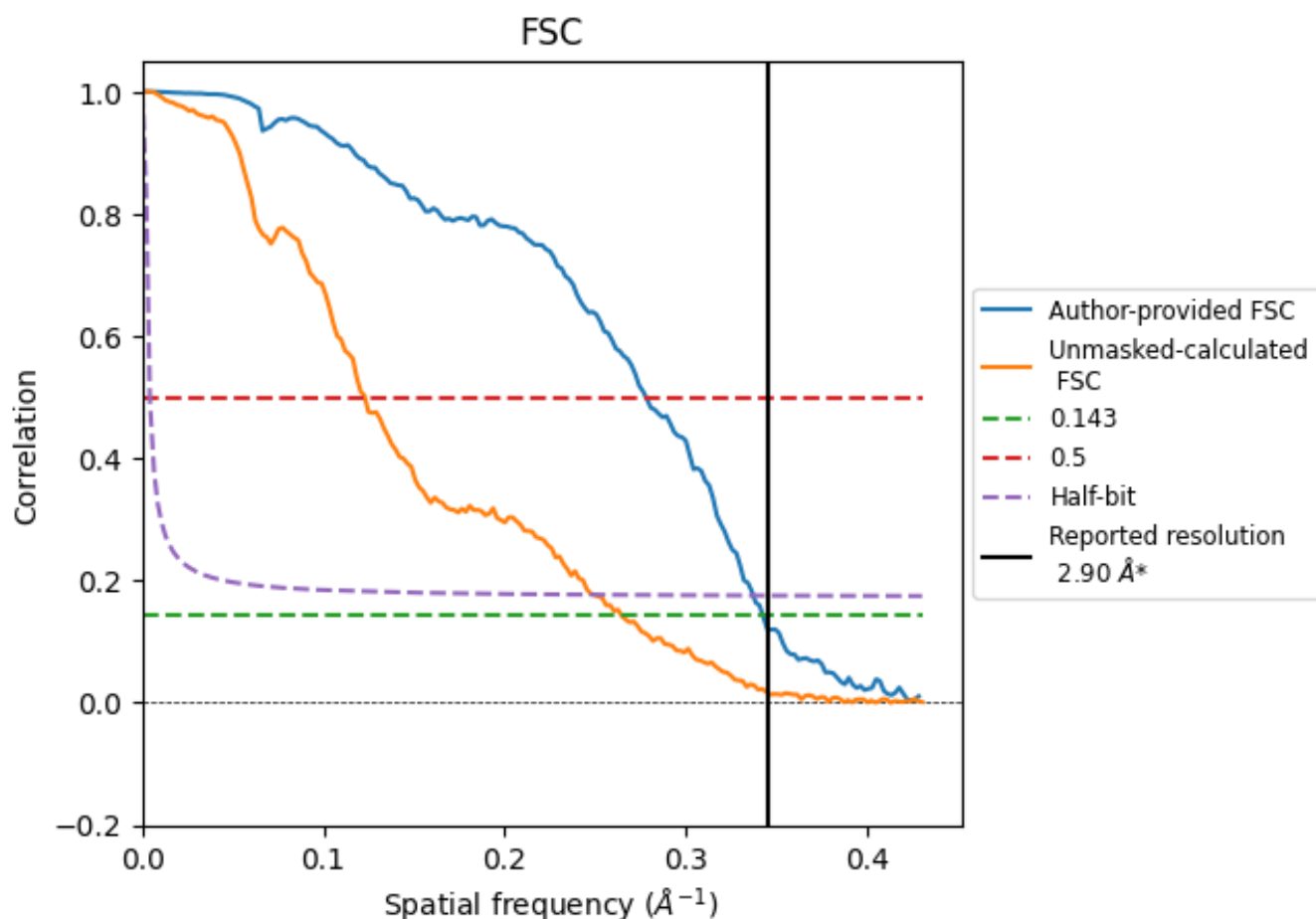


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

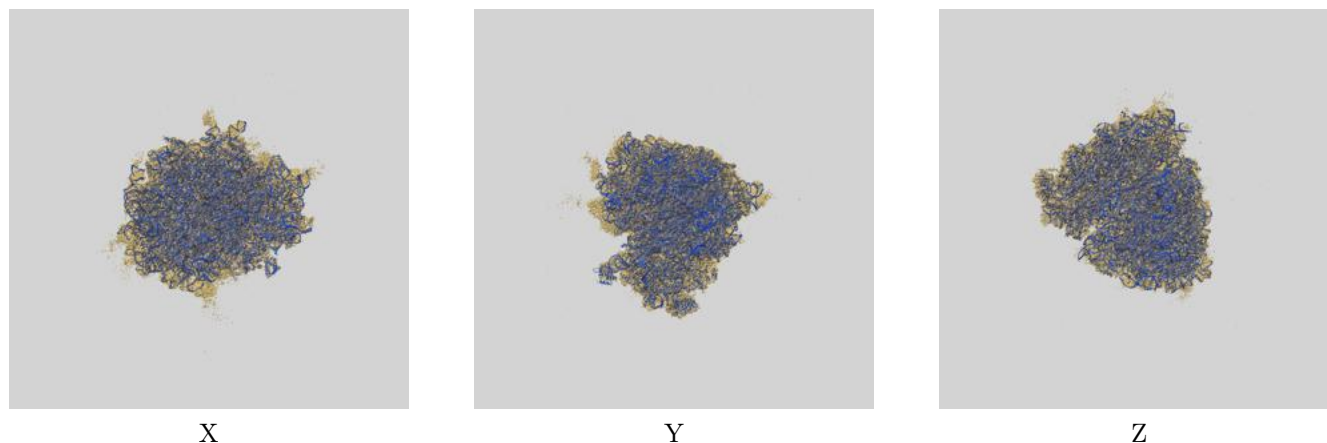
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.92	3.60	2.97
Unmasked-calculated*	3.78	8.14	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

