



Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 08:35 pm BST

PDB ID : 5JB3
EMDB ID : EMD-8148
Title : Cryo-EM structure of a full archaeal ribosomal translation initiation complex in the P-REMOTE conformation
Authors : Coureux, P.-D.; Schmitt, E.; Mechulam, Y.
Deposited on : 2016-04-13
Resolution : 5.34 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

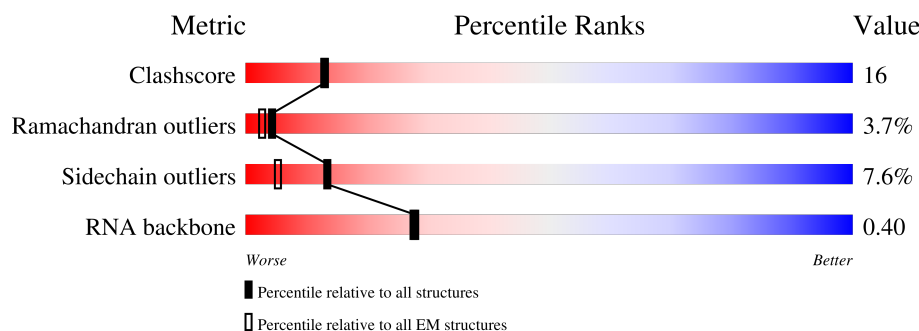
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.34 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2	1519	
2	M	137	
3	N	147	
4	Q	158	
5	R	113	
6	A	198	
7	B	202	

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Mol	Chain	Length	Quality of chain
8	V	99	
9	W	63	
10	Z	210	
11	D	180	
12	E	243	
13	F	236	
14	G	125	
15	I	130	
16	J	127	
17	C	57	
18	3	123	
19	L	102	
20	O	148	
21	P	56	
22	S	67	
23	T	132	
24	U	150	
25	X	71	
26	Y	50	
27	H	215	
28	K	135	
29	0	22	
30	4	76	
31	5	26	
32	1	102	

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Mol	Chain	Length	Quality of chain
33	6	113	
34	7	415	
35	8	139	
36	9	266	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	MET	7	501	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 70678 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1495	Total	C	N	O	P	0	0
			32135	14297	5954	10389	1495		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	-3	U	UNK	conflict	GB 5457433
2	227	C	G	conflict	GB 5457433
2	229	G	C	conflict	GB 5457433
2	715	C	G	conflict	GB 5457433
2	718	G	C	conflict	GB 5457433
2	1216	A	U	conflict	GB 5457433
2	1217	C	G	conflict	GB 5457433
2	1224	U	C	conflict	GB 5457433
2	1234	A	G	conflict	GB 5457433
2	1238	G	U	conflict	GB 5457433
2	1316	U	C	conflict	GB 5457433
2	1383	A	G	conflict	GB 5457433
2	1385	U	C	conflict	GB 5457433
2	1387	C	U	conflict	GB 5457433
2	1388	G	A	conflict	GB 5457433
2	1398	U	C	conflict	GB 5457433
2	1417	A	G	conflict	GB 5457433
2	1427	C	U	conflict	GB 5457433
2	1428	G	A	conflict	GB 5457433
2	1463	A	G	conflict	GB 5457433

- Molecule 2 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	133	Total	C	N	O	S	0	0
			1004	623	200	179	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	23	PHE	TYR	conflict	UNP P62010

- Molecule 3 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	145	Total	C	N	O	S	0	0
			1140	722	222	193	3		

- Molecule 4 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	158	Total	C	N	O	S	0	0
			1310	834	250	221	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	26	VAL	LEU	conflict	UNP Q9V2K9
Q	32	GLU	ASP	conflict	UNP Q9V2K9
Q	62	SER	THR	conflict	UNP Q9V2K9
Q	67	LYS	ARG	conflict	UNP Q9V2K9
Q	75	ASN	LYS	conflict	UNP Q9V2K9
Q	100	ARG	LYS	conflict	UNP Q9V2K9
Q	145	ASN	ASP	conflict	UNP Q9V2K9
Q	152	THR	GLN	conflict	UNP Q9V2K9

- Molecule 5 is a protein called 30S ribosomal protein S17P.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	113	Total	C	N	O	S	0	0
			934	592	177	160	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	2	MET	VAL	conflict	UNP Q9V1U5
R	9	VAL	ILE	conflict	UNP Q9V1U5
R	26	ASN	HIS	conflict	UNP Q9V1U5
R	55	PHE	HIS	conflict	UNP Q9V1U5
R	58	ASN	LYS	conflict	UNP Q9V1U5
R	69	LYS	ARG	conflict	UNP Q9V1U5
R	85	LYS	ARG	conflict	UNP Q9V1U5

- Molecule 6 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	190	Total	C	N	O	S	0	0
			1559	1007	273	274	5		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	ALA	conflict	UNP Q9V2K7
A	3	ALA	LYS	conflict	UNP Q9V2K7
A	4	LYS	ARG	conflict	UNP Q9V2K7
A	6	ALA	VAL	conflict	UNP Q9V2K7
A	7	THR	SER	conflict	UNP Q9V2K7
A	8	THR	ALA	conflict	UNP Q9V2K7
A	9	THR	ALA	conflict	UNP Q9V2K7
A	10	ARG	LYS	conflict	UNP Q9V2K7
A	20	ILE	VAL	conflict	UNP Q9V2K7
A	55	VAL	ILE	conflict	UNP Q9V2K7
A	60	THR	LEU	conflict	UNP Q9V2K7
A	62	SER	GLY	conflict	UNP Q9V2K7
A	99	LYS	ARG	conflict	UNP Q9V2K7
A	123	ALA	VAL	conflict	UNP Q9V2K7
A	126	MET	ALA	conflict	UNP Q9V2K7
A	161	SER	ALA	conflict	UNP Q9V2K7
A	181	ARG	LYS	conflict	UNP Q9V2K7
A	192	GLU	GLY	conflict	UNP Q9V2K7
A	195	GLN	GLU	conflict	UNP Q9V2K7
A	197	ILE	ALA	conflict	UNP Q9V2K7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	202	Total	C	N	O	S	0	0
			1623	1046	282	290	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	LYS	ARG	conflict	UNP Q9V191
B	63	GLU	ASP	conflict	UNP Q9V191
B	115	LEU	ILE	conflict	UNP Q9V191
B	117	VAL	ILE	conflict	UNP Q9V191
B	128	ARG	LYS	conflict	UNP Q9V191

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Chain	Residue	Modelled	Actual	Comment	Reference
B	131	VAL	ILE	conflict	UNP Q9V191
B	183	GLN	SER	conflict	UNP Q9V191
B	187	ASP	GLU	conflict	UNP Q9V191

- Molecule 8 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	99	Total	C	N	O	S	0	0
			823	532	134	154	3		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	4	ARG	LYS	conflict	UNP Q9UY20
V	6	LYS	THR	conflict	UNP Q9UY20
V	8	ILE	VAL	conflict	UNP Q9UY20
V	64	ILE	LYS	conflict	UNP Q9UY20
V	71	ALA	TYR	conflict	UNP Q9UY20
V	73	ASP	TYR	conflict	UNP Q9UY20
V	74	SER	ASP	conflict	UNP Q9UY20
V	76	GLU	ASP	conflict	UNP Q9UY20
V	92	LEU	ILE	conflict	UNP Q9UY20

- Molecule 9 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	63	Total	C	N	O	S	0	0
			478	306	85	81	6		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	1	MET	LEU	conflict	UNP Q9UXZ3
W	2	ALA	PRO	conflict	UNP Q9UXZ3
W	3	LYS	ARG	conflict	UNP Q9UXZ3
W	4	PRO	ASN	conflict	UNP Q9UXZ3
W	5	ILE	VAL	conflict	UNP Q9UXZ3
W	34	LYS	ARG	conflict	UNP Q9UXZ3
W	38	LEU	ASN	conflict	UNP Q9UXZ3
W	39	ILE	VAL	conflict	UNP Q9UXZ3
W	54	VAL	ILE	conflict	UNP Q9UXZ3
W	55	LYS	ARG	conflict	UNP Q9UXZ3

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	186	Total	C	N	O	S	0	0
			1459	933	271	251	4		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	13	ARG	LYS	conflict	UNP Q9V1U1
Z	71	LYS	ARG	conflict	UNP Q9V1U1
Z	81	GLU	ASP	conflict	UNP Q9V1U1
Z	83	GLU	GLN	conflict	UNP Q9V1U1
Z	99	LEU	ILE	conflict	UNP Q9V1U1
Z	117	LEU	MET	conflict	UNP Q9V1U1
Z	122	ASN	SER	conflict	UNP Q9V1U1
Z	132	LEU	ILE	conflict	UNP Q9V1U1
Z	144	ILE	VAL	conflict	UNP Q9V1U1
Z	186	GLY	ASP	conflict	UNP Q9V1U1
Z	205	VAL	SER	conflict	UNP Q9V1U1

- Molecule 11 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	172	Total	C	N	O	S	0	0
			1434	902	273	255	4		

- Molecule 12 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	241	Total	C	N	O	S	0	0
			1976	1277	355	339	5		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	118	ASP	GLU	conflict	UNP Q9V1U8
E	121	PHE	ASN	conflict	UNP Q9V1U8
E	133	ILE	VAL	conflict	UNP Q9V1U8
E	137	ARG	LYS	conflict	UNP Q9V1U8
E	138	VAL	ILE	conflict	UNP Q9V1U8
E	149	ILE	LEU	conflict	UNP Q9V1U8
E	150	VAL	ILE	conflict	UNP Q9V1U8
E	151	SER	PRO	conflict	UNP Q9V1U8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	152	ILE	LEU	conflict	UNP Q9V1U8
E	153	ALA	SER	conflict	UNP Q9V1U8
E	204	ARG	LYS	conflict	UNP Q9V1U8
E	235	THR	ARG	conflict	UNP Q9V1U8
E	239	LYS	ARG	conflict	UNP Q9V1U8

- Molecule 13 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	217	Total	C	N	O	S	0	0
			1716	1084	319	305	8		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	17	GLU	GLN	conflict	UNP Q9V1V5
F	25	MET	LEU	conflict	UNP Q9V1V5
F	40	ARG	LYS	conflict	UNP Q9V1V5
F	65	VAL	ILE	conflict	UNP Q9V1V5
F	104	LYS	ARG	conflict	UNP Q9V1V5
F	144	ALA	THR	conflict	UNP Q9V1V5
F	155	ARG	LYS	conflict	UNP Q9V1V5
F	180	VAL	ILE	conflict	UNP Q9V1V5
F	188	PHE	LEU	conflict	UNP Q9V1V5
F	210	ARG	LYS	conflict	UNP Q9V1V5
F	212	ALA	VAL	conflict	UNP Q9V1V5
F	213	ILE	VAL	conflict	UNP Q9V1V5
F	214	SER	THR	conflict	UNP Q9V1V5
F	231	THR	ALA	conflict	UNP Q9V1V5
F	232	THR	SER	conflict	UNP Q9V1V5

- Molecule 14 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	125	Total	C	N	O	S	0	0
			984	623	180	179	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	13	SER	THR	conflict	UNP Q9UYS3
G	19	VAL	ILE	conflict	UNP Q9UYS3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	24	ALA	PRO	conflict	UNP Q9UYS3
G	26	THR	ALA	conflict	UNP Q9UYS3
G	40	ALA	VAL	conflict	UNP Q9UYS3
G	44	ASN	GLY	conflict	UNP Q9UYS3
G	61	LEU	MET	conflict	UNP Q9UYS3
G	86	VAL	ILE	conflict	UNP Q9UYS3

- Molecule 15 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	68	ARG	LYS	conflict	UNP Q9V1V0
I	83	VAL	ALA	conflict	UNP Q9V1V0
I	84	SER	ARG	conflict	UNP Q9V1V0
I	85	GLU	ASP	conflict	UNP Q9V1V0
I	86	PHE	TYR	conflict	UNP Q9V1V0
I	88	LYS	ARG	conflict	UNP Q9V1V0
I	117	ILE	ARG	conflict	UNP Q9V1V0

- Molecule 16 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	127	Total	C	N	O	S	0	0
			1004	622	207	174	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	10	LYS	ARG	conflict	UNP Q9UZL4
J	53	ARG	LYS	conflict	UNP Q9UZL4

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	C	57	Total	C	N	O	0	0
			286	171	57	58		

- Molecule 18 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	123	Total	C	N	O	S	0	0
			939	599	155	181	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	119	LYS	ARG	conflict	UNP P62008

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	102	Total	C	N	O	S	0	0
			822	507	159	152	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	8	ILE	LEU	conflict	UNP Q9V0V6
L	17	ASP	GLU	conflict	UNP Q9V0V6
L	48	THR	VAL	conflict	UNP Q9V0V6
L	68	VAL	ILE	conflict	UNP Q9V0V6

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	148	Total	C	N	O	S	0	0
			1189	746	237	200	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	3	ASN	ASP	conflict	UNP Q9V1A0
O	31	ILE	VAL	conflict	UNP Q9V1A0
O	67	ALA	GLN	conflict	UNP Q9V1A0

- Molecule 21 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	56	Total	C	N	O	S	0	0
			462	292	95	69	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	34	GLN	HIS	conflict	UNP P62012

- Molecule 22 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	67	Total	C	N	O	S	0	0
			556	353	105	95	3		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	17	VAL	PHE	conflict	UNP Q9V0G0
S	26	THR	ARG	conflict	UNP Q9V0G0
S	36	GLN	GLU	conflict	UNP Q9V0G0
S	54	VAL	ILE	conflict	UNP Q9V0G0
S	62	MET	GLU	conflict	UNP Q9V0G0

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	111	Total	C	N	O	S	0	0
			923	594	173	150	6		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	26	ARG	LYS	conflict	UNP Q9V1T9
T	28	PHE	LEU	conflict	UNP Q9V1T9
T	60	LYS	ASN	conflict	UNP Q9V1T9
T	72	ILE	VAL	conflict	UNP Q9V1T9
T	112	LYS	ARG	conflict	UNP Q9V1T9
T	114	GLU	GLN	conflict	UNP Q9V1T9
T	120	VAL	ILE	conflict	UNP Q9V1T9

- Molecule 24 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	144	Total	C	N	O	S	0	0
			1175	758	212	204	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	89	LYS	ARG	conflict	UNP Q9V0G8

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	71	Total	C	N	O	S	0	0
			568	345	115	107	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	51	ILE	VAL	conflict	UNP P61029

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	50	Total	C	N	O	S	0	0
			409	262	75	66	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	9	GLU	ILE	conflict	UNP P61238
Y	10	ILE	VAL	conflict	UNP P61238
Y	42	LYS	ARG	conflict	UNP P61238

- Molecule 27 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	6	ASN	SER	conflict	UNP Q9V109
H	113	GLN	LYS	conflict	UNP Q9V109
H	176	ASN	THR	conflict	UNP Q9V109

- Molecule 28 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	K	135	Total	C	N	O	S	0	0
			1072	671	205	190	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	35	ILE	LEU	conflict	UNP Q9V195
K	36	ILE	VAL	conflict	UNP Q9V195
K	67	GLU	GLN	conflict	UNP Q9V195
K	80	MET	ILE	conflict	UNP Q9V195
K	94	SER	ASN	conflict	UNP Q9V195
K	100	MET	ILE	conflict	UNP Q9V195

- Molecule 29 is a protein called 30S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	0	22	Total	C	N	O	S	0	0
			213	135	52	25	1		

- Molecule 30 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	76	Total	C	N	O	P	0	0
			1622	724	291	531	76		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	18	Total	C	N	O	P	0	0
			388	173	70	127	18		

- Molecule 32 is a protein called Protein translation factor SUI1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1	83	Total	C	N	O	S	0	0
			662	418	116	124	4		

- Molecule 33 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	95	Total	C	N	O	S	0	0
			777	496	148	130	3		

- Molecule 34 is a protein called Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	409	Total	C	N	O	S	0	0
			3171	2028	541	590	12		

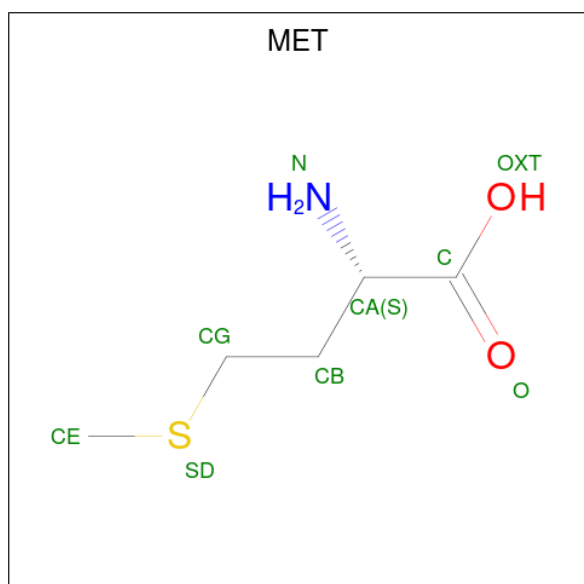
- Molecule 35 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	129	Total	C	N	O	S	0	0
			1034	660	172	192	10		

- Molecule 36 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	254	Total	C	N	O	S	0	0
			2033	1301	346	384	2		

- Molecule 37 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).

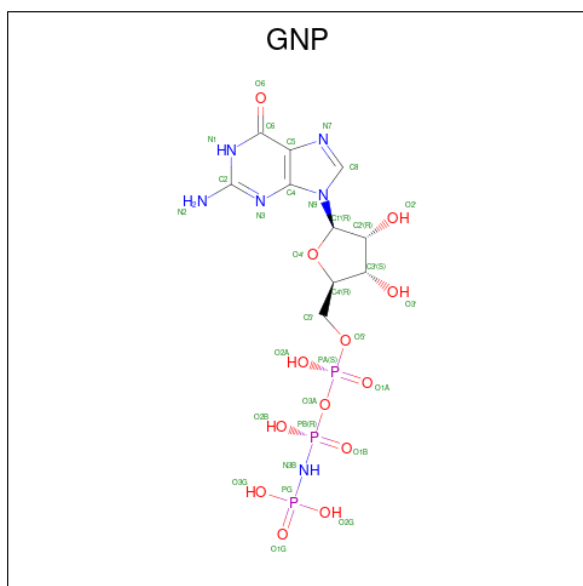


Mol	Chain	Residues	Atoms					AltConf
37	7	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	7	1	Total	Mg	0
			1	1	

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

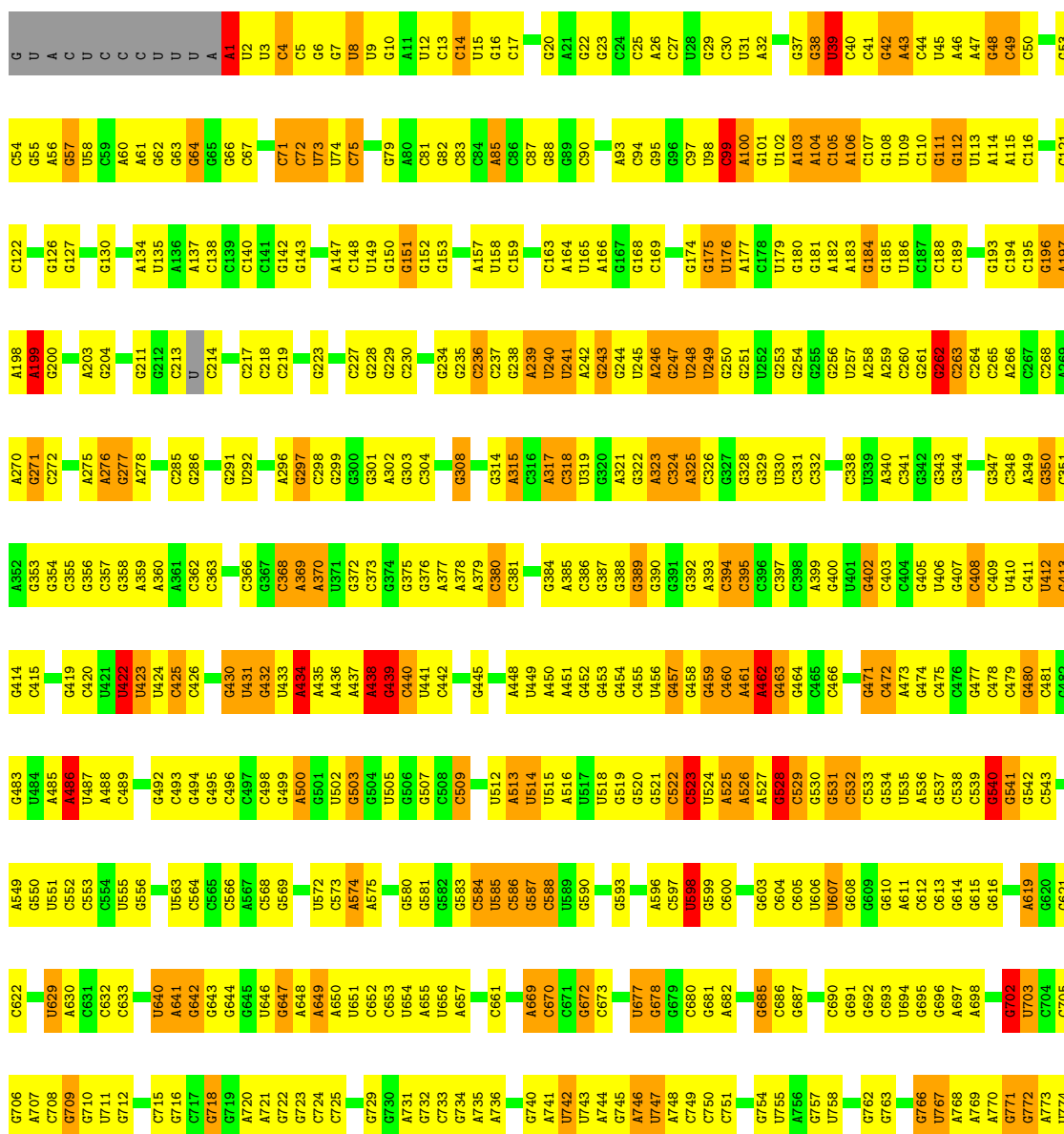
Mol	Chain	Residues	Atoms		AltConf
40	8	1	Total	Zn	0
			1	1	

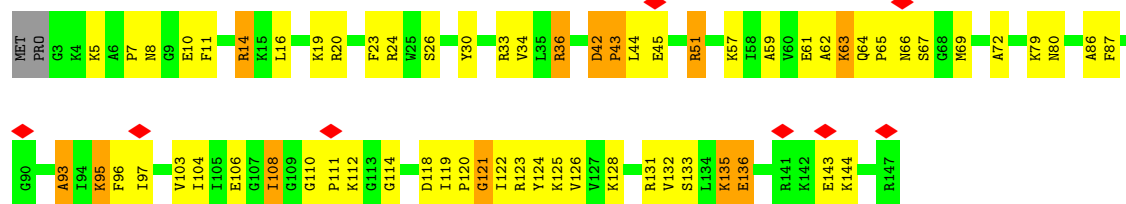
3 Residue-property plots

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.

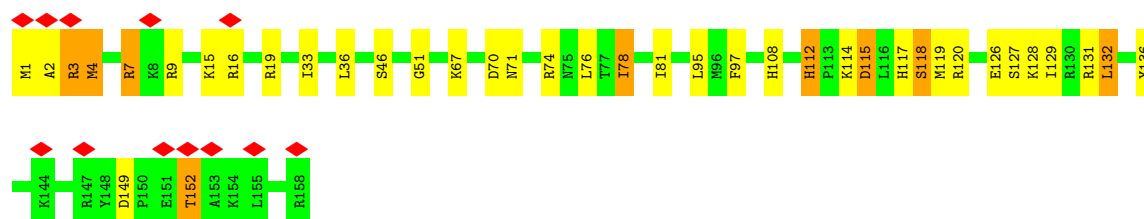
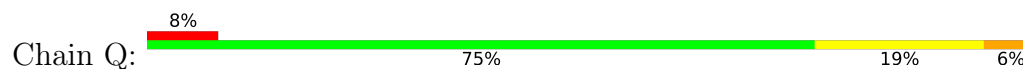
• Molecule 1: 16S ribosomal RNA

Chain 2: 

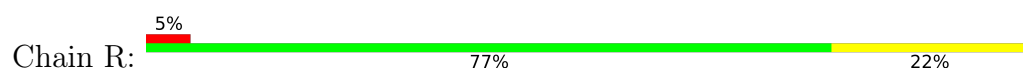




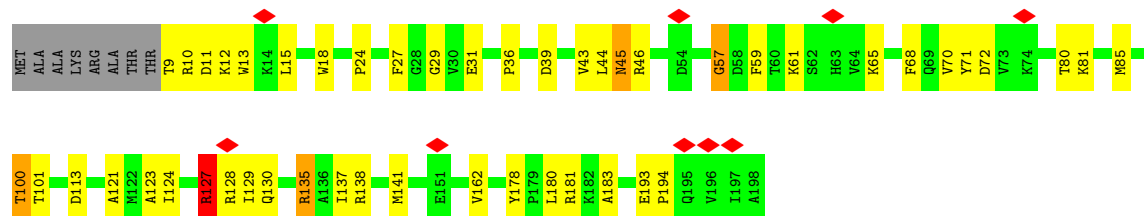
• Molecule 4: 30S ribosomal protein S15



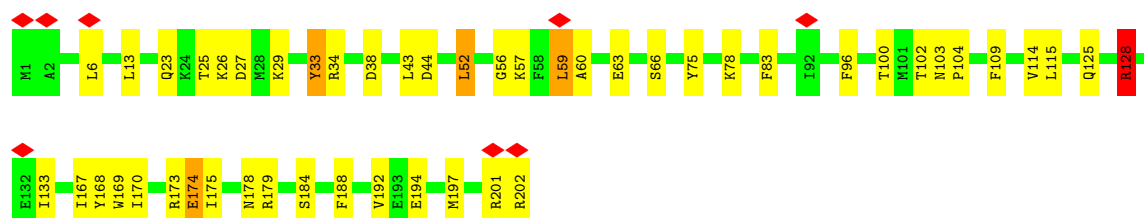
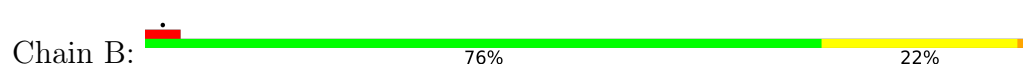
• Molecule 5: 30S ribosomal protein S17P



• Molecule 6: 30S ribosomal protein S3Ae



• Molecule 7: 30S ribosomal protein S2



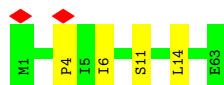
- Molecule 8: 30S ribosomal protein S24e

Chain V:  68% 26% . .




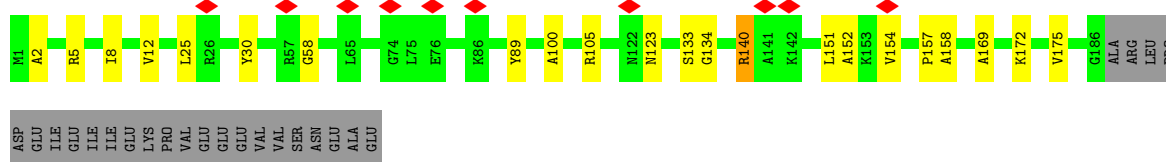
- Molecule 9: 30S ribosomal protein S27e

Chain W:  94% 6%



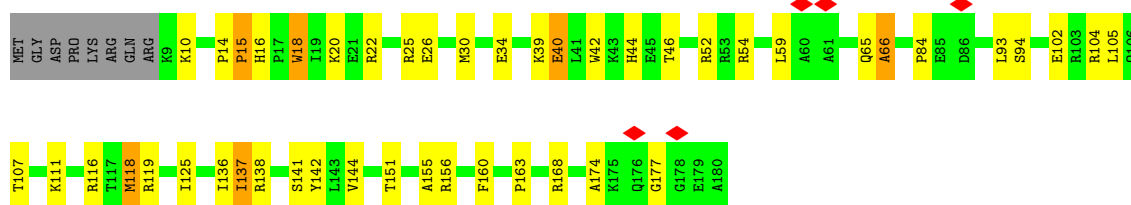
- Molecule 10: 30S ribosomal protein S3

Chain Z:  5% 78% 10% 11%



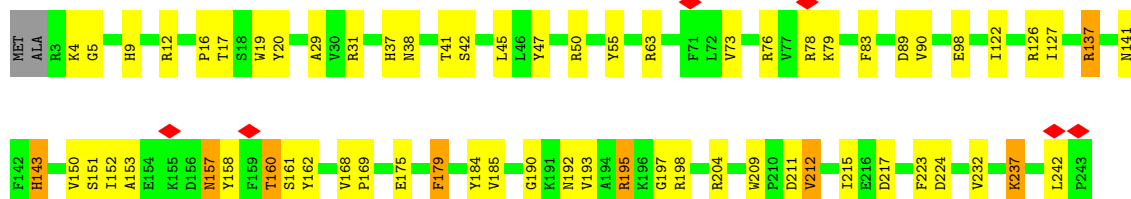
- Molecule 11: 30S ribosomal protein S4

Chain D:  69% 23% . .

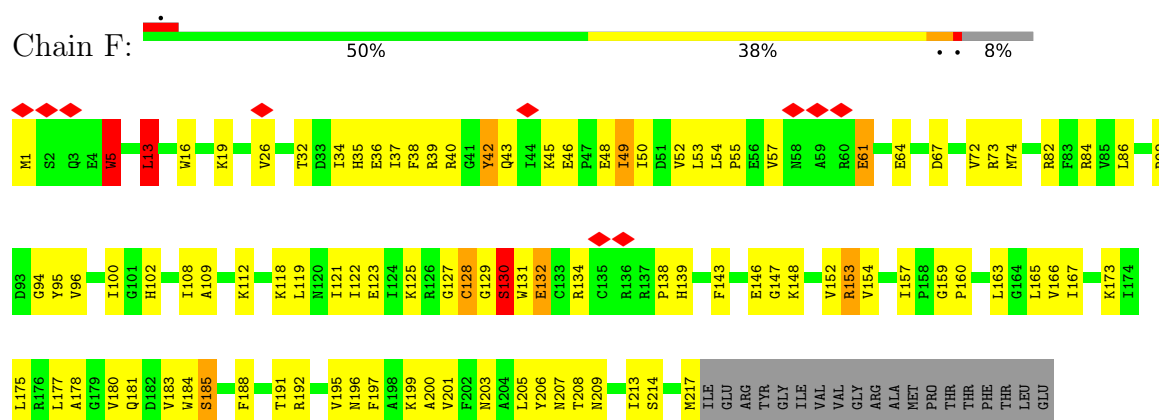


- Molecule 12: 30S ribosomal protein S4e

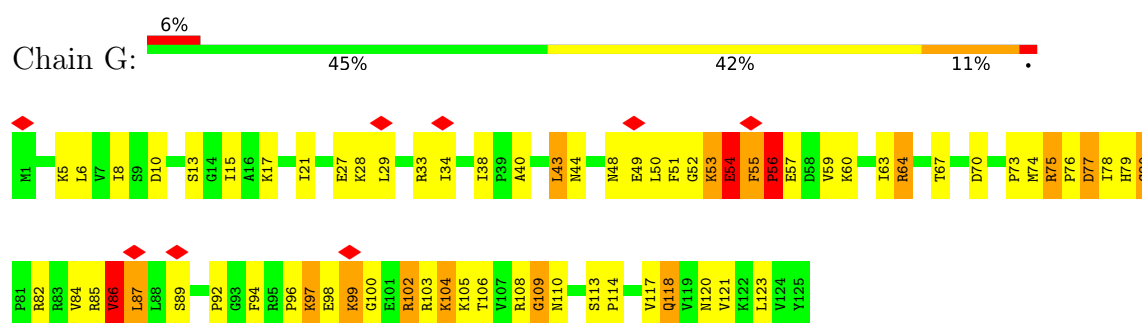
Chain E:  72% 23% . .



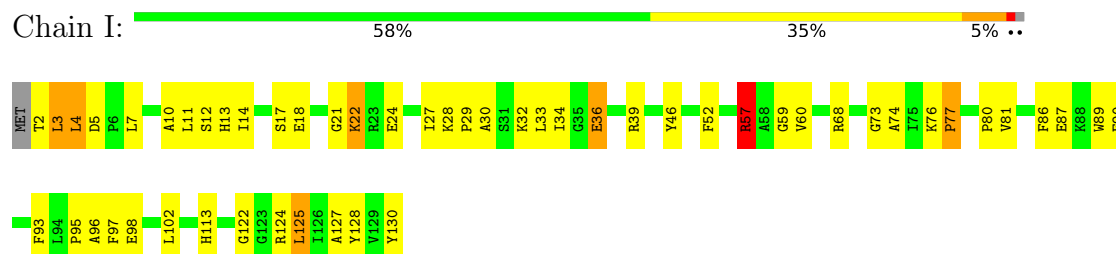
- Molecule 13: 30S ribosomal protein S5



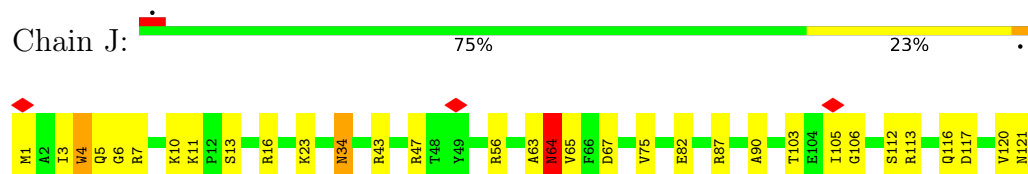
- Molecule 14: 30S ribosomal protein S6e



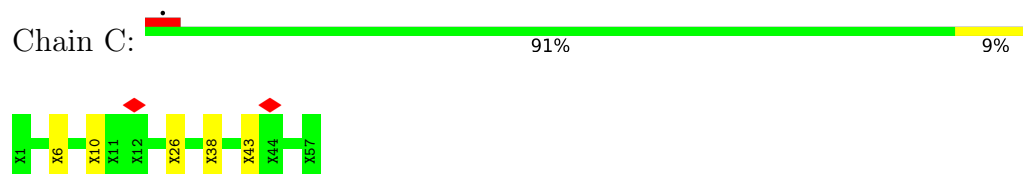
- Molecule 15: 30S ribosomal protein S8



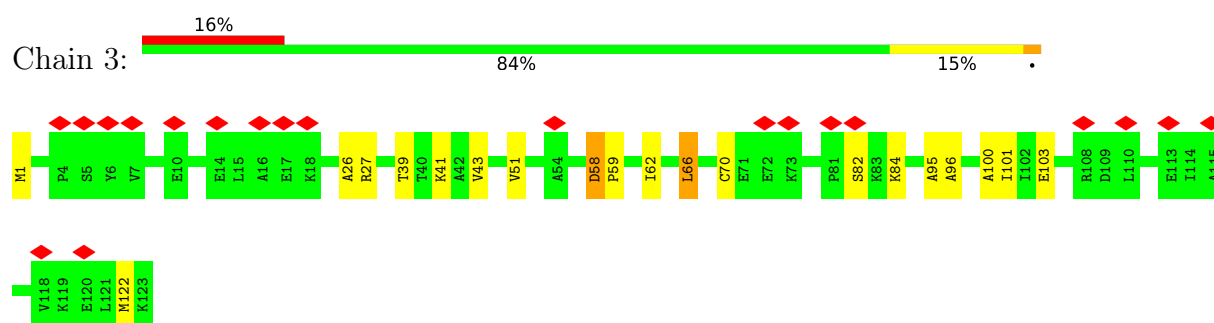
- Molecule 16: 30S ribosomal protein S8e



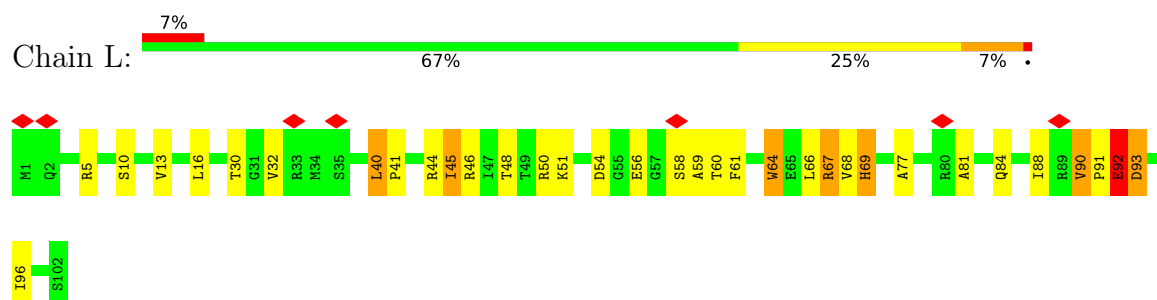
- Molecule 17: 30S ribosomal protein SX



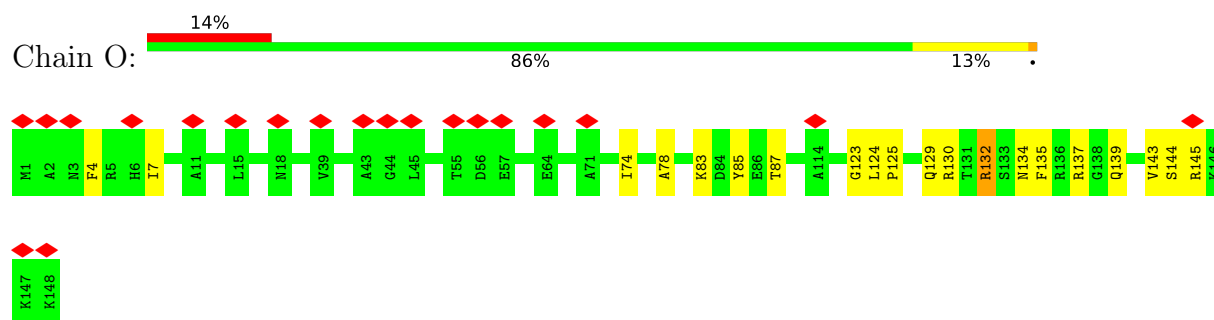
- Molecule 18: 50S ribosomal protein L7Ae



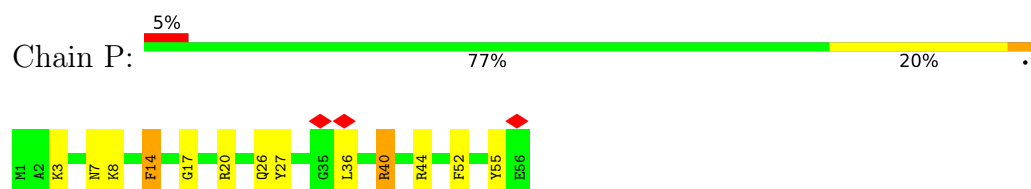
• Molecule 19: 30S ribosomal protein S10



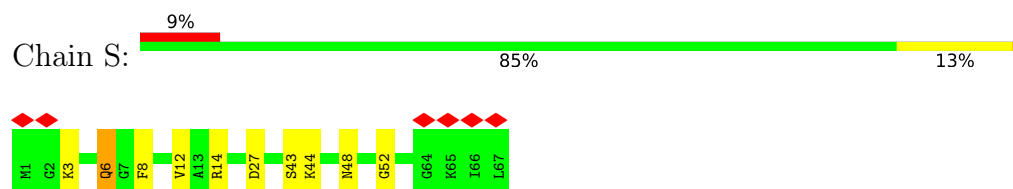
• Molecule 20: 30S ribosomal protein S13



• Molecule 21: 30S ribosomal protein S14 type Z

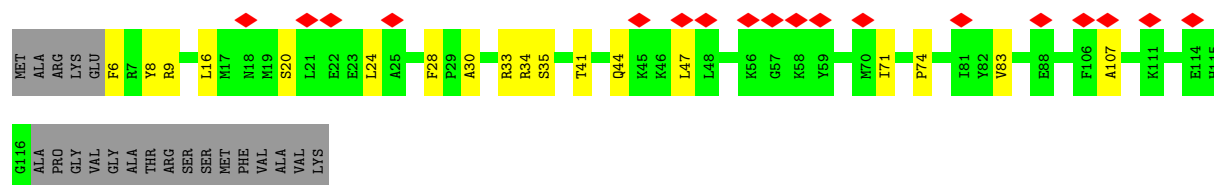


• Molecule 22: 30S ribosomal protein S17e

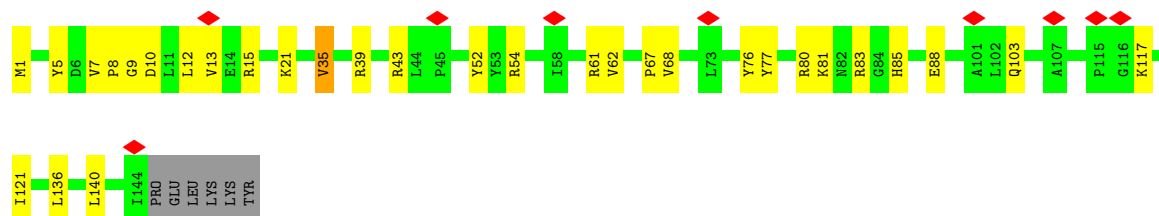
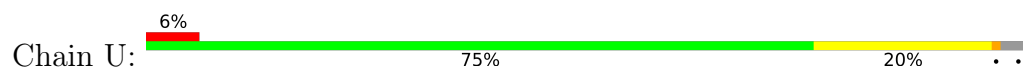


• Molecule 23: 30S ribosomal protein S19

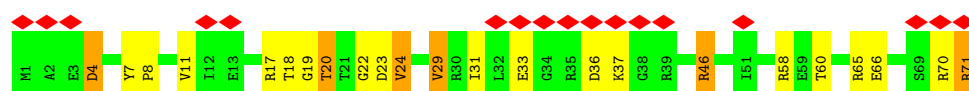




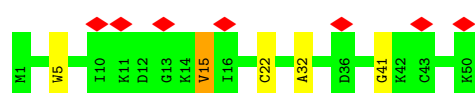
- Molecule 24: 30S ribosomal protein S19e