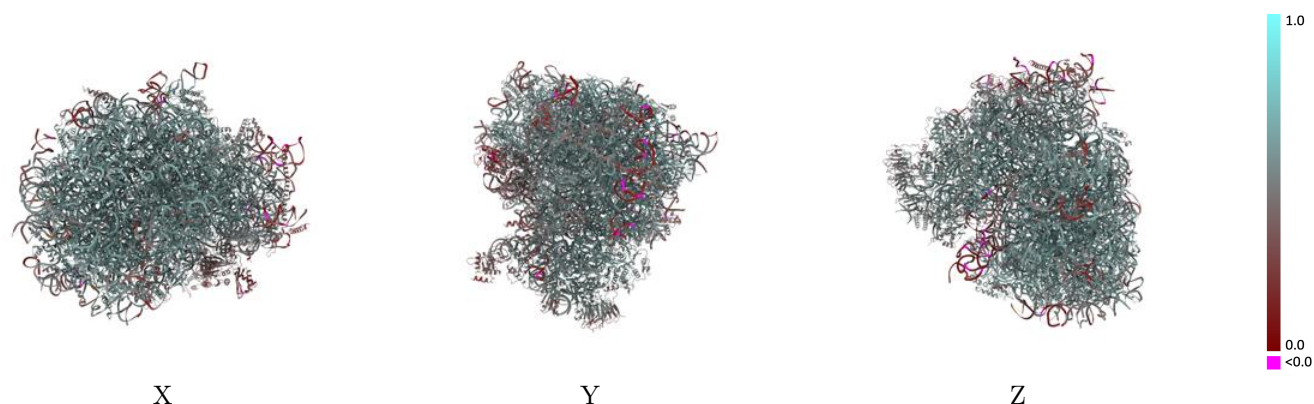
This section contains information regarding the fit between EMDB map EMD-73311 and PDB model 9YPW. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