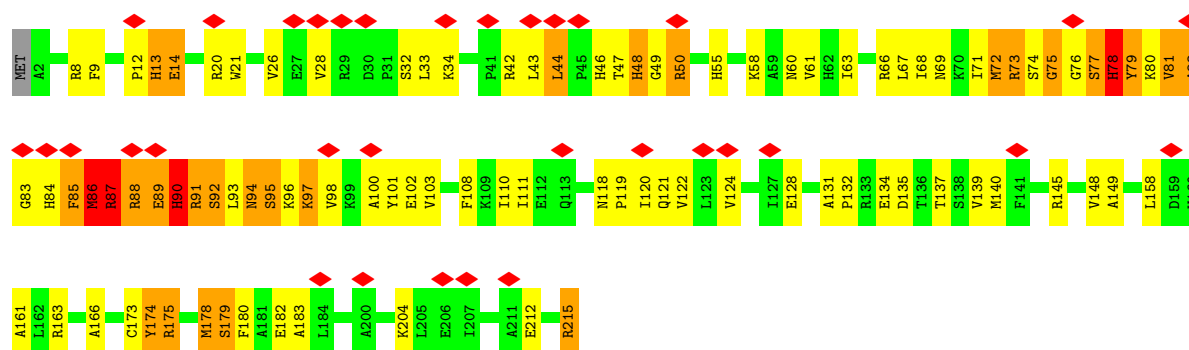
- Molecule 25: 30S ribosomal protein S28e



- Molecule 26: 30S ribosomal protein S27ae



- Molecule 27: 30S ribosomal protein S7

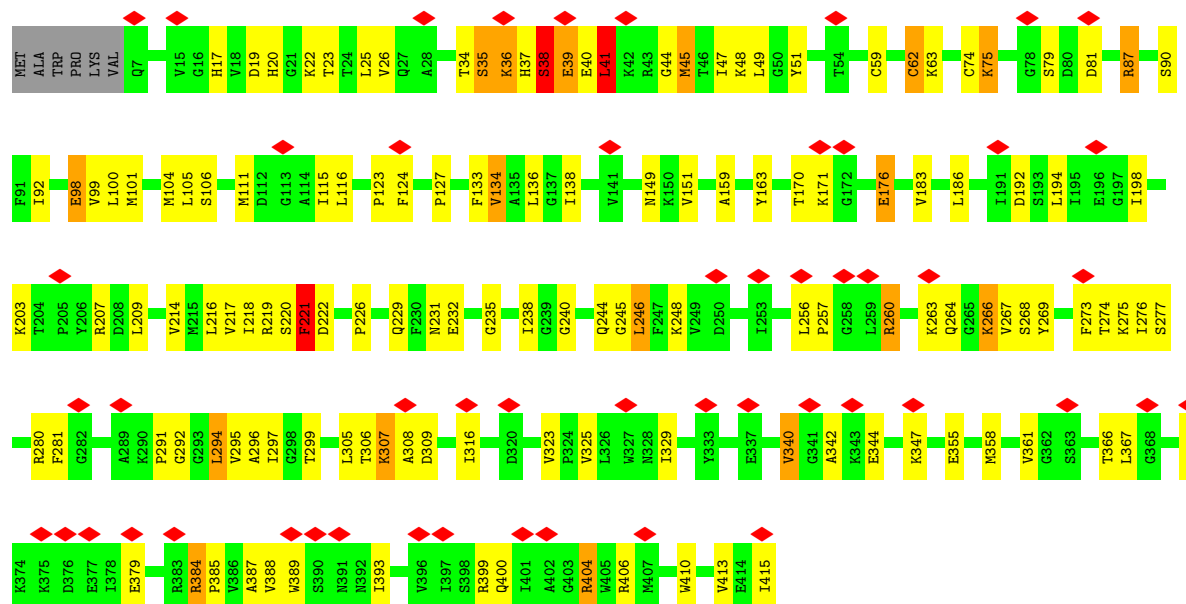


- Molecule 28: 30S ribosomal protein S9



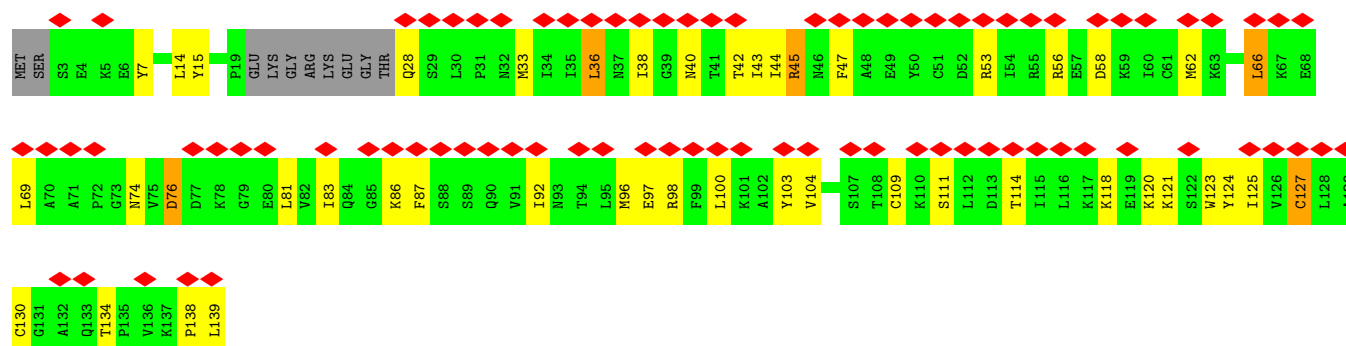
- Molecule 34: Translation initiation factor 2 subunit gamma

Chain 7: 13% 65% 28%



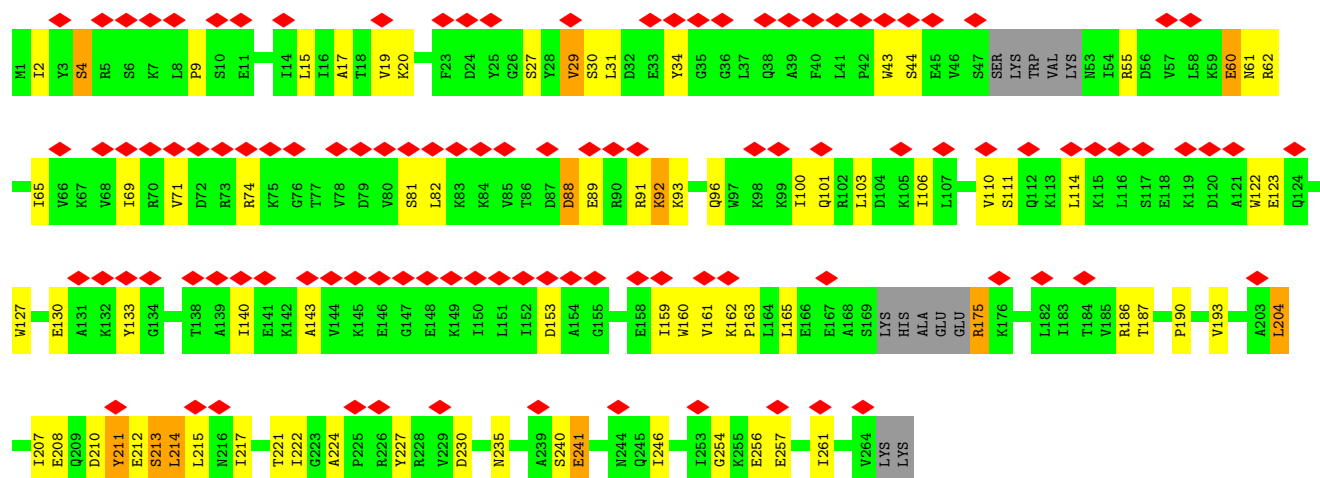
- Molecule 35: Translation initiation factor 2 subunit beta

Chain 8: 60% 60% 29% 7%



- Molecule 36: Translation initiation factor 2 subunit alpha

Chain 9: 40% 66% 26% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.270	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	389.76, 389.76, 389.76	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, OMC, PSU, 5MU, GNP, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.63	17/35964 (0.0%)	0.90	54/56130 (0.1%)
2	M	0.77	0/1022	0.97	3/1375 (0.2%)
3	N	0.81	0/1156	1.07	3/1535 (0.2%)
4	Q	0.75	0/1338	0.99	5/1797 (0.3%)
5	R	0.72	0/956	0.95	2/1287 (0.2%)
6	A	0.68	0/1585	0.88	2/2124 (0.1%)
7	B	0.75	0/1654	0.99	3/2233 (0.1%)
8	V	0.67	0/839	1.00	3/1122 (0.3%)
9	W	0.65	0/485	0.88	0/651
10	Z	0.69	0/1480	0.87	2/1985 (0.1%)
11	D	0.75	2/1457 (0.1%)	0.94	5/1953 (0.3%)
12	E	0.68	0/2025	0.95	8/2732 (0.3%)
13	F	0.77	1/1745 (0.1%)	1.00	3/2350 (0.1%)
14	G	0.74	0/999	1.09	7/1337 (0.5%)
15	I	0.71	1/1049 (0.1%)	0.96	4/1408 (0.3%)
16	J	0.67	0/1013	0.92	0/1349
18	3	0.86	0/951	0.90	1/1281 (0.1%)
19	L	0.76	1/830 (0.1%)	1.08	3/1113 (0.3%)
20	O	0.82	0/1208	0.96	2/1619 (0.1%)
21	P	0.73	0/471	1.11	1/620 (0.2%)
22	S	0.80	0/562	0.96	1/744 (0.1%)
23	T	0.84	0/942	0.91	0/1257
24	U	0.86	0/1203	0.95	3/1621 (0.2%)
25	X	0.78	0/570	1.07	2/760 (0.3%)
26	Y	0.76	0/421	0.78	0/558
27	H	0.95	1/1765 (0.1%)	1.19	12/2371 (0.5%)
28	K	0.78	0/1088	0.92	3/1455 (0.2%)
29	0	1.17	2/216 (0.9%)	1.10	0/279
30	4	0.62	0/1721	0.91	1/2682 (0.0%)
31	5	0.49	0/434	0.77	0/675
32	1	0.61	0/666	0.82	0/882
33	6	0.70	0/791	0.92	2/1066 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	7	0.72	0/3227	0.84	4/4367 (0.1%)
35	8	0.85	0/1048	0.85	0/1406
36	9	0.84	0/2057	0.88	1/2767 (0.0%)
All	All	0.70	25/74938 (0.0%)	0.93	140/108891 (0.1%)

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
3	N	0	2
4	Q	0	1
5	R	0	1
7	B	0	1
8	V	0	3
10	Z	0	1
12	E	0	1
13	F	0	2
14	G	1	7
15	I	0	1
16	J	0	3
20	O	0	1
25	X	0	3
27	H	4	9
28	K	0	2
34	7	0	2
35	8	0	1
36	9	0	1
All	All	5	42

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1019	A	O3'-P	32.96	2.00	1.61
29	0	3	TRP	CB-CG	-7.21	1.37	1.50
1	2	357	C	O3'-P	-6.99	1.52	1.61
1	2	830	A	O3'-P	-6.54	1.53	1.61
1	2	1471	G	O3'-P	-6.51	1.53	1.61
27	H	86	MET	N-CA	6.26	1.58	1.46
1	2	833	C	O3'-P	-6.04	1.53	1.61
1	2	1462	A	O3'-P	-5.85	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	0	22	GLY	C-O	5.70	1.32	1.23
1	2	523	C	O3'-P	-5.67	1.54	1.61
1	2	629	U	C4-O4	-5.63	1.19	1.23
1	2	395	C	O3'-P	-5.57	1.54	1.61
1	2	596	A	O3'-P	-5.56	1.54	1.61
1	2	598	U	O3'-P	-5.47	1.54	1.61
1	2	522	C	O3'-P	-5.44	1.54	1.61
19	L	64	TRP	CB-CG	-5.39	1.40	1.50
1	2	847	A	O3'-P	-5.38	1.54	1.61
11	D	18	TRP	CB-CG	-5.36	1.40	1.50
13	F	42	TYR	CB-CG	-5.32	1.43	1.51
1	2	457	G	O3'-P	-5.30	1.54	1.61
15	I	5	ASP	CB-CG	5.21	1.62	1.51
11	D	40	GLU	CD-OE1	5.14	1.31	1.25
1	2	271	G	O3'-P	-5.12	1.55	1.61
1	2	850	A	O3'-P	-5.02	1.55	1.61
1	2	875	G	O3'-P	-5.01	1.55	1.61

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1019	A	P-O3'-C3'	21.15	145.09	119.70
1	2	1414	G	O5'-P-OP1	-15.20	92.02	105.70
1	2	962	G	O5'-P-OP1	-13.71	93.36	105.70
1	2	1019	A	O3'-P-O5'	10.24	123.46	104.00
27	H	87	ARG	N-CA-C	9.96	137.90	111.00
1	2	540	G	N9-C1'-C2'	-8.77	102.36	112.00
33	6	57	ARG	NE-CZ-NH2	-8.76	115.92	120.30
33	6	57	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	2	985	C	C2'-C3'-O3'	8.41	128.00	109.50
27	H	86	MET	N-CA-C	8.37	133.60	111.00
1	2	962	G	O5'-P-OP2	-8.10	98.41	105.70
1	2	1340	U	C2'-C3'-O3'	8.10	127.32	109.50
1	2	277	G	C2'-C3'-O3'	8.03	127.16	109.50
13	F	5	TRP	CA-CB-CG	8.02	128.94	113.70
1	2	975	A	C2'-C3'-O3'	7.81	126.68	109.50
5	R	62	ARG	NE-CZ-NH1	7.49	124.05	120.30
4	Q	3	ARG	NE-CZ-NH1	7.49	124.04	120.30
14	G	86	VAL	CB-CA-C	-7.48	97.20	111.40
1	2	1343	C	O5'-P-OP1	7.40	119.58	110.70
1	2	462	A	C2'-C3'-O3'	7.28	125.52	109.50
1	2	408	C	C2'-C3'-O3'	7.23	125.41	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1460	G	C2'-C3'-O3'	7.20	125.34	109.50
27	H	79	TYR	CA-CB-CG	7.14	126.96	113.40
1	2	1261	U	C2'-C3'-O3'	7.13	125.18	109.50
21	P	40	ARG	NE-CZ-NH2	7.05	123.83	120.30
6	A	135	ARG	NE-CZ-NH2	-6.79	116.91	120.30
34	7	294	LEU	CA-CB-CG	6.78	130.90	115.30
8	V	85	TYR	CA-CB-CG	6.74	126.20	113.40
11	D	104	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	2	528	G	C2'-C3'-O3'	6.73	124.47	113.70
12	E	78	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	2	1053	A	C2'-C3'-O3'	6.70	124.42	113.70
36	9	92	LYS	CD-CE-NZ	6.57	126.81	111.70
1	2	1453	U	C2'-C3'-O3'	6.54	124.16	113.70
1	2	847	A	C2'-C3'-O3'	-6.48	95.25	109.50
24	U	61	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	2	1306	A	C2'-C3'-O3'	6.40	123.94	113.70
34	7	221	PHE	N-CA-C	6.39	128.25	111.00
14	G	109	GLY	N-CA-C	6.39	129.06	113.10
1	2	742	U	C2'-C3'-O3'	6.37	123.89	113.70
8	V	85	TYR	N-CA-CB	6.37	122.06	110.60
1	2	924	U	C2'-C3'-O3'	6.35	123.86	113.70
1	2	422	U	N1-C1'-C2'	-6.34	105.02	112.00
15	I	57	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	2	462	A	O4'-C4'-C3'	-6.30	97.70	104.00
7	B	128	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	2	1	A	O5'-P-OP1	-6.26	100.06	105.70
1	2	434	A	C2'-C3'-O3'	6.21	123.63	113.70
22	S	14	ARG	NE-CZ-NH1	6.20	123.40	120.30
11	D	25	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	2	486	A	C2'-C3'-O3'	6.15	123.54	113.70
5	R	51	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	2	99	C	C2'-C3'-O3'	6.14	123.52	113.70
1	2	1483	U	C2'-C3'-O3'	6.13	123.51	113.70
10	Z	140	ARG	NE-CZ-NH1	6.06	123.33	120.30
11	D	25	ARG	NE-CZ-NH2	-6.06	117.27	120.30
7	B	115	LEU	CA-CB-CG	6.06	129.23	115.30
13	F	13	LEU	CA-CB-CG	6.04	129.19	115.30
19	L	92	GLU	N-CA-C	6.02	127.25	111.00
1	2	438	A	C4'-C3'-O3'	6.02	125.03	113.00
2	M	66	ARG	NE-CZ-NH2	-6.01	117.30	120.30
27	H	86	MET	C-N-CA	5.99	136.69	121.70
14	G	75	ARG	NE-CZ-NH1	5.98	123.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	262	G	C2'-C3'-O3'	5.98	123.26	113.70
1	2	1368	A	C2'-C3'-O3'	5.97	123.25	113.70
25	X	71	ARG	NE-CZ-NH1	5.92	123.26	120.30
14	G	86	VAL	CG1-CB-CG2	5.90	120.33	110.90
1	2	439	G	C2'-C3'-O3'	5.88	123.10	113.70
3	N	51	ARG	NE-CZ-NH1	5.86	123.23	120.30
15	I	4	LEU	CA-CB-CG	5.83	128.72	115.30
1	2	196	G	C4'-C3'-O3'	-5.83	97.16	109.40
27	H	85	PHE	CB-CA-C	5.81	122.02	110.40
15	I	33	LEU	CA-CB-CG	5.80	128.63	115.30
6	A	127	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	2	1262	U	C2'-C3'-O3'	5.75	122.90	113.70
12	E	76	ARG	NE-CZ-NH1	5.75	123.17	120.30
27	H	215	ARG	NE-CZ-NH1	5.73	123.17	120.30
15	I	5	ASP	CB-CG-OD2	-5.71	113.16	118.30
19	L	92	GLU	C-N-CA	5.71	135.98	121.70
1	2	1423	A	C2'-C3'-O3'	5.71	122.83	113.70
27	H	14	GLU	N-CA-C	5.71	126.42	111.00
14	G	54	GLU	N-CA-CB	5.70	120.86	110.60
1	2	1343	C	O5'-P-OP2	5.67	117.50	110.70
27	H	79	TYR	N-CA-CB	-5.64	100.45	110.60
1	2	199	A	P-O3'-C3'	5.64	126.46	119.70
20	O	132	ARG	NE-CZ-NH2	5.64	123.12	120.30
12	E	63	ARG	NE-CZ-NH1	5.63	123.11	120.30
14	G	53	LYS	CB-CA-C	5.61	121.62	110.40
1	2	977	G	C2'-C3'-O3'	5.54	122.56	113.70
24	U	43	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	M	41	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	2	1249	A	O5'-P-OP1	-5.46	100.79	105.70
1	2	176	U	C2'-C3'-O3'	5.45	122.41	113.70
11	D	119	ARG	NE-CZ-NH1	5.44	123.02	120.30
19	L	67	ARG	NE-CZ-NH1	5.44	123.02	120.30
34	7	87	ARG	NE-CZ-NH1	5.43	123.02	120.30
4	Q	3	ARG	NE-CZ-NH2	-5.38	117.61	120.30
25	X	71	ARG	NE-CZ-NH2	-5.37	117.61	120.30
24	U	43	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	2	1378	A	N9-C1'-C2'	-5.37	106.10	112.00
28	K	79	ARG	NE-CZ-NH1	5.36	122.98	120.30
11	D	52	ARG	NE-CZ-NH2	-5.35	117.62	120.30
27	H	8	ARG	NE-CZ-NH1	5.35	122.97	120.30
4	Q	74	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	2	669	A	C4-N9-C1'	5.31	135.86	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	136	ARG	NE-CZ-NH1	5.29	122.94	120.30
28	K	127	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	2	39	U	C5'-C4'-O4'	5.28	115.43	109.10
34	7	41	LEU	CA-CB-CG	5.27	127.42	115.30
12	E	78	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	2	438	A	C2'-C3'-O3'	-5.26	97.93	109.50
13	F	42	TYR	CA-CB-CG	-5.25	103.42	113.40
27	H	163	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	2	962	G	OP1-P-OP2	5.21	127.42	119.60
8	V	33	ARG	NE-CZ-NH2	5.21	122.90	120.30
18	3	27	ARG	NE-CZ-NH1	5.19	122.90	120.30
4	Q	19	ARG	NE-CZ-NH1	5.19	122.89	120.30
3	N	36	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	2	702	G	N9-C1'-C2'	5.15	120.69	114.00
4	Q	7	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	2	669	A	C8-N9-C1'	-5.13	118.46	127.70
12	E	50	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	2	175	G	C4'-C3'-O3'	5.13	123.26	113.00
12	E	137	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	2	1318	U	O4'-C1'-N1	5.13	112.30	108.20
28	K	104	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	2	111	G	C2'-C3'-O3'	5.10	121.86	113.70
3	N	14	ARG	NE-CZ-NH1	5.08	122.84	120.30
7	B	34	ARG	NE-CZ-NH1	5.08	122.84	120.30
14	G	80	GLY	N-CA-C	-5.06	100.44	113.10
1	2	1143	G	C2'-C3'-O3'	5.06	121.80	113.70
12	E	137	ARG	NE-CZ-NH2	-5.05	117.77	120.30
20	O	145	ARG	NE-CZ-NH1	5.04	122.82	120.30
27	H	75	GLY	N-CA-C	5.04	125.70	113.10
10	Z	105	ARG	NE-CZ-NH2	-5.04	117.78	120.30
12	E	209	TRP	CA-CB-CG	5.03	123.26	113.70
1	2	1458	A	C2'-C3'-O3'	5.03	121.74	113.70
1	2	1337	A	C4'-C3'-O3'	5.02	123.04	113.00
30	4	74	C	O5'-P-OP1	-5.00	101.20	105.70
27	H	91	ARG	NE-CZ-NH1	5.00	122.80	120.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	G	53	LYS	CA
27	H	85	PHE	CA
27	H	86	MET	CA

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Mol	Chain	Res	Type	Atom
27	H	87	ARG	CA
27	H	96	LYS	CA

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	7	38	SER	Peptide
34	7	79	SER	Peptide
35	8	28	GLN	Peptide
36	9	211	TYR	Peptide
7	B	6	LEU	Peptide
12	E	143	HIS	Peptide
13	F	130	SER	Peptide
13	F	72	VAL	Peptide
14	G	17	LYS	Peptide
14	G	43	LEU	Peptide
14	G	49	GLU	Peptide
14	G	56	PRO	Peptide
14	G	74	MET	Peptide
14	G	97	LYS	Peptide
14	G	98	GLU	Peptide
27	H	12	PRO	Peptide
27	H	14	GLU	Peptide
27	H	178	MET	Peptide
27	H	42	ARG	Peptide
27	H	78	HIS	Peptide
27	H	84	HIS	Peptide
27	H	86	MET	Peptide
27	H	87	ARG	Peptide
27	H	90	HIS	Peptide
15	I	21	GLY	Peptide
16	J	6	GLY	Peptide
16	J	63	ALA	Peptide
16	J	64	ASN	Peptide
28	K	110	ASP	Peptide
28	K	12	THR	Peptide
3	N	121	GLY	Peptide
3	N	5	LYS	Peptide
20	O	124	LEU	Peptide
4	Q	2	ALA	Peptide
5	R	34	PHE	Peptide
8	V	55	TYR	Peptide

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Mol	Chain	Res	Type	Group
8	V	94	GLU	Peptide
8	V	96	LYS	Peptide
25	X	22	GLY	Peptide
25	X	4	ASP	Peptide
25	X	66	GLU	Peptide
10	Z	157	PRO	Peptide

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	2	32135	0	16233	1310	0
2	M	1004	0	1041	15	0
3	N	1140	0	1235	48	0
4	Q	1310	0	1392	21	0
5	R	934	0	960	17	0
6	A	1559	0	1648	32	0
7	B	1623	0	1685	36	0
8	V	823	0	847	26	0
9	W	478	0	524	2	0
10	Z	1459	0	1549	11	0
11	D	1434	0	1498	27	0
12	E	1976	0	2046	36	0
13	F	1716	0	1770	105	0
14	G	984	0	1044	98	0
15	I	1028	0	1065	45	0
16	J	1004	0	1088	16	0
17	C	286	0	61	3	0
18	3	939	0	994	6	0
19	L	822	0	870	26	0
20	O	1189	0	1248	11	0
21	P	462	0	492	7	0
22	S	556	0	604	5	0
23	T	923	0	986	6	0
24	U	1175	0	1216	22	0
25	X	568	0	600	23	0
26	Y	409	0	410	4	0
27	H	1728	0	1775	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	K	1072	0	1128	14	0
29	0	213	0	250	10	0
30	4	1622	0	830	71	0
31	5	388	0	193	19	0
32	1	662	0	705	22	0
33	6	777	0	804	18	0
34	7	3171	0	3292	111	0
35	8	1034	0	1078	31	0
36	9	2033	0	2144	40	0
37	7	8	0	8	11	0
38	7	1	0	0	0	0
39	7	32	0	13	1	0
40	8	1	0	0	1	0
All	All	70678	0	55326	2020	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 16.