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

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

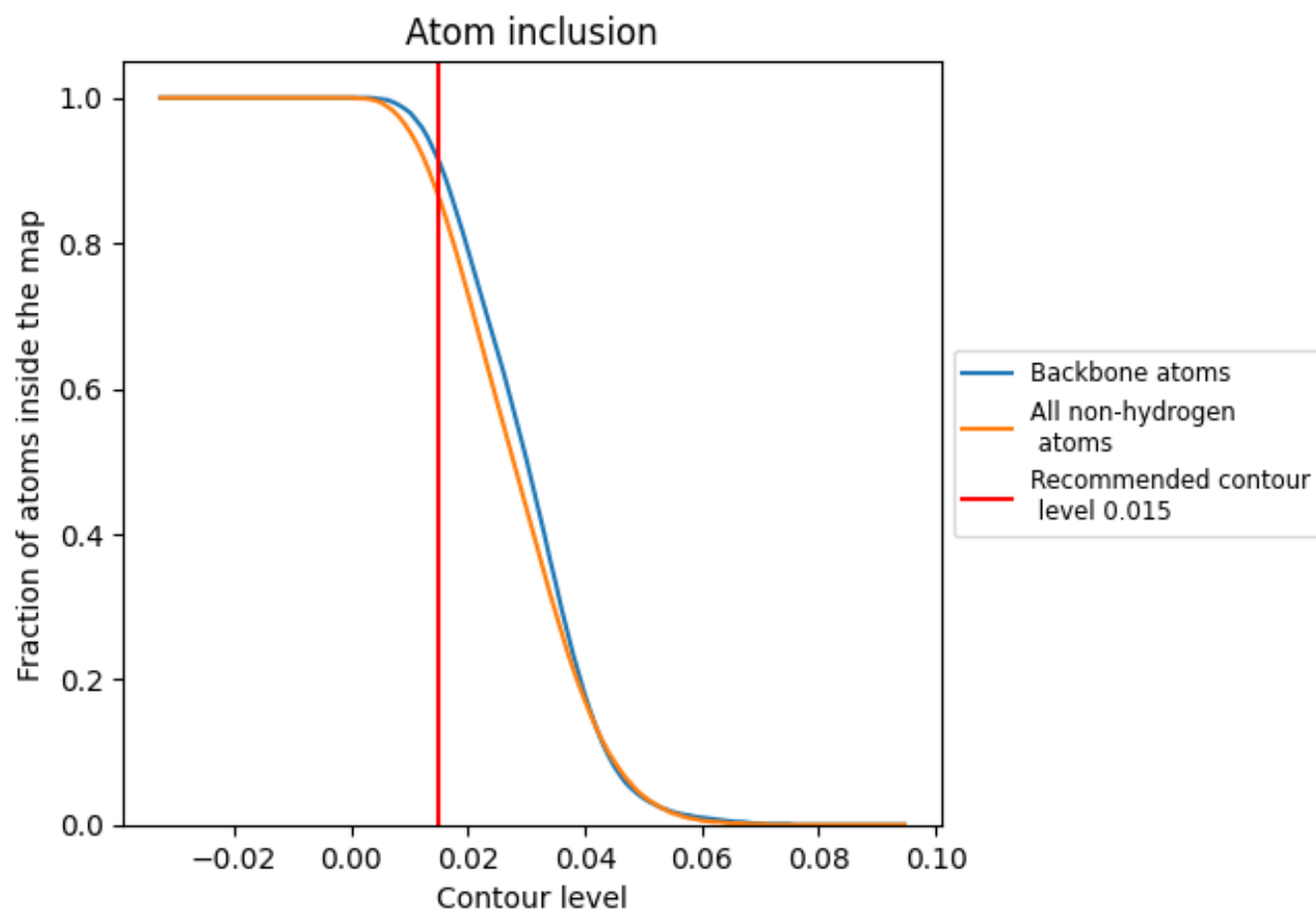


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 86% 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	 0.8650	 0.5420
10	 0.9490	 0.5690
11	 0.3260	 0.2380
12	 0.7910	 0.3880
13	 0.7350	 0.4610
5	 0.9240	 0.5540
7	 0.9910	 0.6060
8	 0.9590	 0.5790
9	 0.9120	 0.5340
A	 0.9480	 0.6130
AA	 0.8050	 0.5500
B	 0.8910	 0.5920
BB	 0.8080	 0.5560
C	 0.9160	 0.5950
CC	 0.8530	 0.5600
D	 0.8430	 0.5660
DD	 0.7420	 0.5130
E	 0.8550	 0.5560
EE	 0.7710	 0.5100
FF	 0.7790	 0.5270
G	 0.7840	 0.5390
GG	 0.6620	 0.4600
H	 0.8190	 0.5750
HH	 0.6410	 0.4870
I	 0.8680	 0.5780
II	 0.8170	 0.5450
J	 0.7820	 0.5460
JJ	 0.7220	 0.4550
K	 0.9230	 0.5980
KK	 0.7490	 0.5020
L	 0.8420	 0.5710
LL	 0.8470	 0.5570
M	 0.8700	 0.5660
MM	 0.2780	 0.3270
N	 0.9560	 0.6100



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Chain	Atom inclusion	Q-score
NN	 0.8590	 0.5600
O	 0.9120	 0.5940
OO	 0.8500	 0.5560
P	 0.9050	 0.5980
PP	 0.7030	 0.4950
Q	 0.9120	 0.6000
QQ	 0.8130	 0.5380
R	 0.8580	 0.5630
RR	 0.7220	 0.5050
S	 0.9170	 0.6020
SS	 0.7560	 0.5070
T	 0.8610	 0.5760
TT	 0.7760	 0.5150
U	 0.7500	 0.5090
UU	 0.6900	 0.4790
V	 0.9090	 0.5980
VV	 0.7740	 0.5390
W	 0.6530	 0.4710
WW	 0.8850	 0.5850
X	 0.8660	 0.5700
XX	 0.8670	 0.5740
Y	 0.8380	 0.5700
YY	 0.6930	 0.4660
Z	 0.8460	 0.5640
ZZ	 0.6790	 0.4850
a	 0.9310	 0.6050
aa	 0.8500	 0.5610
b	 0.8160	 0.5410
bb	 0.7430	 0.5270
c	 0.8560	 0.5650
cc	 0.7380	 0.5300
d	 0.8500	 0.5650
dd	 0.8530	 0.5630
e	 0.9140	 0.6020
ee	 0.6640	 0.4640
f	 0.9300	 0.6130
ff	 0.3960	 0.3640
g	 0.8710	 0.5810
gg	 0.6190	 0.4510
h	 0.8420	 0.5660
i	 0.8380	 0.5520
j	 0.9600	 0.6100

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Chain	Atom inclusion	Q-score
jj	 0.4440	 0.3520
k	 0.7330	 0.5230
l	 0.9200	 0.5900
m	 0.8610	 0.5740
n	 0.9130	 0.5970
o	 0.9060	 0.5910
p	 0.8820	 0.5820
r	 0.9070	 0.5930