All (2020) 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)
35:8:127:CYS:SG	40:8:201:ZN:ZN	1.06	1.41
1:2:8:U:N3	1:2:873:A:N6	1.70	1.36
1:2:1019:A:O3'	1:2:1020:G:P	2.00	1.18
1:2:920:U:H3	1:2:1161:A:N6	1.42	1.16
1:2:516:A:N6	1:2:842:U:H3	1.48	1.11
1:2:822:A:H2'	1:2:823:A:C8	1.89	1.07
1:2:314:G:O2'	1:2:1424:G:OP1	1.73	1.06
30:4:74:C:C4	34:7:37:HIS:HB2	1.91	1.06
1:2:315:A:H1'	1:2:1423:A:H1'	1.38	1.06
1:2:1402:C:H2'	1:2:1403:U:O4'	1.54	1.05
29:0:1:MET:SD	29:0:4:LYS:NZ	2.29	1.05
1:2:6:G:O6	1:2:7:G:O6	1.75	1.03
1:2:648:A:N6	1:2:741:A:O2'	1.96	0.99
1:2:1487:U:H2'	1:2:1488:C:C6	1.98	0.97
1:2:8:U:C4	1:2:873:A:N6	2.34	0.96
1:2:60:A:N1	1:2:64:G:O6	1.97	0.96
1:2:507:G:OP1	3:N:111:PRO:HG3	1.64	0.96
1:2:1403:U:O2'	14:G:110:ASN:ND2	2.00	0.95
30:4:19:G:C5	36:9:61:ASN:HB2	2.02	0.94
1:2:619:A:N6	1:2:678:G:O6	2.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:229:G:C2	1:2:230:C:C5	2.56	0.93
1:2:1412:A:O2'	14:G:92:PRO:HG3	1.69	0.92
1:2:1378:A:O2'	34:7:373:VAL:HB	1.69	0.92
1:2:1414:G:OP1	14:G:86:VAL:HG13	1.70	0.91
1:2:516:A:H61	1:2:842:U:H3	0.94	0.91
1:2:1414:G:OP1	14:G:86:VAL:CG1	2.19	0.90
1:2:920:U:H3	1:2:1161:A:H61	0.94	0.90
30:4:76:A:O3'	37:7:501:MET:HA	1.72	0.90
1:2:229:G:C2	1:2:230:C:C4	2.60	0.90
30:4:73:A:C2	34:7:38:SER:HA	2.07	0.90
1:2:1318:U:H3	1:2:1323:A:N6	1.69	0.89
1:2:1367:C:H1'	32:1:65:ALA:HB2	1.53	0.89
1:2:975:A:H2'	1:2:976:A:H5'	1.53	0.89
1:2:151:G:O2'	14:G:64:ARG:NE	2.06	0.89
1:2:229:G:N2	1:2:230:C:C2	2.40	0.89
1:2:1313:G:OP1	27:H:81:VAL:HG23	1.73	0.89
1:2:8:U:N3	1:2:873:A:C6	2.32	0.89
1:2:439:G:H1'	1:2:440:C:C5	2.08	0.89
1:2:1472:G:OP1	32:1:58:LYS:HD2	1.72	0.89
1:2:8:U:H3	1:2:873:A:N6	1.58	0.88
1:2:1031:G:O3'	13:F:84:ARG:NH1	2.06	0.88
1:2:483:G:C8	33:6:57:ARG:NH2	2.40	0.87
1:2:920:U:N3	1:2:1161:A:N6	2.09	0.87
1:2:8:U:C2	1:2:873:A:N6	2.42	0.87
1:2:516:A:N1	1:2:842:U:O4	2.08	0.87
30:4:19:G:N7	36:9:61:ASN:HB2	1.90	0.86
1:2:1367:C:H1'	32:1:65:ALA:CB	2.06	0.86
1:2:368:C:O2'	1:2:369:A:OP2	1.94	0.85
1:2:1342:C:H3'	1:2:1343:C:P	2.16	0.85
1:2:460:C:H5'	1:2:461:A:H5''	1.59	0.85
1:2:229:G:N1	1:2:230:C:C4	2.43	0.85
1:2:184:G:O2'	1:2:185:G:C8	2.30	0.84
30:4:74:C:N3	34:7:37:HIS:HB2	1.91	0.84
1:2:1195:U:OP1	27:H:79:TYR:HB2	1.76	0.84
27:H:87:ARG:HG3	27:H:90:HIS:HA	1.57	0.84
1:2:6:G:C6	1:2:7:G:C6	2.65	0.84
1:2:1348:C:H2'	1:2:1349:C:C6	2.13	0.84
1:2:1200:U:N3	27:H:180:PHE:HB2	1.92	0.83
14:G:53:LYS:HA	14:G:54:GLU:HB2	1.58	0.83
1:2:1338:C:O2	25:X:23:ASP:HA	1.78	0.83
1:2:1347:U:O2'	1:2:1348:C:H5'	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:540:G:O2'	1:2:541:G:OP2	1.97	0.82
1:2:1128:U:O4	7:B:202:ARG:N	2.13	0.81
1:2:1400:A:H2'	1:2:1401:U:C6	2.14	0.81
1:2:1494:C:O2	31:5:806:G:N2	2.13	0.81
1:2:1333:G:C8	27:H:48:HIS:CE1	2.69	0.81
1:2:459:G:H3'	1:2:460:C:C4'	2.11	0.80
1:2:846:G:H4'	1:2:1443:G:H4'	1.64	0.80
1:2:1392:G:O2'	1:2:1423:A:N6	2.13	0.80
36:9:123:GLU:HA	36:9:127:TRP:CD1	2.17	0.80
12:E:37:HIS:CE1	12:E:41:THR:HB	2.17	0.79
1:2:1413:G:H2'	1:2:1414:G:C8	2.16	0.79
8:V:56:ILE:HG13	8:V:67:GLY:HA3	1.63	0.79
1:2:1318:U:N3	1:2:1323:A:N6	2.29	0.79
1:2:1200:U:H3	27:H:180:PHE:HB2	1.48	0.79
1:2:1248:A:O2'	27:H:81:VAL:HG22	1.84	0.78
1:2:437:A:OP2	1:2:439:G:O6	2.01	0.78
1:2:1041:C:H5''	25:X:71:ARG:NE	1.98	0.78
1:2:1443:G:H2'	1:2:1444:G:C8	2.18	0.78
1:2:8:U:O2	1:2:873:A:N7	2.17	0.78
1:2:880:G:H2'	1:2:881:G:C8	2.19	0.78
9:W:4:PRO:HB3	15:I:28:LYS:HE3	1.66	0.78
1:2:1402:C:O2	14:G:79:HIS:HB2	1.83	0.78
1:2:1248:A:O3'	27:H:81:VAL:HG13	1.83	0.77
1:2:1311:C:OP1	27:H:76:GLY:C	2.21	0.77
1:2:516:A:N6	1:2:842:U:N3	2.19	0.77
1:2:867:A:O2'	1:2:1374:C:H4'	1.84	0.77
1:2:152:G:H2'	1:2:153:G:C8	2.18	0.77
1:2:644:G:N2	1:2:651:U:O4	2.18	0.77
6:A:10:ARG:HB2	36:9:92:LYS:CD	2.14	0.77
14:G:78:ILE:HB	14:G:109:GLY:HA2	1.67	0.77
14:G:40:ALA:HB3	14:G:59:VAL:HG13	1.67	0.77
30:4:26:G:H4'	35:8:38:ILE:CG2	2.15	0.77
1:2:62:G:N7	1:2:63:G:N7	2.32	0.77
1:2:879:U:O2'	13:F:74:MET:O	2.00	0.77
11:D:59:LEU:HD11	13:F:132:GLU:HG3	1.68	0.76
1:2:1042:U:OP1	25:X:70:ARG:NH2	2.19	0.76
27:H:90:HIS:HB2	27:H:94:ASN:HB2	1.66	0.76
1:2:471:G:N2	3:N:65:PRO:O	2.19	0.76
1:2:643:G:C2	1:2:653:C:N3	2.54	0.75
1:2:1037:U:H1'	1:2:1046:G:C6	2.20	0.75
30:4:73:A:H2	34:7:38:SER:HA	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:276:A:H4'	3:N:14:ARG:NH2	2.01	0.75
1:2:1096:G:H21	24:U:1:MET:HA	1.51	0.75
1:2:431:U:H4'	8:V:33:ARG:HH21	1.52	0.75
19:L:32:VAL:HG22	19:L:77:ALA:HB2	1.69	0.74
1:2:830:A:C8	1:2:832:G:C8	2.75	0.74
1:2:324:C:O2'	1:2:325:A:OP2	2.04	0.74
1:2:868:C:H5''	1:2:1373:A:O2'	1.88	0.74
1:2:1413:G:N3	14:G:77:ASP:OD2	2.21	0.74
1:2:394:C:H2'	1:2:395:C:H6	1.52	0.74
1:2:879:U:H4'	13:F:73:ARG:CZ	2.17	0.74
30:4:74:C:H4'	30:4:75:C:O5'	1.88	0.74
1:2:438:A:H3'	1:2:439:G:H5''	1.70	0.74
1:2:1041:C:H5''	25:X:71:ARG:CZ	2.16	0.73
1:2:642:G:H2'	1:2:643:G:O4'	1.87	0.73
13:F:157:ILE:HB	13:F:184:TRP:HB2	1.70	0.73
34:7:235:GLY:HA2	36:9:193:VAL:HG21	1.70	0.73
1:2:643:G:N2	1:2:653:C:C2	2.57	0.73
1:2:1413:G:C2	14:G:77:ASP:OD2	2.41	0.73
1:2:359:A:OP1	3:N:51:ARG:N	2.22	0.73
1:2:1403:U:C2	14:G:77:ASP:CG	2.62	0.73
12:E:16:PRO:HG2	12:E:19:TRP:NE1	2.04	0.72
1:2:179:U:H3	1:2:184:G:H1	1.35	0.72
1:2:1080:C:O2'	1:2:1082:A:OP2	2.05	0.72
1:2:1403:U:C2	14:G:77:ASP:OD1	2.42	0.72
1:2:344:G:OP1	14:G:106:THR:HG21	1.90	0.72
1:2:1485:G:H2'	1:2:1486:A:H5''	1.70	0.72
1:2:134:A:H2'	1:2:135:U:C6	2.23	0.72
1:2:1459:G:O2'	1:2:1460:G:OP2	2.05	0.72
34:7:218:ILE:HD11	34:7:294:LEU:HD11	1.70	0.72
1:2:321:A:H2'	1:2:322:G:O4'	1.89	0.72
30:4:2:G:N2	30:4:3:C:C2	2.58	0.72
1:2:229:G:N3	1:2:230:C:C6	2.58	0.71
30:4:49:G:C2	30:4:66:C:C2	2.77	0.71
1:2:433:U:O5'	1:2:433:U:O2	2.07	0.71
27:H:44:LEU:HD13	28:K:44:THR:OG1	1.90	0.71
27:H:178:MET:HB3	27:H:183:ALA:HB2	1.71	0.71
1:2:1346:C:H2'	1:2:1347:U:C6	2.25	0.71
1:2:1404:C:H2'	1:2:1405:C:O4'	1.91	0.71
1:2:495:G:N2	1:2:496:C:C2	2.58	0.71
1:2:1032:A:OP1	13:F:84:ARG:CZ	2.38	0.71
30:4:2:G:N1	30:4:3:C:C4	2.58	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:129:GLY:HA2	13:F:134:ARG:HB3	1.73	0.70
1:2:1290:U:O4	1:2:1291:G:C2	2.43	0.70
19:L:45:ILE:HG23	19:L:66:LEU:HB3	1.72	0.70
1:2:1032:A:P	13:F:84:ARG:CZ	2.80	0.70
27:H:71:ILE:HG23	27:H:180:PHE:CE1	2.26	0.70
1:2:317:A:O2'	14:G:102:ARG:NH2	2.24	0.70
1:2:607:U:H4'	15:I:57:ARG:HH21	1.56	0.70
1:2:17:C:H4'	1:2:843:G:C8	2.26	0.70
1:2:359:A:P	3:N:51:ARG:H	2.14	0.70
1:2:650:A:N3	1:2:740:G:O2'	2.23	0.70
30:4:73:A:H3'	34:7:221:PHE:CZ	2.27	0.70
34:7:37:HIS:N	34:7:41:LEU:HB2	2.07	0.70
1:2:113:U:OP1	5:R:30:HIS:CE1	2.44	0.70
34:7:17:HIS:O	34:7:22:LYS:NZ	2.25	0.70
1:2:400:G:O2'	1:2:423:U:O2	2.09	0.70
1:2:1346:C:H2'	1:2:1347:U:C5	2.27	0.70
1:2:495:G:C2	1:2:496:C:C4	2.80	0.69
1:2:394:C:H2'	1:2:395:C:C6	2.26	0.69
1:2:930:G:C5	1:2:1325:C:H4'	2.27	0.69
5:R:1:MET:C	5:R:15:LYS:HG2	2.12	0.69
1:2:892:C:O2'	1:2:894:A:OP2	2.08	0.69
12:E:12:ARG:HA	12:E:29:ALA:HB2	1.72	0.69
27:H:87:ARG:C	27:H:88:ARG:HD3	2.12	0.69
1:2:909:U:OP2	20:O:130:ARG:HD2	1.92	0.69
1:2:1448:A:H62	33:6:51:ILE:HD13	1.56	0.69
1:2:6:G:N7	13:F:192:ARG:NH2	2.40	0.69
1:2:121:C:N3	1:2:122:C:C5	2.61	0.69
1:2:251:G:O6	1:2:262:G:O6	2.11	0.69
1:2:318:C:H4'	14:G:102:ARG:HD3	1.73	0.69
1:2:152:G:H4'	14:G:64:ARG:HD2	1.74	0.69
1:2:1118:C:N3	1:2:1141:G:N2	2.41	0.69
15:I:11:LEU:O	15:I:14:ILE:HG22	1.92	0.69
1:2:229:G:C2	1:2:230:C:C6	2.80	0.69
1:2:585:U:H3'	1:2:586:C:H4'	1.74	0.69
1:2:648:A:N6	1:2:741:A:HO2'	1.86	0.69
13:F:203:ASN:O	13:F:206:TYR:HB3	1.92	0.69
15:I:80:PRO:HA	15:I:124:ARG:HA	1.74	0.69
27:H:110:ILE:HD13	27:H:182:GLU:HG2	1.74	0.69
1:2:478:C:H2'	1:2:479:C:C6	2.29	0.69
1:2:1402:C:H42	1:2:1413:G:H22	1.38	0.68
1:2:1452:G:H2'	1:2:1453:U:H6	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:H:87:ARG:HA	27:H:88:ARG:HD3	1.75	0.68
1:2:229:G:N3	1:2:230:C:C5	2.61	0.68
1:2:771:G:C5	1:2:773:A:O4'	2.46	0.68
6:A:10:ARG:HB2	36:9:92:LYS:HD2	1.75	0.68
34:7:260:ARG:HD2	34:7:267:VAL:HG13	1.75	0.68
1:2:1424:G:C5	1:2:1425:C:C4	2.81	0.68
27:H:137:THR:HB	27:H:139:VAL:HG13	1.75	0.68
1:2:642:G:C6	1:2:654:U:N3	2.60	0.68
1:2:1178:C:H2'	1:2:1179:C:C6	2.28	0.68
1:2:1313:G:H5'	27:H:81:VAL:HG21	1.74	0.68
30:4:76:A:H1'	34:7:296:ALA:CB	2.24	0.68
1:2:6:G:O6	1:2:7:G:C6	2.47	0.68
1:2:957:A:C2	1:2:991:C:N4	2.61	0.68
1:2:151:G:N3	14:G:64:ARG:NH2	2.42	0.68
1:2:507:G:P	3:N:111:PRO:HG3	2.33	0.68
1:2:460:C:H4'	1:2:460:C:OP1	1.94	0.67
1:2:6:G:C6	1:2:7:G:O6	2.47	0.67
13:F:203:ASN:O	13:F:207:ASN:ND2	2.28	0.67
1:2:127:G:C2	1:2:218:C:C2	2.83	0.67
1:2:315:A:Cl'	1:2:1423:A:H1'	2.20	0.67
34:7:207:ARG:HE	34:7:291:PRO:HB2	1.57	0.67
1:2:112:G:H8	1:2:112:G:O5'	1.77	0.67
1:2:315:A:H4'	1:2:1423:A:H4'	1.75	0.67
1:2:1049:U:O2'	1:2:1129:A:N3	2.26	0.67
1:2:1032:A:P	13:F:84:ARG:NH2	2.67	0.67
1:2:607:U:H4'	15:I:57:ARG:NH2	2.09	0.67
1:2:906:G:C6	1:2:907:C:N3	2.64	0.66
1:2:513:A:O2'	1:2:514:U:OP2	2.10	0.66
1:2:1413:G:H2'	1:2:1414:G:H8	1.59	0.66
1:2:1131:G:H2'	1:2:1132:C:C6	2.29	0.66
12:E:20:TYR:O	12:E:47:TYR:OH	2.13	0.66
36:9:204:LEU:HD23	36:9:207:ILE:HG21	1.77	0.66
1:2:495:G:N1	1:2:496:C:C4	2.64	0.66
1:2:1341:C:H2'	1:2:1342:C:C6	2.29	0.66
13:F:143:PHE:CZ	15:I:96:ALA:HB3	2.31	0.66
1:2:643:G:C2	1:2:653:C:C2	2.84	0.66
1:2:642:G:C6	1:2:654:U:C2	2.84	0.66
1:2:1041:C:O3'	25:X:71:ARG:NH2	2.28	0.66
34:7:59:CYS:CB	34:7:74:CYS:HG	2.09	0.66
1:2:152:G:H2'	1:2:153:G:H8	1.58	0.65
1:2:1371:C:N4	1:2:1372:C:N4	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:26:GLU:O	11:D:30:MET:N	2.29	0.65
7:B:104:PRO:HG2	13:F:19:LYS:HE2	1.77	0.65
1:2:1349:C:O5'	1:2:1349:C:H6	1.80	0.65
1:2:406:U:H2'	1:2:407:G:N7	2.12	0.65
1:2:540:G:H4'	15:I:4:LEU:HB2	1.77	0.65
13:F:165:LEU:HD23	13:F:183:VAL:HG12	1.77	0.65
1:2:1424:G:C6	1:2:1425:C:C4	2.84	0.65
1:2:1452:G:H2'	1:2:1453:U:C6	2.32	0.65
1:2:1475:C:OP2	29:O:4:LYS:HG2	1.96	0.65
1:2:2:U:C6	13:F:184:TRP:CZ3	2.85	0.65
1:2:1348:C:O2'	1:2:1349:C:H5'	1.97	0.65
12:E:192:ASN:HA	12:E:195:ARG:NH2	2.11	0.65
36:9:217:ILE:HD13	36:9:246:ILE:HD11	1.77	0.65
1:2:16:G:H2'	1:2:17:C:C6	2.31	0.65
1:2:434:A:C4	8:V:85:TYR:HD1	2.14	0.65
1:2:1371:C:N4	1:2:1372:C:H41	1.95	0.65
34:7:238:ILE:HG21	34:7:316:ILE:HD11	1.78	0.65
1:2:199:A:C6	1:2:217:C:H4'	2.32	0.64
1:2:867:A:O2'	1:2:1374:C:O3'	2.14	0.64
1:2:434:A:C5	8:V:85:TYR:HD1	2.15	0.64
1:2:1403:U:N3	1:2:1404:C:C5	2.66	0.64
1:2:121:C:C2	1:2:122:C:C5	2.85	0.64
1:2:572:U:H1'	8:V:60:PHE:CZ	2.31	0.64
1:2:6:G:O6	13:F:192:ARG:NH2	2.30	0.64
1:2:151:G:H1'	14:G:120:ASN:ND2	2.11	0.64
1:2:740:G:N2	1:2:751:C:C2	2.65	0.64
1:2:1316:U:H3	1:2:1326:G:H1	1.46	0.64
31:5:812:G:H3'	31:5:813:A:O4'	1.98	0.64
1:2:1131:G:H2'	1:2:1132:C:H6	1.63	0.64
3:N:103:VAL:HG13	3:N:126:VAL:HG13	1.80	0.64
1:2:1154:G:H2'	1:2:1155:U:C6	2.32	0.64
1:2:1401:U:O4	1:2:1402:C:N4	2.31	0.64
1:2:1412:A:HO2'	14:G:92:PRO:HG3	1.63	0.64
1:2:1488:C:N4	31:5:812:G:O6	2.19	0.64
27:H:43:LEU:HD11	28:K:43:PHE:HB3	1.79	0.64
34:7:59:CYS:HA	34:7:74:CYS:SG	2.38	0.64
1:2:1371:C:C4	1:2:1372:C:N4	2.66	0.64
3:N:87:PHE:N	3:N:122:ILE:HG21	2.13	0.64
14:G:29:LEU:HD11	14:G:63:ILE:HD11	1.79	0.64
15:I:46:TYR:HA	15:I:68:ARG:HD3	1.80	0.64
1:2:498:C:O2'	1:2:502:U:OP1	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:78:ILE:CG2	14:G:109:GLY:HA2	2.28	0.64
1:2:332:C:O2	1:2:1424:G:O2'	2.11	0.63
1:2:439:G:H1'	1:2:440:C:H5	1.61	0.63
7:B:56:GLY:HA3	7:B:174:GLU:CG	2.28	0.63
1:2:302:A:C2	1:2:303:G:N7	2.67	0.63
1:2:1060:G:O3'	1:2:1061:A:P	2.56	0.63
1:2:1128:U:O4	7:B:201:ARG:C	2.36	0.63
1:2:1352:G:N2	1:2:1353:C:C2	2.65	0.63
1:2:1462:A:C8	1:2:1486:A:C6	2.87	0.63
1:2:127:G:N2	1:2:218:C:C2	2.67	0.63
1:2:1028:C:H5'	7:B:128:ARG:NH2	2.14	0.63
1:2:1041:C:C5'	25:X:71:ARG:CZ	2.76	0.63
14:G:53:LYS:HA	14:G:54:GLU:CB	2.28	0.63
1:2:317:A:O2'	14:G:102:ARG:CZ	2.46	0.63
1:2:459:G:H3'	1:2:460:C:O4'	1.98	0.63
1:2:901:G:N2	1:2:1302:C:C2	2.66	0.63
27:H:46:HIS:O	27:H:48:HIS:N	2.32	0.63
3:N:72:ALA:HA	3:N:86:ALA:O	1.99	0.63
1:2:1489:A:C2'	1:2:1490:C:H5'	2.28	0.63
13:F:86:LEU:HG	13:F:100:ILE:HG22	1.81	0.62
30:4:12:G:N1	30:4:13:C:C2	2.67	0.62
1:2:1413:G:O3'	14:G:86:VAL:HG21	1.99	0.62
19:L:92:GLU:HB2	19:L:93:ASP:HB2	1.80	0.62
1:2:60:A:C2	1:2:64:G:O6	2.52	0.62
1:2:483:G:N7	33:6:57:ARG:NH2	2.46	0.62
1:2:677:U:C4	1:2:1493:C:H4'	2.33	0.62
15:I:7:LEU:HA	15:I:34:ILE:CG1	2.29	0.62
1:2:126:G:N2	1:2:219:C:C2	2.67	0.62
1:2:1333:G:N7	27:H:48:HIS:NE2	2.48	0.62
2:M:97:GLY:HA2	2:M:100:ALA:HB3	1.81	0.62
11:D:118:MET:SD	11:D:118:MET:N	2.73	0.62
15:I:76:LYS:HB3	15:I:77:PRO:HD3	1.81	0.62
1:2:641:A:H2	1:2:642:G:C4	2.18	0.62
1:2:780:C:H4'	15:I:13:HIS:CG	2.34	0.62
1:2:1347:U:O5'	1:2:1347:U:H6	1.81	0.62
13:F:152:VAL:C	13:F:153:ARG:HD2	2.20	0.62
1:2:711:U:H2'	1:2:712:G:O4'	1.99	0.62
1:2:1424:G:C2	1:2:1425:C:C2	2.87	0.62
4:Q:4:MET:HA	4:Q:7:ARG:HG3	1.81	0.62
13:F:54:LEU:HD13	13:F:61:GLU:HB3	1.81	0.62
1:2:975:A:H2'	1:2:976:A:C5'	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:17:ASP:HB3	5:R:21:CYS:SG	2.39	0.62
12:E:157:ASN:OD1	12:E:162:TYR:CE1	2.52	0.62
14:G:33:ARG:O	14:G:63:ILE:HD12	2.00	0.62
1:2:584:C:H4'	1:2:585:U:OP1	2.00	0.62
4:Q:132:LEU:O	4:Q:136:TYR:CD2	2.53	0.62
13:F:130:SER:HB3	13:F:139:HIS:CE1	2.35	0.62
13:F:196:ASN:O	13:F:200:ALA:N	2.27	0.62
34:7:138:ILE:HG23	34:7:410:TRP:CG	2.35	0.62
1:2:534:G:O6	1:2:712:G:C8	2.53	0.62
1:2:1465:C:OP1	29:0:2:ARG:HB2	2.00	0.62
1:2:330:U:H4'	14:G:104:LYS:HB2	1.82	0.61
1:2:884:G:N2	31:5:818:A:H5''	2.15	0.61
1:2:1307:G:N2	27:H:48:HIS:CE1	2.68	0.61
4:Q:126:GLU:HA	4:Q:129:ILE:HD12	1.82	0.61
14:G:84:VAL:O	14:G:106:THR:OG1	2.12	0.61
30:4:15:G:N7	30:4:16:C:H5	1.98	0.61
1:2:1028:C:C2	1:2:1034:G:C2	2.87	0.61
30:4:50:U:H2'	30:4:51:C:C6	2.34	0.61
1:2:121:C:C2	1:2:122:C:C6	2.87	0.61
1:2:1269:G:H2'	1:2:1270:C:O4'	1.99	0.61
1:2:533:C:C4	1:2:534:G:N1	2.68	0.61
1:2:29:G:H1'	3:N:135:LYS:HZ3	1.65	0.61
1:2:472:C:H2'	1:2:473:A:C8	2.35	0.61
1:2:540:G:C6	1:2:709:G:C6	2.89	0.61
1:2:996:A:C2	1:2:997:G:C8	2.88	0.61
24:U:62:VAL:HG22	24:U:68:VAL:HG11	1.83	0.61
30:4:26:G:H4'	35:8:38:ILE:HG22	1.81	0.61
1:2:380:C:H2'	1:2:381:C:C6	2.34	0.61
1:2:607:U:OP2	4:Q:16:ARG:HD3	2.00	0.61
6:A:100:THR:HA	6:A:127:ARG:O	2.00	0.61
27:H:73:ARG:NH1	27:H:166:ALA:O	2.34	0.61
30:4:2:G:O6	30:4:71:C:N3	2.34	0.61
1:2:227:C:H2'	1:2:228:G:C8	2.35	0.61
1:2:702:G:H22	1:2:706:G:H1	1.49	0.61
1:2:930:G:C4	1:2:1325:C:H4'	2.36	0.61
1:2:1378:A:O2'	34:7:373:VAL:CB	2.47	0.61
30:4:2:G:C2	30:4:3:C:C4	2.89	0.61
34:7:62:CYS:SG	34:7:63:LYS:N	2.74	0.61
1:2:867:A:C2'	1:2:1374:C:H4'	2.31	0.61
1:2:1013:G:C5	1:2:1014:C:C4	2.89	0.61
34:7:37:HIS:C	34:7:41:LEU:HG	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:7:51:TYR:CG	37:7:501:MET:HE2	2.36	0.61
31:5:812:G:C3'	31:5:813:A:O4'	2.49	0.60
1:2:99:C:O2'	1:2:100:A:OP2	2.19	0.60
1:2:876:A:H2'	1:2:877:A:C8	2.36	0.60
12:E:45:LEU:HD12	12:E:83:PHE:HB3	1.82	0.60
16:J:120:VAL:O	16:J:121:ASN:ND2	2.33	0.60
34:7:41:LEU:HD22	34:7:47:ILE:HB	1.83	0.60
1:2:985:C:H3'	1:2:986:G:C2	2.36	0.60
16:J:64:ASN:ND2	16:J:75:VAL:HG12	2.16	0.60
27:H:13:HIS:CE1	28:K:50:ILE:HD11	2.36	0.60
33:6:89:THR:C	33:6:90:GLN:N	2.54	0.60
1:2:868:C:H4'	1:2:1373:A:C2'	2.32	0.60
16:J:10:LYS:HD3	16:J:16:ARG:HA	1.82	0.60
6:A:71:TYR:CE1	6:A:81:LYS:HB2	2.36	0.60
14:G:55:PHE:N	14:G:56:PRO:HA	2.16	0.60
24:U:80:ARG:HE	27:H:81:VAL:HG11	1.66	0.60
27:H:21:TRP:CH2	27:H:108:PHE:HB3	2.36	0.60
1:2:599:G:C6	1:2:600:C:C4	2.90	0.60
1:2:1032:A:OP1	13:F:84:ARG:NH2	2.33	0.60
13:F:148:LYS:HB3	13:F:153:ARG:NH2	2.17	0.60
14:G:76:PRO:O	14:G:77:ASP:HB2	1.99	0.60
30:4:8:U:O2'	30:4:21:A:N1	2.29	0.60
36:9:214:LEU:HD11	36:9:217:ILE:HD11	1.83	0.60
1:2:533:C:N3	1:2:534:G:C2	2.69	0.60
30:4:5:G:O6	30:4:6:G:O6	2.19	0.60
1:2:909:U:OP2	20:O:130:ARG:CD	2.50	0.60
30:4:5:G:C6	30:4:6:G:C6	2.90	0.60
35:8:62:MET:O	35:8:66:LEU:HB2	2.01	0.60
1:2:260:C:H2'	1:2:261:G:O4'	2.02	0.60
1:2:649:A:H2	1:2:740:G:O2'	1.85	0.60
1:2:742:U:C4	1:2:743:U:C4	2.90	0.60
1:2:822:A:C2'	1:2:823:A:C8	2.78	0.60
1:2:1339:G:H21	1:2:1341:C:H41	1.48	0.60
14:G:78:ILE:CB	14:G:109:GLY:HA2	2.31	0.60
16:J:64:ASN:O	16:J:121:ASN:OD1	2.18	0.60
30:4:18:G:H4'	30:4:60:U:O2	2.01	0.60
1:2:1370:U:C2	1:2:1446:G:C2	2.90	0.59
1:2:229:G:N1	1:2:230:C:N4	2.50	0.59
1:2:1401:U:H3	1:2:1414:G:H1	1.51	0.59
1:2:1452:G:OP1	32:1:78:GLN:NE2	2.35	0.59
34:7:35:SER:O	35:8:121:LYS:NZ	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:380:C:H2'	1:2:381:C:H6	1.65	0.59
1:2:537:G:H2'	1:2:538:C:C6	2.37	0.59
1:2:1275:U:O4	1:2:1276:G:N1	2.35	0.59
1:2:1448:A:N6	33:6:51:ILE:HD13	2.16	0.59
1:2:947:G:O2'	1:2:976:A:N6	2.36	0.59
1:2:1053:A:N7	7:B:125:GLN:NE2	2.47	0.59
34:7:294:LEU:HB3	37:7:501:MET:HG3	1.84	0.59
1:2:1401:U:C4	1:2:1402:C:N4	2.71	0.59
13:F:191:THR:HG23	13:F:197:PHE:CD1	2.37	0.59
1:2:82:G:C6	1:2:83:C:C4	2.91	0.59
1:2:229:G:N2	1:2:230:C:N3	2.50	0.59
1:2:1053:A:C8	7:B:125:GLN:NE2	2.71	0.59
19:L:51:LYS:HB2	19:L:60:THR:O	2.03	0.59
1:2:151:G:O2'	14:G:64:ARG:CZ	2.50	0.59
1:2:607:U:H4'	15:I:57:ARG:HE	1.67	0.59
1:2:746:A:O2'	1:2:747:U:OP2	2.19	0.59
6:A:10:ARG:NE	36:9:88:ASP:O	2.36	0.59
1:2:1049:U:O2'	1:2:1129:A:C2	2.56	0.59
1:2:122:C:C2	1:2:223:G:N2	2.71	0.58
1:2:315:A:H4'	1:2:1423:A:C4'	2.32	0.58
1:2:461:A:O3'	1:2:462:A:H3'	2.02	0.58
1:2:615:G:O6	1:2:698:A:C6	2.56	0.58
1:2:1414:G:P	14:G:86:VAL:HG11	2.43	0.58
12:E:193:VAL:O	12:E:195:ARG:NH1	2.36	0.58
1:2:369:A:H4'	1:2:434:A:C5	2.38	0.58
1:2:921:G:H1'	1:2:1161:A:N6	2.17	0.58
1:2:1414:G:H1'	14:G:78:ILE:HA	1.85	0.58
1:2:1423:A:H2'	1:2:1424:G:C8	2.38	0.58
1:2:884:G:H22	31:5:818:A:H5''	1.68	0.58
1:2:1382:G:N2	1:2:1434:C:C2	2.71	0.58
1:2:774:U:H4'	1:2:775:G:OP2	2.02	0.58
1:2:1311:C:OP1	27:H:76:GLY:CA	2.51	0.58
30:4:73:A:C3'	34:7:221:PHE:CZ	2.86	0.58
30:4:76:A:H1'	34:7:296:ALA:HB1	1.84	0.58
1:2:353:G:C2	1:2:354:G:C8	2.91	0.58
1:2:509:C:OP2	3:N:33:ARG:NH2	2.37	0.58
1:2:1312:C:C2	1:2:1331:G:C2	2.91	0.58
1:2:1397:C:C2	1:2:1419:G:C2	2.91	0.58
1:2:271:G:C6	1:2:272:C:C4	2.92	0.58
1:2:1489:A:H1'	31:5:812:G:N2	2.19	0.58
1:2:442:C:O5'	1:2:442:C:H6	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:495:G:C6	1:2:496:C:N4	2.71	0.58
1:2:661:C:H4'	2:M:18:HIS:CD2	2.39	0.58
1:2:1062:G:H1'	22:S:6:GLN:NE2	2.17	0.58
1:2:1448:A:H4'	1:2:1449:G:OP1	2.04	0.58
34:7:41:LEU:HD13	34:7:47:ILE:HB	1.85	0.58
1:2:459:G:N1	1:2:460:C:C2	2.72	0.58
1:2:920:U:C2	1:2:1161:A:N6	2.69	0.58
1:2:1059:C:C4	1:2:1060:G:N7	2.71	0.58
1:2:1399:G:C6	1:2:1417:A:N6	2.72	0.58
1:2:1414:G:H4'	14:G:84:VAL:HG11	1.86	0.58
24:U:62:VAL:HG22	24:U:68:VAL:CG1	2.34	0.58
34:7:186:LEU:HD11	35:8:124:TYR:CZ	2.39	0.58
1:2:4:C:C2	1:2:5:C:C5	2.91	0.57
1:2:297:G:C2	1:2:298:C:C2	2.92	0.57
1:2:1048:G:O2'	1:2:1130:A:O2'	2.22	0.57
1:2:1443:G:C6	1:2:1444:G:O6	2.56	0.57
6:A:9:THR:HG22	36:9:92:LYS:HE2	1.86	0.57
13:F:197:PHE:O	13:F:200:ALA:HB3	2.03	0.57
1:2:303:G:C8	1:2:304:C:C5	2.92	0.57
1:2:607:U:H4'	15:I:57:ARG:NE	2.19	0.57
1:2:360:A:OP1	3:N:131:ARG:NH2	2.37	0.57
1:2:434:A:C5	8:V:85:TYR:CD1	2.92	0.57
1:2:585:U:H3'	1:2:586:C:C4'	2.34	0.57
1:2:1142:G:O5'	1:2:1142:G:C8	2.57	0.57
27:H:21:TRP:CD1	27:H:119:PRO:HD2	2.39	0.57
27:H:87:ARG:CA	27:H:88:ARG:HD3	2.34	0.57
32:1:83:LYS:O	32:1:87:GLU:HG2	2.04	0.57
1:2:71:C:C2	1:2:79:G:C2	2.92	0.57
1:2:199:A:N6	1:2:217:C:H4'	2.19	0.57
1:2:872:A:C6	1:2:873:A:C6	2.92	0.57
1:2:441:U:C4	1:2:442:C:N4	2.72	0.57
1:2:615:G:C6	1:2:698:A:N1	2.73	0.57
1:2:1329:C:H2'	1:2:1330:G:C8	2.40	0.57
11:D:59:LEU:HD11	13:F:132:GLU:CG	2.34	0.57
13:F:165:LEU:HD21	13:F:180:VAL:O	2.05	0.57
1:2:495:G:C2	1:2:496:C:C5	2.91	0.57
1:2:1050:G:O4'	1:2:1127:A:N1	2.37	0.57
13:F:5:TRP:HB3	13:F:57:VAL:CG2	2.35	0.57
1:2:142:G:H4'	14:G:5:LYS:HG2	1.87	0.57
1:2:394:C:C2	1:2:395:C:C5	2.93	0.57
1:2:441:U:O4	1:2:442:C:N4	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:616:G:C2	1:2:698:A:C6	2.93	0.57
19:L:54:ASP:HB3	19:L:56:GLU:HB2	1.87	0.57
34:7:149:ASN:O	34:7:183:VAL:O	2.22	0.57
1:2:553:C:C2	1:2:593:G:C2	2.93	0.57
1:2:1009:G:H5'	10:Z:134:GLY:HA2	1.87	0.57
1:2:1348:C:H2'	1:2:1349:C:C5	2.39	0.57
1:2:1403:U:C3'	1:2:1404:C:H5'	2.34	0.57
1:2:110:C:H4'	1:2:588:C:O2	2.04	0.57
1:2:38:G:C6	1:2:39:U:C5	2.93	0.56
1:2:297:G:C6	1:2:298:C:C4	2.93	0.56
1:2:555:U:H3	1:2:590:G:H1	1.53	0.56
1:2:1040:A:C2'	1:2:1041:C:H5'	2.35	0.56
1:2:1096:G:N2	24:U:1:MET:HA	2.20	0.56
1:2:1332:C:O2	27:H:96:LYS:HG3	2.05	0.56
6:A:18:TRP:CZ2	6:A:36:PRO:HB3	2.40	0.56
34:7:37:HIS:H	34:7:41:LEU:HB2	1.70	0.56
1:2:93:A:O2'	12:E:5:GLY:HA3	2.05	0.56
1:2:549:A:C2	1:2:550:G:C8	2.94	0.56
1:2:586:C:O2'	1:2:587:G:C2	2.58	0.56
1:2:531:G:C4	1:2:718:G:N2	2.73	0.56
1:2:607:U:C4'	15:I:57:ARG:HE	2.18	0.56
1:2:879:U:O3'	13:F:73:ARG:NH2	2.38	0.56
1:2:1041:C:OP1	25:X:71:ARG:HD3	2.05	0.56
1:2:1311:C:H4'	27:H:95:SER:HA	1.86	0.56
1:2:1424:G:C5	1:2:1425:C:C5	2.93	0.56
7:B:56:GLY:HA3	7:B:174:GLU:HG3	1.85	0.56
27:H:179:SER:O	27:H:183:ALA:N	2.37	0.56
32:1:36:PHE:CD1	32:1:36:PHE:C	2.78	0.56
34:7:260:ARG:HA	34:7:268:SER:O	2.05	0.56
1:2:324:C:H4'	1:2:325:A:O5'	2.06	0.56
1:2:324:C:HO2'	1:2:325:A:P	2.27	0.56
1:2:452:G:H2'	1:2:453:G:C8	2.40	0.56
1:2:1195:U:OP2	27:H:78:HIS:HA	2.05	0.56
1:2:1424:G:O5'	1:2:1424:G:H8	1.87	0.56
6:A:10:ARG:NE	36:9:92:LYS:HD2	2.21	0.56
13:F:34:ILE:HB	13:F:53:LEU:HG	1.88	0.56
1:2:150:G:H2'	1:2:151:G:C8	2.40	0.56
1:2:1275:U:C4	1:2:1276:G:C6	2.94	0.56
1:2:1320:A:H8	1:2:1320:A:OP1	1.89	0.56
15:I:32:LYS:O	15:I:36:GLU:N	2.30	0.56
1:2:459:G:C5	1:2:460:C:C6	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:649:A:H2	1:2:740:G:HO2'	1.52	0.56
1:2:1025:U:O2	7:B:103:ASN:ND2	2.37	0.56
1:2:1347:U:H2'	1:2:1348:C:C6	2.40	0.56
1:2:1352:G:C2	1:2:1353:C:C4	2.94	0.56
1:2:6:G:C6	1:2:7:G:C5	2.94	0.56
1:2:10:G:N7	1:2:1356:A:C6	2.73	0.56
1:2:537:G:C6	1:2:538:C:C4	2.94	0.56
1:2:647:G:O6	1:2:742:U:H5'	2.06	0.56
1:2:821:G:N2	1:2:824:G:OP2	2.34	0.56
1:2:1061:A:OP2	10:Z:154:VAL:HG22	2.06	0.56
1:2:1269:G:C6	1:2:1270:C:C4	2.93	0.56
1:2:1385:U:H2'	1:2:1386:C:C6	2.41	0.56
1:2:1486:A:H5'	1:2:1487:U:OP2	2.06	0.56
6:A:43:VAL:HG23	6:A:46:ARG:HB2	1.86	0.56
8:V:33:ARG:O	8:V:53:ILE:HG21	2.05	0.56
1:2:229:G:C4	1:2:230:C:C5	2.93	0.56
1:2:250:G:OP1	5:R:97:THR:OG1	2.20	0.56
6:A:123:ALA:HA	6:A:183:ALA:HA	1.88	0.56
12:E:45:LEU:CD1	12:E:83:PHE:HB3	2.36	0.56
1:2:12:U:H2'	1:2:13:C:C6	2.40	0.56
1:2:234:G:H5'	5:R:55:PHE:CZ	2.41	0.56
1:2:1382:G:C2	1:2:1434:C:N3	2.74	0.56
1:2:372:G:C6	1:2:373:C:C4	2.94	0.56
1:2:610:G:N2	1:2:705:C:C2	2.74	0.56
1:2:680:C:H2'	1:2:681:G:O4'	2.06	0.56
1:2:1414:G:H21	14:G:79:HIS:HB3	1.71	0.56
1:2:60:A:N6	1:2:85:A:N6	2.54	0.55
1:2:649:A:C2	1:2:650:A:C4	2.94	0.55
1:2:839:G:C6	1:2:840:C:C4	2.93	0.55
1:2:1341:C:H2'	1:2:1342:C:H6	1.71	0.55
13:F:131:TRP:NE1	15:I:97:PHE:CE2	2.75	0.55
1:2:439:G:H4'	1:2:440:C:O5'	2.05	0.55
1:2:672:G:C8	2:M:123:HIS:HA	2.41	0.55
1:2:732:G:C6	1:2:733:C:C4	2.94	0.55
1:2:891:A:H4'	1:2:892:C:OP1	2.06	0.55
1:2:1342:C:C3'	1:2:1343:C:P	2.94	0.55
1:2:1403:U:N3	14:G:77:ASP:CG	2.59	0.55
30:4:74:C:OP1	34:7:221:PHE:CD1	2.59	0.55
30:4:76:A:O3'	37:7:501:MET:CA	2.49	0.55
1:2:607:U:OP1	15:I:57:ARG:HG2	2.07	0.55
1:2:1395:G:C5'	14:G:87:LEU:HD13	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1487:U:H2'	1:2:1488:C:H6	1.65	0.55
1:2:616:G:N1	1:2:697:A:C2	2.74	0.55
1:2:955:G:H2'	1:2:956:C:O4'	2.07	0.55
1:2:236:C:H2'	1:2:237:C:H6	1.71	0.55
1:2:1031:G:N2	1:2:1032:A:C2	2.74	0.55
1:2:1372:C:H2'	1:2:1373:A:C8	2.41	0.55
3:N:43:PRO:O	3:N:45:GLU:N	2.40	0.55
16:J:34:ASN:C	16:J:34:ASN:HD22	2.09	0.55
17:C:38:UNK:HA	17:C:43:UNK:CB	2.36	0.55
1:2:505:U:H5''	3:N:108:ILE:HD12	1.88	0.55
1:2:513:A:H2'	13:F:188:PHE:CE1	2.42	0.55
1:2:1013:G:C6	1:2:1014:C:N3	2.74	0.55
1:2:1264:G:C6	1:2:1265:G:C2	2.94	0.55
1:2:1311:C:C4'	27:H:95:SER:HA	2.37	0.55
1:2:41:C:C2	1:2:392:G:C2	2.94	0.55
1:2:583:G:C6	1:2:584:C:C4	2.94	0.55
27:H:43:LEU:HD11	28:K:43:PHE:CB	2.37	0.55
1:2:539:C:OP1	3:N:10:GLU:N	2.40	0.55
1:2:1343:C:C5	1:2:1344:U:C5	2.95	0.55
4:Q:126:GLU:O	4:Q:129:ILE:HB	2.07	0.55
1:2:526:A:O2'	1:2:527:A:O4'	2.15	0.55
1:2:607:U:C4'	15:I:57:ARG:HH21	2.19	0.55
1:2:1070:C:H2'	1:2:1071:C:C6	2.42	0.55
1:2:1317:G:C5	1:2:1318:U:C4	2.95	0.55
1:2:1443:G:N1	1:2:1444:G:C6	2.75	0.55
3:N:59:ALA:O	33:6:79:ARG:NH1	2.40	0.55
35:8:56:ARG:HH12	35:8:104:VAL:HA	1.71	0.55
1:2:26:A:H2'	1:2:27:C:O4'	2.07	0.54
1:2:642:G:N2	1:2:643:G:H1'	2.21	0.54
1:2:1424:G:C6	1:2:1425:C:N3	2.76	0.54
1:2:1424:G:C4	1:2:1425:C:C6	2.95	0.54
27:H:87:ARG:HG3	27:H:90:HIS:CA	2.34	0.54
30:4:2:G:C2	30:4:3:C:C5	2.95	0.54
1:2:1448:A:H61	33:6:61:ILE:HB	1.72	0.54
13:F:50:ILE:HD12	13:F:118:LYS:HB3	1.89	0.54
27:H:89:GLU:N	27:H:94:ASN:HB3	2.22	0.54
1:2:426:C:C2	1:2:445:G:C2	2.95	0.54
1:2:884:G:O2'	1:2:885:G:OP2	2.19	0.54
30:4:49:G:C6	30:4:66:C:C4	2.95	0.54
1:2:1249:A:OP1	27:H:82:ALA:HB3	2.07	0.54
14:G:75:ARG:O	14:G:78:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:533:C:N4	1:2:534:G:N1	2.55	0.54
1:2:1024:G:H2'	1:2:1025:U:C6	2.42	0.54
7:B:169:TRP:CE2	7:B:192:VAL:HG22	2.43	0.54
22:S:44:LYS:O	22:S:48:ASN:ND2	2.40	0.54
34:7:214:VAL:HB	34:7:244:GLN:CG	2.38	0.54
1:2:106:A:HO2'	1:2:308:G:HO2'	1.53	0.54
1:2:1131:G:C6	1:2:1132:C:N4	2.75	0.54
1:2:1367:C:C1'	32:1:65:ALA:HB2	2.34	0.54
13:F:86:LEU:HD21	13:F:195:VAL:HA	1.90	0.54
30:4:74:C:OP1	34:7:221:PHE:CG	2.61	0.54
1:2:55:G:H5'	1:2:384:G:OP1	2.07	0.54
1:2:1219:C:C2	1:2:1237:G:N2	2.75	0.54
1:2:1313:G:H5'	27:H:81:VAL:CG2	2.37	0.54
27:H:72:MET:HE2	27:H:97:LYS:N	2.23	0.54
27:H:78:HIS:HB2	27:H:88:ARG:HG3	1.89	0.54
1:2:94:C:OP1	12:E:5:GLY:N	2.37	0.54
1:2:291:G:H2'	1:2:292:U:O4'	2.07	0.54
1:2:787:U:C2	1:2:788:C:C5	2.96	0.54
1:2:813:G:C6	1:2:814:C:C4	2.95	0.54
1:2:1307:G:C2	27:H:48:HIS:CE1	2.96	0.54
1:2:1311:C:H1'	27:H:96:LYS:HG2	1.89	0.54
1:2:1323:A:N3	1:2:1323:A:O2'	2.36	0.54
5:R:60:TYR:O	5:R:61:GLU:HB2	2.08	0.54
1:2:754:G:N2	1:2:755:U:O4	2.41	0.54
1:2:1031:G:O3'	13:F:84:ARG:CZ	2.56	0.54
1:2:642:G:C2	1:2:643:G:H1'	2.43	0.54
1:2:709:G:OP2	4:Q:131:ARG:NE	2.41	0.54
1:2:1312:C:H5''	27:H:80:LYS:HB3	1.90	0.54
27:H:71:ILE:HG23	27:H:180:PHE:CZ	2.43	0.54
34:7:245:GLY:O	34:7:291:PRO:HD3	2.08	0.54
36:9:4:SER:HB2	36:9:34:TYR:HA	1.89	0.54
1:2:236:C:H2'	1:2:237:C:C6	2.42	0.53
1:2:462:A:N6	11:D:18:TRP:CE2	2.76	0.53
1:2:492:G:C6	1:2:493:C:C4	2.96	0.53
1:2:1382:G:C2	1:2:1434:C:C2	2.95	0.53
13:F:167:ILE:HG21	13:F:175:LEU:HD12	1.91	0.53
19:L:54:ASP:HB3	19:L:56:GLU:CB	2.38	0.53
30:4:76:A:H3'	37:7:501:MET:C	2.28	0.53
1:2:5:C:O2'	1:2:459:G:O3'	2.26	0.53
1:2:459:G:O6	1:2:460:C:C4	2.62	0.53
1:2:1131:G:N2	1:2:1132:C:C2	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:33:TYR:HB2	7:B:44:ASP:N	2.23	0.53
8:V:56:ILE:HA	8:V:66:LYS:O	2.08	0.53
15:I:7:LEU:O	15:I:10:ALA:HB3	2.08	0.53
36:9:221:THR:HB	36:9:227:TYR:CE2	2.43	0.53
1:2:31:U:H2'	1:2:32:A:O4'	2.09	0.53
1:2:193:G:H2'	1:2:194:C:C6	2.44	0.53
1:2:378:A:H2'	1:2:379:A:C8	2.43	0.53
1:2:607:U:H4'	15:I:57:ARG:CZ	2.37	0.53
1:2:988:A:O2'	1:2:989:C:H5'	2.08	0.53
1:2:1460:G:O2'	31:5:815:U:O4	2.26	0.53
13:F:166:VAL:O	13:F:185:SER:HB3	2.08	0.53
1:2:60:A:H61	1:2:85:A:N6	2.06	0.53
1:2:262:G:C8	1:2:262:G:H5''	2.43	0.53
1:2:855:C:O2	1:2:861:G:C2	2.62	0.53
1:2:872:A:C6	1:2:873:A:C5	2.97	0.53
1:2:900:G:N2	1:2:1303:C:C2	2.77	0.53
1:2:1338:C:C2	25:X:23:ASP:HA	2.43	0.53
19:L:61:PHE:HB2	28:K:119:PRO:HB3	1.90	0.53
1:2:616:G:C2	1:2:698:A:C5	2.96	0.53
1:2:629:U:H2'	1:2:630:A:C8	2.43	0.53
1:2:1290:U:O4	1:2:1291:G:N2	2.40	0.53
3:N:63:LYS:HB2	3:N:118:ASP:O	2.08	0.53
13:F:34:ILE:HA	13:F:37:ILE:HD12	1.91	0.53
13:F:96:VAL:O	13:F:122:ILE:N	2.39	0.53
1:2:8:U:OP1	1:2:9:U:H5	1.91	0.53
1:2:182:A:H2'	1:2:183:A:C8	2.44	0.53
1:2:650:A:C2	1:2:740:G:H1'	2.44	0.53
1:2:872:A:C4	1:2:873:A:N7	2.77	0.53
1:2:999:G:O2'	1:2:1176:C:OP1	2.26	0.53
7:B:60:ALA:HA	7:B:179:ARG:HE	1.72	0.53
13:F:13:LEU:O	13:F:13:LEU:HD12	2.09	0.53
1:2:87:C:H2'	1:2:88:G:H5'	1.89	0.53
1:2:1193:G:H2'	1:2:1194:C:C6	2.44	0.53
1:2:1385:U:H2'	1:2:1386:C:H6	1.73	0.53
1:2:1414:G:OP1	14:G:86:VAL:HG11	2.07	0.53
1:2:607:U:C5'	15:I:57:ARG:HE	2.22	0.53
1:2:947:G:HO2'	1:2:976:A:N6	2.07	0.53
1:2:1290:U:C4	1:2:1291:G:C2	2.96	0.53
1:2:1311:C:H4'	27:H:94:ASN:O	2.09	0.53
7:B:96:PHE:CE2	7:B:100:THR:HB	2.44	0.53
1:2:331:C:H4'	1:2:1393:A:O2'	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:868:C:H4'	1:2:1373:A:O2'	2.08	0.53
1:2:906:G:C6	1:2:907:C:C4	2.97	0.53
1:2:1144:G:C6	1:2:1145:C:C4	2.97	0.53
2:M:21:SER:OG	2:M:95:GLY:N	2.41	0.53
27:H:94:ASN:O	27:H:95:SER:OG	2.27	0.53
34:7:269:TYR:CE2	34:7:384:ARG:HG3	2.44	0.53
1:2:434:A:N1	8:V:83:PRO:HB3	2.24	0.52
1:2:725:C:C2	1:2:763:G:C2	2.97	0.52
1:2:784:G:OP1	7:B:25:THR:HA	2.09	0.52
1:2:1131:G:C4	1:2:1132:C:C5	2.98	0.52
1:2:1443:G:H2'	1:2:1444:G:H8	1.72	0.52
12:E:126:ARG:NH1	12:E:127:ILE:O	2.42	0.52
19:L:90:VAL:HG11	19:L:96:ILE:HD11	1.91	0.52
1:2:100:A:H2'	1:2:101:G:O4'	2.09	0.52
1:2:166:A:C2	1:2:197:A:C8	2.98	0.52
1:2:229:G:C6	1:2:230:C:N4	2.78	0.52
1:2:462:A:H5''	11:D:20:LYS:HE2	1.91	0.52
1:2:531:G:C6	1:2:532:C:C4	2.97	0.52
1:2:1156:A:C8	10:Z:140:ARG:NH1	2.78	0.52
1:2:1347:U:C4	1:2:1348:C:N4	2.78	0.52
1:2:1403:U:C2	1:2:1404:C:C6	2.97	0.52
33:6:19:PRO:CD	33:6:25:PHE:CZ	2.92	0.52
34:7:99:VAL:C	34:7:101:MET:H	2.12	0.52
1:2:95:G:H4'	12:E:9:HIS:CD2	2.45	0.52
1:2:213:C:C5	1:2:214:C:C5	2.97	0.52
1:2:642:G:O6	1:2:654:U:C4	2.62	0.52
1:2:677:U:C2	1:2:1493:C:H1'	2.45	0.52
8:V:60:PHE:N	8:V:60:PHE:CD1	2.78	0.52
24:U:8:PRO:HD2	24:U:140:LEU:HD11	1.92	0.52
27:H:101:TYR:CD2	27:H:101:TYR:C	2.82	0.52
1:2:143:G:H4'	14:G:117:VAL:HG11	1.92	0.52
1:2:315:A:H1'	1:2:1423:A:C1'	2.27	0.52
14:G:103:ARG:HE	14:G:105:LYS:HE2	1.74	0.52
15:I:73:GLY:O	15:I:128:TYR:N	2.41	0.52
15:I:86:PHE:O	15:I:90:GLU:N	2.40	0.52
27:H:67:LEU:O	27:H:71:ILE:HG12	2.09	0.52
28:K:52:ALA:HB2	28:K:95:LEU:HD11	1.91	0.52
1:2:48:G:C6	1:2:49:C:C4	2.97	0.52
1:2:95:G:H5'	12:E:9:HIS:ND1	2.24	0.52
1:2:181:G:H2'	1:2:182:A:C8	2.45	0.52
1:2:458:G:C2	1:2:479:C:O2	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:879:U:H4'	13:F:73:ARG:NE	2.24	0.52
1:2:1031:G:C3'	13:F:84:ARG:NH1	2.73	0.52
1:2:1463:A:OP2	2:M:133:ARG:NH1	2.42	0.52
1:2:1131:G:C2	1:2:1132:C:C4	2.98	0.52
1:2:1206:G:O2'	24:U:9:GLY:O	2.27	0.52
1:2:1363:C:O5'	1:2:1363:C:H6	1.93	0.52
25:X:7:TYR:CE2	25:X:31:ILE:HG12	2.44	0.52
1:2:1313:G:P	27:H:81:VAL:HG23	2.50	0.52
1:2:1441:G:H2'	1:2:1442:G:O4'	2.10	0.52
1:2:952:A:H2'	1:2:953:C:H5'	1.92	0.52
1:2:1388:G:H2'	1:2:1389:G:O4'	2.10	0.52
1:2:1475:C:H2'	1:2:1476:C:C6	2.44	0.52
14:G:52:GLY:CA	14:G:54:GLU:HB2	2.40	0.52
34:7:393:ILE:HB	34:7:413:VAL:HB	1.92	0.52
1:2:359:A:H2'	1:2:360:A:C8	2.45	0.52
1:2:642:G:N1	1:2:654:U:C2	2.78	0.52
1:2:920:U:O4	1:2:1161:A:N1	2.43	0.52
1:2:1026:A:O3'	7:B:102:THR:HB	2.09	0.52
1:2:1335:A:C6	1:2:1336:U:C2	2.98	0.52
1:2:1345:G:C6	1:2:1346:C:C4	2.98	0.52
32:1:66:CYS:SG	32:1:77:LEU:HB3	2.50	0.52
1:2:256:G:OP1	16:J:56:ARG:NH1	2.42	0.52
1:2:573:C:H4'	11:D:142:TYR:CE1	2.44	0.52
1:2:1324:U:OP1	24:U:83:ARG:NH1	2.42	0.52
6:A:127:ARG:HG3	6:A:128:ARG:HG3	1.91	0.52
34:7:209:LEU:HD22	34:7:246:LEU:HB3	1.91	0.52
1:2:460:C:C5'	1:2:461:A:H5''	2.34	0.51
1:2:1120:G:C6	1:2:1121:C:C4	2.98	0.51
1:2:149:U:H4'	14:G:94:PHE:CD1	2.45	0.51
1:2:612:C:H2'	1:2:613:C:C6	2.45	0.51
1:2:1333:G:N7	27:H:48:HIS:CE1	2.78	0.51
34:7:59:CYS:HA	34:7:74:CYS:HG	1.76	0.51
6:A:10:ARG:CZ	36:9:89:GLU:HA	2.41	0.51
1:2:459:G:N3	1:2:460:C:O4'	2.43	0.51
1:2:900:G:H5''	27:H:74:SER:HA	1.92	0.51
1:2:1253:G:C6	1:2:1254:C:C4	2.98	0.51
1:2:1415:U:H2'	1:2:1416:C:C6	2.45	0.51
15:I:52:PHE:HA	15:I:60:VAL:O	2.10	0.51
31:5:817:A:H4'	31:5:818:A:OP2	2.10	0.51
35:8:125:ILE:HB	35:8:134:THR:HB	1.92	0.51
1:2:140:C:C2	1:2:152:G:N2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1298:G:H2'	1:2:1299:A:C8	2.46	0.51
1:2:1414:G:H5''	14:G:84:VAL:HG11	1.92	0.51
1:2:1453:U:C6	1:2:1453:U:O5'	2.63	0.51
30:4:26:G:H4'	35:8:38:ILE:HG23	1.91	0.51
1:2:372:G:C2	1:2:373:C:C2	2.99	0.51
1:2:516:A:N1	1:2:842:U:C4	2.78	0.51
1:2:725:C:C2	1:2:763:G:N2	2.79	0.51
1:2:910:G:C6	1:2:911:C:C4	2.99	0.51
11:D:39:LYS:HA	11:D:42:TRP:CE3	2.45	0.51
27:H:96:LYS:HE3	27:H:96:LYS:HA	1.91	0.51
1:2:61:A:N6	1:2:377:A:C2	2.78	0.51
1:2:203:A:C2	1:2:204:G:C5	2.99	0.51
1:2:431:U:C4'	8:V:33:ARG:HH21	2.22	0.51
1:2:603:G:C6	1:2:604:C:C4	2.99	0.51
1:2:1009:G:C5'	10:Z:134:GLY:HA2	2.40	0.51
1:2:1013:G:H1	1:2:1155:U:H3	1.58	0.51
27:H:71:ILE:HD12	27:H:180:PHE:HE1	1.75	0.51
30:4:38:A:C2	30:4:39:C:C2	2.99	0.51
34:7:41:LEU:CD1	34:7:47:ILE:HB	2.41	0.51
1:2:458:G:H2'	1:2:459:G:H5''	1.92	0.51
1:2:458:G:N2	1:2:479:C:O2	2.43	0.51
1:2:607:U:H5'	1:2:702:G:O6	2.11	0.51
1:2:874:G:C2	1:2:875:G:C5	2.99	0.51
1:2:898:G:N1	1:2:899:G:C6	2.79	0.51
27:H:71:ILE:HD12	27:H:180:PHE:CE1	2.46	0.51
34:7:23:THR:HG23	34:7:34:THR:HG23	1.93	0.51
34:7:355:GLU:OE2	34:7:399:ARG:NE	2.44	0.51
1:2:525:A:C2	1:2:822:A:C6	2.99	0.51
1:2:599:G:C5	1:2:600:C:C5	2.99	0.51
1:2:740:G:C2	1:2:751:C:C2	2.98	0.51
1:2:845:G:O2'	1:2:1444:G:OP1	2.29	0.51
1:2:1006:C:O2	1:2:1006:C:O4'	2.28	0.51
23:T:83:VAL:HB	23:T:107:ALA:HB2	1.93	0.51
27:H:87:ARG:C	27:H:88:ARG:CD	2.78	0.51
27:H:93:LEU:C	27:H:95:SER:N	2.64	0.51
34:7:36:LYS:HE2	34:7:45:MET:HA	1.93	0.51
1:2:1332:C:H2'	1:2:1333:G:O4'	2.11	0.51
1:2:130:G:N2	1:2:163:C:C2	2.79	0.50
1:2:168:G:C2	1:2:195:C:C2	3.00	0.50
1:2:461:A:OP1	11:D:16:HIS:NE2	2.44	0.50
1:2:531:G:C2	1:2:532:C:C2	2.98	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:742:U:C5	1:2:743:U:C4	2.99	0.50
1:2:875:G:H2'	1:2:876:A:C8	2.45	0.50
1:2:1058:G:C6	1:2:1059:C:C4	2.98	0.50
1:2:1352:G:N1	1:2:1353:C:C4	2.78	0.50
1:2:1453:U:H6	1:2:1453:U:O5'	1.93	0.50
1:2:1486:A:H3'	1:2:1487:U:C5	2.45	0.50
27:H:26:VAL:HG21	27:H:120:ILE:HG23	1.93	0.50
27:H:111:ILE:HD11	27:H:122:VAL:HG11	1.93	0.50
34:7:294:LEU:HB3	37:7:501:MET:CG	2.41	0.50
1:2:524:U:H5''	1:2:773:A:C5	2.46	0.50
1:2:553:C:C2	1:2:593:G:N2	2.79	0.50
1:2:621:G:C6	1:2:622:C:C4	2.99	0.50
1:2:964:A:N6	1:2:989:C:H4'	2.26	0.50
1:2:1390:G:C2	1:2:1426:C:C2	2.98	0.50
24:U:39:ARG:HA	24:U:39:ARG:HE	1.76	0.50
27:H:89:GLU:HB2	27:H:95:SER:HB2	1.93	0.50
34:7:41:LEU:CD2	34:7:47:ILE:HB	2.40	0.50
1:2:93:A:O2'	1:2:322:G:N2	2.44	0.50
1:2:229:G:H2'	1:2:230:C:H6	1.77	0.50
1:2:869:U:O5'	1:2:869:U:H6	1.93	0.50
1:2:1028:C:C2	1:2:1034:G:N2	2.79	0.50
13:F:1:MET:CB	13:F:57:VAL:HG22	2.41	0.50
24:U:21:LYS:HG2	24:U:52:TYR:CE1	2.47	0.50
27:H:148:VAL:HG12	27:H:149:ALA:N	2.27	0.50
34:7:138:ILE:HG23	34:7:410:TRP:CD1	2.47	0.50
1:2:142:G:O6	1:2:150:G:C6	2.64	0.50
1:2:271:G:C4	1:2:272:C:C5	2.99	0.50
1:2:369:A:H2'	1:2:370:A:C8	2.46	0.50
1:2:985:C:H1'	26:Y:41:GLY:CA	2.41	0.50
1:2:1276:G:H8	1:2:1276:G:O5'	1.94	0.50
1:2:1311:C:H4'	27:H:95:SER:CA	2.42	0.50
32:1:61:LYS:HA	32:1:64:CYS:SG	2.51	0.50
1:2:149:U:H2'	1:2:150:G:O4'	2.12	0.50
1:2:276:A:H4'	3:N:14:ARG:CZ	2.41	0.50
1:2:988:A:C2'	1:2:989:C:H5'	2.41	0.50
1:2:1394:G:H5''	14:G:104:LYS:CE	2.42	0.50
1:2:1472:G:P	32:1:58:LYS:HD2	2.51	0.50
18:3:39:THR:HG23	18:3:100:ALA:HB2	1.93	0.50
1:2:540:G:C6	1:2:709:G:O6	2.65	0.50
1:2:556:G:N2	1:2:590:G:C5	2.80	0.50
1:2:566:C:H4'	11:D:54:ARG:CZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1311:C:H4'	27:H:95:SER:N	2.26	0.50
1:2:1327:C:OP1	28:K:119:PRO:O	2.29	0.50
12:E:37:HIS:CG	12:E:38:ASN:N	2.80	0.50
1:2:1118:C:C5	1:2:1120:G:C8	2.99	0.50
1:2:1348:C:H2'	1:2:1349:C:H6	1.74	0.50
1:2:1402:C:N4	1:2:1413:G:H22	2.05	0.50
1:2:1409:G:N2	1:2:1410:G:C8	2.80	0.50
1:2:1489:A:H1'	31:5:812:G:H22	1.76	0.50
34:7:41:LEU:HB3	34:7:45:MET:O	2.12	0.50
35:8:56:ARG:NH1	35:8:103:TYR:O	2.44	0.50
1:2:459:G:N3	1:2:459:G:H5'	2.27	0.50
1:2:533:C:C4	1:2:534:G:C2	3.00	0.50
1:2:551:U:H2'	1:2:552:C:C6	2.46	0.50
1:2:771:G:C4	1:2:773:A:O4'	2.64	0.50
1:2:1479:C:H5''	2:M:127:ARG:HH22	1.75	0.50
31:5:812:G:C8	31:5:813:A:C8	2.99	0.50
34:7:134:VAL:HG11	34:7:340:VAL:HG21	1.94	0.50
1:2:29:G:H1'	3:N:135:LYS:NZ	2.27	0.50
1:2:262:G:H5''	1:2:262:G:H8	1.76	0.50
1:2:368:C:H4'	1:2:369:A:O5'	2.11	0.50
1:2:1403:U:C2	1:2:1404:C:C5	3.00	0.50
8:V:60:PHE:N	8:V:60:PHE:HD1	2.10	0.50
13:F:86:LEU:HD11	13:F:195:VAL:HG22	1.93	0.50
14:G:28:LYS:HE2	14:G:38:ILE:HG23	1.94	0.50
27:H:44:LEU:HD11	28:K:40:ILE:HG22	1.93	0.50
27:H:90:HIS:HB3	27:H:92:SER:H	1.76	0.50
1:2:372:G:H2'	1:2:373:C:C6	2.47	0.49
1:2:431:U:H3'	1:2:432:G:C8	2.47	0.49
1:2:649:A:H2'	1:2:650:A:C8	2.47	0.49
1:2:930:G:C6	1:2:1325:C:H5'	2.47	0.49
1:2:1196:A:OP1	27:H:88:ARG:CZ	2.61	0.49
1:2:1336:U:H2'	1:2:1337:A:O4'	2.11	0.49
1:2:1403:U:H2'	1:2:1404:C:H5'	1.93	0.49
8:V:21:PHE:CE1	8:V:69:ALA:HB3	2.47	0.49
19:L:77:ALA:HB1	19:L:81:ALA:HB3	1.93	0.49
30:4:11:A:H2'	30:4:12:G:C8	2.47	0.49
34:7:294:LEU:O	37:7:501:MET:HB2	2.12	0.49
1:2:2:U:C5	13:F:184:TRP:CZ3	3.00	0.49
1:2:471:G:OP2	33:6:54:LYS:HD2	2.11	0.49
1:2:786:G:H2'	1:2:787:U:O4'	2.12	0.49
1:2:866:A:H2'	1:2:867:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1352:G:C6	1:2:1353:C:N4	2.80	0.49
7:B:33:TYR:HB2	7:B:43:LEU:C	2.32	0.49
10:Z:2:ALA:HB3	10:Z:5:ARG:NH1	2.27	0.49
27:H:93:LEU:HG	27:H:96:LYS:O	2.11	0.49
27:H:124:VAL:O	27:H:128:GLU:HG3	2.12	0.49
30:4:67:C:H2'	30:4:68:C:C6	2.47	0.49
34:7:115:ILE:HD11	34:7:198:ILE:CG2	2.42	0.49
1:2:432:G:H2'	1:2:433:U:O4'	2.11	0.49
1:2:556:G:C2	1:2:590:G:C6	3.00	0.49
1:2:975:A:C2'	1:2:976:A:H5'	2.32	0.49
1:2:1260:G:O2'	1:2:1263:C:N4	2.45	0.49
4:Q:112:HIS:O	4:Q:114:LYS:N	2.45	0.49
6:A:137:ILE:HD13	6:A:180:LEU:HD21	1.95	0.49
19:L:64:TRP:CE3	21:P:52:PHE:HB3	2.47	0.49
1:2:30:C:C4	1:2:31:U:C4	3.01	0.49
1:2:242:A:O3'	1:2:243:G:H4'	2.12	0.49
1:2:537:G:C6	1:2:538:C:N4	2.80	0.49
1:2:723:G:N2	1:2:724:C:C2	2.80	0.49
14:G:78:ILE:HG22	14:G:109:GLY:HA2	1.94	0.49
27:H:174:TYR:CG	27:H:174:TYR:O	2.65	0.49
30:4:73:A:H5''	34:7:221:PHE:CZ	2.47	0.49
34:7:263:LYS:O	34:7:266:LYS:HG2	2.13	0.49
1:2:419:G:C2	1:2:420:C:C6	3.01	0.49
1:2:431:U:C2'	1:2:432:G:OP1	2.59	0.49
1:2:861:G:C6	1:2:862:C:C4	3.01	0.49
1:2:1118:C:O2'	22:S:52:GLY:HA3	2.12	0.49
6:A:135:ARG:HA	6:A:138:ARG:HG3	1.93	0.49
8:V:56:ILE:HG13	8:V:67:GLY:CA	2.38	0.49
12:E:184:TYR:HA	12:E:197:GLY:O	2.13	0.49
13:F:129:GLY:O	13:F:130:SER:CB	2.61	0.49
14:G:80:GLY:C	14:G:82:ARG:H	2.16	0.49
15:I:7:LEU:HA	15:I:34:ILE:HG12	1.93	0.49
32:1:32:THR:HB	32:1:42:ILE:HG12	1.94	0.49
1:2:166:A:H61	1:2:196:G:H1'	1.77	0.49
1:2:314:G:O2'	1:2:1424:G:H5'	2.13	0.49
1:2:872:A:N3	1:2:873:A:C8	2.81	0.49
1:2:1028:C:H5'	7:B:128:ARG:HH22	1.78	0.49
15:I:2:THR:OG1	15:I:3:LEU:N	2.45	0.49
25:X:18:THR:HG22	25:X:19:GLY:H	1.78	0.49
34:7:281:PHE:CZ	34:7:295:VAL:HG22	2.47	0.49
1:2:53:G:C5	1:2:54:C:C4	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:81:C:C2	1:2:82:G:C8	3.01	0.49
1:2:193:G:H2'	1:2:194:C:H6	1.78	0.49
1:2:526:A:H2'	1:2:527:A:C8	2.47	0.49
1:2:629:U:O4	1:2:669:A:N1	2.46	0.49
1:2:762:G:C6	1:2:763:G:C5	3.01	0.49
1:2:963:A:C8	1:2:987:G:N2	2.81	0.49
1:2:1139:A:H2'	1:2:1140:A:O4'	2.13	0.49
1:2:244:G:C6	1:2:245:U:C4	3.01	0.49
1:2:271:G:N3	1:2:272:C:C6	2.81	0.49
1:2:1309:A:C2	1:2:1334:A:C5	3.00	0.49
1:2:1454:A:N3	1:2:1455:A:C8	2.80	0.49
14:G:29:LEU:CD1	14:G:63:ILE:HD11	2.42	0.49
34:7:281:PHE:CE2	34:7:295:VAL:HG13	2.47	0.49
1:2:260:C:H4'	5:R:92:ARG:NH1	2.27	0.49
1:2:355:C:H2'	1:2:356:G:C8	2.48	0.49
1:2:898:G:N1	1:2:899:G:O6	2.46	0.49
1:2:1308:U:C5	1:2:1333:G:N2	2.81	0.49
1:2:1472:G:OP1	32:1:58:LYS:CD	2.52	0.49
18:3:43:VAL:HG11	18:3:66:LEU:HD21	1.94	0.49
27:H:81:VAL:HG12	27:H:82:ALA:N	2.27	0.49
30:4:76:A:HO2'	37:7:501:MET:N	2.10	0.49
1:2:20:G:H4'	1:2:477:G:C2	2.47	0.49
1:2:175:G:N2	1:2:188:C:C2	2.81	0.49
1:2:244:G:C5	1:2:245:U:C5	3.00	0.49
1:2:438:A:C3'	1:2:439:G:H5''	2.41	0.49
1:2:515:U:O4	3:N:26:SER:HB2	2.12	0.49
1:2:715:C:C2	1:2:716:G:C8	3.00	0.49
1:2:1219:C:N3	1:2:1237:G:C2	2.81	0.49
1:2:1312:C:OP1	27:H:78:HIS:O	2.31	0.49
1:2:1414:G:C4'	14:G:84:VAL:HG11	2.43	0.49
12:E:37:HIS:CD2	12:E:38:ASN:N	2.81	0.49
14:G:84:VAL:CG1	14:G:85:ARG:N	2.75	0.49
35:8:33:MET:HG3	35:8:44:ILE:HG23	1.95	0.49
1:2:4:C:H2'	1:2:5:C:H6	1.78	0.48
1:2:8:U:C4	1:2:874:G:C6	3.00	0.48
1:2:297:G:H2'	1:2:298:C:H6	1.78	0.48
1:2:452:G:C6	1:2:499:G:C2	3.01	0.48
1:2:492:G:C2	1:2:493:C:C2	3.01	0.48
1:2:836:G:P	15:I:76:LYS:HG3	2.53	0.48
1:2:868:C:C5'	1:2:1373:A:O2'	2.58	0.48
1:2:1031:G:H8	1:2:1031:G:O5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1311:C:OP1	27:H:77:SER:N	2.46	0.48
1:2:1311:C:H4'	27:H:94:ASN:C	2.33	0.48
27:H:140:MET:HB3	27:H:145:ARG:HA	1.95	0.48
1:2:6:G:C5	1:2:7:G:N7	2.81	0.48
1:2:62:G:C8	1:2:63:G:C8	3.01	0.48
1:2:93:A:C6	1:2:322:G:C6	3.01	0.48
1:2:541:G:C5	1:2:707:A:C5	3.01	0.48
1:2:556:G:H4'	12:E:224:ASP:HB2	1.94	0.48
1:2:1412:A:H2'	1:2:1413:G:C8	2.48	0.48
1:2:1454:A:C2	1:2:1455:A:C5	3.01	0.48
3:N:119:ILE:HD12	3:N:122:ILE:HB	1.95	0.48
30:4:11:A:H2'	30:4:12:G:H8	1.79	0.48
32:1:32:THR:HG21	32:1:42:ILE:HD11	1.94	0.48
1:2:541:G:C8	1:2:707:A:C2	3.01	0.48
1:2:1040:A:H2'	1:2:1041:C:H5'	1.95	0.48
14:G:52:GLY:HA3	14:G:54:GLU:HB2	1.95	0.48
19:L:59:ALA:HB3	19:L:61:PHE:CE1	2.49	0.48
1:2:103:A:O2'	1:2:104:A:OP2	2.25	0.48
1:2:318:C:O2'	14:G:102:ARG:HG3	2.13	0.48
1:2:944:C:C2	1:2:1181:G:C2	3.01	0.48
1:2:1377:G:O2'	1:2:1438:A:N6	2.46	0.48
1:2:1395:G:H5''	14:G:87:LEU:HD13	1.94	0.48
7:B:63:GLU:HA	7:B:179:ARG:NH2	2.29	0.48
8:V:27:GLY:HA2	11:D:156:ARG:NH2	2.28	0.48
12:E:37:HIS:CD2	12:E:38:ASN:H	2.30	0.48
13:F:5:TRP:HB3	13:F:57:VAL:HG21	1.94	0.48
30:4:74:C:N3	34:7:37:HIS:CB	2.70	0.48
1:2:152:G:H1'	14:G:64:ARG:NH1	2.29	0.48
1:2:453:G:H2'	1:2:454:G:C8	2.48	0.48
1:2:1312:C:H4'	27:H:80:LYS:HG2	1.94	0.48
1:2:1404:C:C4	1:2:1405:C:C5	3.01	0.48
1:2:1489:A:C2	31:5:812:G:C6	3.01	0.48
7:B:56:GLY:HA3	7:B:174:GLU:HG2	1.96	0.48
7:B:56:GLY:CA	7:B:174:GLU:HG2	2.44	0.48
8:V:60:PHE:CD1	8:V:60:PHE:O	2.66	0.48
13:F:175:LEU:HD23	13:F:205:LEU:HD21	1.96	0.48
31:5:813:A:H4'	31:5:814:U:OP1	2.05	0.48
34:7:163:TYR:CE1	35:8:7:TYR:CG	3.01	0.48
1:2:50:C:O2	1:2:354:G:C2	2.67	0.48
1:2:157:A:C8	1:2:159:C:C6	3.02	0.48
1:2:694:U:O2'	4:Q:118:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:843:G:C2	1:2:844:G:C8	3.01	0.48
1:2:848:G:OP1	29:0:9:ARG:NH2	2.46	0.48
1:2:1079:G:N2	1:2:1106:A:H62	2.10	0.48
1:2:1390:G:N2	1:2:1426:C:C2	2.82	0.48
1:2:1414:G:C1'	14:G:78:ILE:HA	2.44	0.48
7:B:59:LEU:HB3	7:B:175:ILE:HG21	1.95	0.48
13:F:125:LYS:O	13:F:208:THR:HG21	2.13	0.48
27:H:58:LYS:O	27:H:66:ARG:CZ	2.61	0.48
30:4:19:G:O2'	36:9:60:GLU:N	2.47	0.48
31:5:819:A:C2	32:1:36:PHE:CD1	3.01	0.48
36:9:69:ILE:HD11	36:9:81:SER:HB2	1.96	0.48
1:2:459:G:H3'	1:2:460:C:H4'	1.92	0.48
1:2:521:G:C6	1:2:522:C:C4	3.01	0.48
1:2:640:U:HO2'	1:2:641:A:H8	1.60	0.48
1:2:1193:G:C2	1:2:1194:C:C2	3.02	0.48
3:N:23:PHE:CD1	3:N:23:PHE:N	2.78	0.48
5:R:1:MET:O	5:R:23:TRP:HB3	2.14	0.48
13:F:38:PHE:CE2	13:F:95:TYR:CE1	3.01	0.48
35:8:42:THR:HG21	35:8:92:ILE:HD11	1.95	0.48
1:2:297:G:H2'	1:2:298:C:C6	2.48	0.48
1:2:762:G:C6	1:2:763:G:N7	2.82	0.48
1:2:1312:C:O2	1:2:1331:G:C2	2.67	0.48
1:2:1317:G:C4	1:2:1326:G:N2	2.81	0.48
1:2:1450:U:H2'	1:2:1451:C:C6	2.48	0.48
11:D:40:GLU:O	11:D:44:HIS:ND1	2.47	0.48
19:L:92:GLU:HB2	19:L:93:ASP:CB	2.42	0.48
25:X:23:ASP:OD1	25:X:46:ARG:NH1	2.46	0.48
27:H:212:GLU:O	27:H:215:ARG:HG2	2.14	0.48
1:2:462:A:O2'	1:2:463:G:O4'	2.20	0.48
1:2:518:U:H2'	1:2:519:G:C8	2.48	0.48
1:2:962:G:H1'	1:2:988:A:N6	2.29	0.48
1:2:1411:G:H2'	1:2:1412:A:C8	2.49	0.48
3:N:108:ILE:HD13	3:N:125:LYS:HD2	1.96	0.48
8:V:9:LYS:HE2	12:E:55:TYR:HA	1.96	0.48
12:E:9:HIS:O	12:E:31:ARG:NH1	2.47	0.48
19:L:10:SER:HB3	19:L:16:LEU:HB2	1.95	0.48
1:2:692:G:C6	1:2:693:C:C4	3.02	0.48
1:2:881:G:C6	1:2:882:C:C4	3.01	0.48
1:2:1307:G:HO2'	1:2:1308:U:P	2.37	0.48
1:2:1414:G:O4'	14:G:78:ILE:HG23	2.13	0.48
1:2:1424:G:C4	1:2:1425:C:C5	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:62:ALA:HB3	3:N:67:SER:HA	1.96	0.48
13:F:5:TRP:HB2	13:F:55:PRO:HB2	1.96	0.48
16:J:103:THR:OG1	16:J:106:GLY:O	2.32	0.48
32:1:31:VAL:HG13	32:1:82:ARG:HD2	1.96	0.48
34:7:269:TYR:CE1	34:7:385:PRO:HD3	2.49	0.48
34:7:280:ARG:O	37:7:501:MET:N	2.47	0.48
36:9:240:SER:O	36:9:241:GLU:C	2.51	0.48
1:2:75:C:O2	1:2:75:C:O4'	2.31	0.47
1:2:419:G:N2	1:2:420:C:C2	2.82	0.47
1:2:839:G:C5	1:2:840:C:C5	3.02	0.47
1:2:898:G:C6	1:2:899:G:O6	2.67	0.47
1:2:1048:G:HO2'	1:2:1130:A:HO2'	1.53	0.47
1:2:1144:G:C2	1:2:1145:C:C2	3.02	0.47
1:2:1186:C:H4'	1:2:1187:A:OP1	2.14	0.47
1:2:1488:C:C2	1:2:1489:A:C8	3.01	0.47
3:N:128:LYS:HA	3:N:133:SER:HA	1.96	0.47
8:V:28:GLU:HB3	8:V:29:PRO:HD2	1.96	0.47
10:Z:100:ALA:HA	10:Z:169:ALA:HB2	1.96	0.47
16:J:87:ARG:HD2	16:J:90:ALA:HB3	1.96	0.47
34:7:276:ILE:HG23	34:7:297:ILE:HG23	1.95	0.47
1:2:106:A:H62	1:2:235:G:N2	2.12	0.47
1:2:541:G:C4	1:2:707:A:C6	3.01	0.47
1:2:974:G:H2'	1:2:974:G:N3	2.28	0.47
1:2:1239:A:H2'	1:2:1239:A:N3	2.29	0.47
1:2:1389:G:N2	1:2:1427:C:C2	2.82	0.47
1:2:1390:G:C6	1:2:1391:U:C4	3.02	0.47
13:F:146:GLU:HG2	13:F:147:GLY:N	2.29	0.47
13:F:148:LYS:N	13:F:148:LYS:HD2	2.29	0.47
35:8:100:LEU:HA	35:8:104:VAL:HG12	1.96	0.47
35:8:118:LYS:HG2	35:8:123:TRP:NE1	2.29	0.47
1:2:29:G:C6	1:2:30:C:C4	3.01	0.47
1:2:338:C:C2	1:2:344:G:C2	3.01	0.47
1:2:402:G:C6	1:2:403:C:C4	3.02	0.47
1:2:459:G:C6	1:2:460:C:C2	3.03	0.47
1:2:646:U:O4	2:M:51:ASP:HB3	2.14	0.47
1:2:991:C:C5	1:2:992:G:N7	2.82	0.47
1:2:1120:G:C2	1:2:1121:C:C6	3.03	0.47
1:2:1215:G:C2	1:2:1243:C:C2	3.02	0.47
1:2:1352:G:C4	1:2:1353:C:C5	3.02	0.47
1:2:1383:A:C2	1:2:1433:C:C2	3.03	0.47
23:T:16:LEU:HB3	23:T:74:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:73:A:N1	34:7:38:SER:HA	2.29	0.47
34:7:59:CYS:CA	34:7:74:CYS:HG	2.27	0.47
1:2:87:C:C4	1:2:88:G:N7	2.83	0.47
1:2:151:G:O2'	14:G:64:ARG:HB3	2.14	0.47
1:2:229:G:N2	1:2:230:C:N1	2.62	0.47
1:2:262:G:O2'	1:2:263:C:OP2	2.25	0.47
1:2:669:A:H2'	1:2:670:C:O4'	2.14	0.47
1:2:723:G:N1	1:2:724:C:C4	2.82	0.47
1:2:1450:U:H2'	1:2:1451:C:H6	1.78	0.47
1:2:1483:U:O2'	1:2:1484:C:P	2.73	0.47
6:A:59:PHE:CE2	6:A:162:VAL:HG12	2.49	0.47
25:X:7:TYR:CG	25:X:60:THR:HG22	2.48	0.47
1:2:318:C:O2	14:G:100:GLY:HA2	2.14	0.47
1:2:893:U:OP1	1:2:893:U:H3'	2.15	0.47
1:2:1120:G:N2	1:2:1121:C:C2	2.83	0.47
1:2:1124:G:C2	1:2:1133:C:C2	3.03	0.47
1:2:1273:G:C6	1:2:1274:C:C4	3.02	0.47
12:E:127:ILE:HG22	12:E:141:ASN:O	2.14	0.47
27:H:72:MET:CE	27:H:97:LYS:HB2	2.44	0.47
32:1:32:THR:HG23	32:1:40:MET:HB3	1.96	0.47
1:2:93:A:H2'	1:2:322:G:N2	2.28	0.47
1:2:329:G:H4'	14:G:103:ARG:NH1	2.29	0.47
1:2:632:C:H2'	1:2:633:C:O4'	2.15	0.47
1:2:921:G:C6	1:2:933:G:O6	2.68	0.47
1:2:1200:U:O4'	27:H:103:VAL:HG22	2.15	0.47
1:2:1318:U:C2	1:2:1323:A:N6	2.80	0.47
4:Q:67:LYS:HD3	4:Q:76:LEU:HB3	1.96	0.47
1:2:87:C:OP1	14:G:97:LYS:HG2	2.14	0.47
1:2:296:A:C2	1:2:519:G:O6	2.68	0.47
1:2:507:G:OP1	3:N:111:PRO:CG	2.51	0.47
1:2:583:G:C2	1:2:584:C:C2	3.02	0.47
1:2:612:C:C2	1:2:613:C:C5	3.03	0.47
1:2:685:G:C6	1:2:686:C:C4	3.02	0.47
1:2:779:G:H2'	1:2:780:C:C6	2.50	0.47
1:2:916:U:O2	1:2:918:A:C8	2.68	0.47
1:2:1249:A:H5'	27:H:81:VAL:HA	1.97	0.47
1:2:1364:C:H2'	1:2:1365:G:C8	2.50	0.47
10:Z:89:TYR:HB2	10:Z:123:ASN:CG	2.35	0.47
11:D:102:GLU:HA	11:D:107:THR:HG21	1.96	0.47
12:E:168:VAL:N	12:E:169:PRO:HD2	2.30	0.47
13:F:48:GLU:O	13:F:52:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:40:LEU:HB3	19:L:41:PRO:CD	2.45	0.47
20:O:78:ALA:HB2	24:U:35:VAL:HG21	1.96	0.47
25:X:8:PRO:HD2	25:X:33:GLU:HG3	1.97	0.47
27:H:118:ASN:OD1	27:H:120:ILE:HG22	2.14	0.47
33:6:54:LYS:HG2	33:6:58:ARG:NH1	2.29	0.47
34:7:342:ALA:HB3	34:7:344:GLU:O	2.14	0.47
1:2:453:G:H2'	1:2:454:G:H8	1.80	0.47
1:2:909:U:O4	20:O:130:ARG:NH2	2.48	0.47
1:2:1131:G:N1	1:2:1132:C:C4	2.83	0.47
1:2:1421:C:H4'	16:J:1:MET:O	2.15	0.47
1:2:1447:A:C1'	33:6:34:ALA:HB2	2.44	0.47
7:B:133:ILE:HA	13:F:43:GLN:OE1	2.14	0.47
31:5:812:G:H2'	31:5:813:A:O4'	2.15	0.47
33:6:89:THR:HG22	33:6:89:THR:O	2.15	0.47
1:2:385:A:H2'	1:2:386:C:C5'	2.45	0.47
1:2:540:G:HO2'	1:2:541:G:P	2.30	0.47
1:2:757:G:H2'	1:2:758:U:O4'	2.15	0.47
1:2:1264:G:C6	1:2:1265:G:N1	2.83	0.47
1:2:1302:C:H2'	1:2:1303:C:C6	2.50	0.47
1:2:1485:G:N3	1:2:1486:A:N7	2.63	0.47
6:A:43:VAL:HA	6:A:46:ARG:HG2	1.97	0.47
10:Z:5:ARG:O	10:Z:8:ILE:HG13	2.14	0.47
13:F:86:LEU:CD2	13:F:195:VAL:HA	2.45	0.47
36:9:2:ILE:HG23	36:9:122:TRP:CH2	2.49	0.47
36:9:204:LEU:CD2	36:9:207:ILE:HG21	2.42	0.47
1:2:82:G:C2	1:2:83:C:C2	3.03	0.47
1:2:323:A:C2	1:2:325:A:C4	3.03	0.47
1:2:1249:A:O2'	27:H:80:LYS:NZ	2.40	0.47
1:2:1284:C:H2'	1:2:1285:C:C6	2.49	0.47
1:2:1318:U:O4	1:2:1323:A:N1	2.47	0.47
1:2:1323:A:N3	1:2:1323:A:C2'	2.78	0.47
1:2:1443:G:C2	1:2:1444:G:C5	3.03	0.47
11:D:93:LEU:HD13	13:F:160:PRO:HB3	1.96	0.47
18:3:43:VAL:HG21	18:3:70:CYS:SG	2.55	0.47
27:H:89:GLU:CB	27:H:95:SER:HB2	2.45	0.47
29:0:14:LYS:O	29:0:18:LYS:N	2.37	0.47
1:2:10:G:N7	1:2:1356:A:C5	2.83	0.46
1:2:239:A:O2'	1:2:240:U:OP2	2.27	0.46
1:2:434:A:N3	8:V:85:TYR:N	2.64	0.46
1:2:480:G:C6	1:2:481:C:C4	3.03	0.46
1:2:537:G:C2	1:2:538:C:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:572:U:O4	11:D:138:ARG:CZ	2.63	0.46
1:2:779:G:C6	1:2:780:C:C4	3.03	0.46
1:2:780:C:OP1	15:I:28:LYS:HE2	2.15	0.46
1:2:1206:G:H4'	24:U:13:VAL:HG21	1.96	0.46
1:2:1346:C:O2'	1:2:1347:U:H5'	2.15	0.46
8:V:24:TYR:HA	8:V:63:TYR:O	2.15	0.46
13:F:82:ARG:HD3	13:F:102:HIS:NE2	2.29	0.46
25:X:46:ARG:HH21	27:H:135:ASP:HB3	1.80	0.46
27:H:132:PRO:HB3	27:H:204:LYS:O	2.15	0.46
30:4:7:G:H5'	30:4:8:U:C5	2.50	0.46
34:7:38:SER:HB2	34:7:41:LEU:CD2	2.45	0.46
35:8:38:ILE:HD12	35:8:43:ILE:HD12	1.96	0.46
1:2:271:G:C2	1:2:272:C:C2	3.03	0.46
1:2:424:U:C4	1:2:425:C:C2	3.03	0.46
1:2:459:G:C6	1:2:460:C:C4	3.03	0.46
1:2:521:G:C2	1:2:522:C:C2	3.04	0.46
1:2:839:G:C2	1:2:840:C:C2	3.03	0.46
1:2:992:G:C6	1:2:993:C:N3	2.82	0.46
1:2:1430:G:C6	1:2:1431:C:C4	3.03	0.46
1:2:1472:G:C6	1:2:1473:A:C5	3.04	0.46
3:N:136:GLU:OE2	3:N:143:GLU:N	2.47	0.46
12:E:190:GLY:O	12:E:193:VAL:HG13	2.16	0.46
12:E:204:ARG:HA	12:E:212:VAL:HG12	1.97	0.46
13:F:35:HIS:CE1	13:F:95:TYR:HH	2.34	0.46
30:4:14:A:N6	30:4:15:G:C2	2.83	0.46
30:4:70:G:C6	30:4:71:C:C5	3.03	0.46
35:8:138:PRO:O	35:8:139:LEU:HD12	2.15	0.46
1:2:495:G:C4	1:2:496:C:C5	3.02	0.46
1:2:537:G:C4	1:2:538:C:C5	3.03	0.46
1:2:910:G:C2	1:2:911:C:C2	3.03	0.46
11:D:65:GLN:O	11:D:66:ALA:C	2.52	0.46
13:F:46:GLU:OE1	13:F:46:GLU:HA	2.15	0.46
27:H:28:VAL:HG11	27:H:34:LYS:HA	1.96	0.46
27:H:33:LEU:HD22	27:H:128:GLU:HG2	1.96	0.46
27:H:75:GLY:HA2	27:H:94:ASN:CG	2.36	0.46
30:4:76:A:C3'	37:7:501:MET:C	2.84	0.46
1:2:137:A:C8	1:2:138:C:C5	3.03	0.46
1:2:358:G:C5'	3:N:79:LYS:HB2	2.46	0.46
1:2:720:A:H2'	1:2:721:A:O4'	2.15	0.46
1:2:971:G:H1	1:2:979:U:H3	1.62	0.46
1:2:1341:C:H1'	25:X:20:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:24:PRO:HA	6:A:27:PHE:O	2.15	0.46
7:B:60:ALA:HB2	7:B:178:ASN:HB2	1.97	0.46
30:4:17:C:O2	30:4:17:C:O4'	2.31	0.46
34:7:274:THR:HG21	34:7:299:THR:HB	1.97	0.46
1:2:106:A:H62	1:2:235:G:H21	1.64	0.46
1:2:431:U:H2'	1:2:432:G:OP1	2.16	0.46
4:Q:95:LEU:HD13	4:Q:132:LEU:HB3	1.97	0.46
4:Q:128:LYS:O	4:Q:132:LEU:HD23	2.16	0.46
34:7:217:VAL:HA	34:7:240:GLY:HA3	1.98	0.46
35:8:97:GLU:HA	35:8:100:LEU:HD12	1.97	0.46
1:2:42:G:H4'	1:2:43:A:OP2	2.16	0.46
1:2:768:A:N7	1:2:770:A:C4	2.84	0.46
1:2:788:C:C2	1:2:811:G:C2	3.04	0.46
1:2:837:C:OP1	3:N:8:ASN:N	2.48	0.46
1:2:998:A:H2'	1:2:999:G:H5'	1.97	0.46
1:2:1463:A:H61	1:2:1482:C:H42	1.64	0.46
1:2:1489:A:C6	1:2:1490:C:N4	2.84	0.46
8:V:55:TYR:O	8:V:67:GLY:CA	2.64	0.46
27:H:86:MET:C	27:H:88:ARG:HB2	2.36	0.46
34:7:361:VAL:HG23	34:7:361:VAL:O	2.16	0.46
34:7:399:ARG:HG2	34:7:400:GLN:N	2.31	0.46
36:9:19:VAL:O	36:9:61:ASN:ND2	2.48	0.46
1:2:127:G:C2	1:2:218:C:N3	2.84	0.46
1:2:164:A:H2'	1:2:165:U:C6	2.50	0.46
1:2:768:A:H4'	1:2:1466:G:H5'	1.98	0.46
1:2:1352:G:H2'	1:2:1353:C:H6	1.80	0.46
1:2:1370:U:C2	1:2:1446:G:N2	2.84	0.46
1:2:1414:G:P	14:G:86:VAL:CG1	3.04	0.46
7:B:59:LEU:O	7:B:179:ARG:NH2	2.49	0.46
9:W:4:PRO:HB3	15:I:28:LYS:CG	2.45	0.46
12:E:37:HIS:NE2	12:E:41:THR:HB	2.31	0.46
34:7:49:LEU:HD12	34:7:218:ILE:HD12	1.98	0.46
36:9:254:GLY:HA3	36:9:261:ILE:HD12	1.98	0.46
1:2:53:G:C6	1:2:54:C:C4	3.04	0.46
1:2:53:G:C6	1:2:54:C:N3	2.84	0.46
1:2:184:G:O2'	1:2:185:G:H8	1.90	0.46
5:R:74:ASN:ND2	5:R:78:ILE:O	2.45	0.46
34:7:41:LEU:HD22	34:7:47:ILE:CB	2.46	0.46
1:2:113:U:P	5:R:30:HIS:CE1	3.09	0.46
1:2:193:G:C6	1:2:194:C:C4	3.04	0.46
1:2:457:G:H2'	1:2:458:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:629:U:H2'	1:2:630:A:O4'	2.16	0.46
1:2:878:U:C2	1:2:879:U:C6	3.04	0.46
1:2:934:G:O2'	1:2:935:G:OP2	2.24	0.46
1:2:955:G:C6	1:2:956:C:C4	3.04	0.46
1:2:1073:C:O5'	1:2:1073:C:H6	1.99	0.46
1:2:1379:G:C6	1:2:1380:C:C4	3.04	0.46
1:2:1483:U:HO2'	1:2:1484:C:H3'	1.81	0.46
4:Q:3:ARG:O	4:Q:7:ARG:NH2	2.42	0.46
7:B:83:PHE:HB2	7:B:168:TYR:HB3	1.97	0.46
12:E:89:ASP:OD2	12:E:90:VAL:N	2.49	0.46
30:4:26:G:C5	30:4:27:U:C5	3.04	0.46
1:2:454:G:H2'	1:2:455:C:C6	2.51	0.46
1:2:901:G:C2	1:2:1302:C:N3	2.84	0.46
1:2:906:G:C2	1:2:907:C:C2	3.04	0.46
1:2:1277:C:H2'	1:2:1278:A:O4'	2.16	0.46
1:2:1395:G:H5'	14:G:87:LEU:HD13	1.97	0.46
1:2:1403:U:C2'	1:2:1404:C:H5'	2.45	0.46
13:F:16:TRP:CE2	13:F:48:GLU:HB2	2.51	0.46
13:F:36:GLU:O	13:F:40:ARG:NH1	2.48	0.46
13:F:139:HIS:NE2	13:F:159:GLY:O	2.45	0.46
14:G:6:LEU:HD13	14:G:21:ILE:HD12	1.97	0.46
14:G:6:LEU:HD23	14:G:121:VAL:HG21	1.98	0.46
24:U:12:LEU:HA	24:U:136:LEU:HD13	1.97	0.46
34:7:183:VAL:HG11	34:7:194:LEU:HD22	1.98	0.46
1:2:147:A:C5	1:2:148:C:H1'	2.51	0.45
1:2:929:C:P	28:K:130:ARG:HH12	2.40	0.45
1:2:1260:G:C2'	1:2:1261:U:OP2	2.64	0.45
1:2:1404:C:C4'	14:G:76:PRO:HB2	2.46	0.45
12:E:73:VAL:HG11	12:E:83:PHE:HE2	1.80	0.45
12:E:192:ASN:HA	12:E:195:ARG:HH21	1.81	0.45
13:F:146:GLU:HA	13:F:154:VAL:O	2.14	0.45
15:I:74:ALA:HA	15:I:127:ALA:HA	1.99	0.45
15:I:87:GLU:O	15:I:90:GLU:HB3	2.15	0.45
27:H:97:LYS:HA	27:H:100:ALA:HB3	1.97	0.45
34:7:329:ILE:O	34:7:379:GLU:HA	2.16	0.45
1:2:677:U:O2	1:2:1493:C:H1'	2.16	0.45
1:2:710:G:OP1	4:Q:3:ARG:NH1	2.49	0.45
1:2:889:G:N1	1:2:890:C:C4	2.84	0.45
1:2:1320:A:C8	21:P:14:PHE:CD2	3.04	0.45
1:2:1489:A:H2'	1:2:1490:C:H5'	1.98	0.45
5:R:1:MET:O	5:R:23:TRP:CD1	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:67:ASP:HB3	13:F:86:LEU:HD13	1.98	0.45
13:F:94:GLY:O	13:F:95:TYR:CD2	2.69	0.45
20:O:87:THR:HG21	23:T:6:PHE:CD1	2.51	0.45
30:4:3:C:H5''	30:4:3:C:H6	1.81	0.45
33:6:72:TRP:CE3	33:6:79:ARG:HD2	2.51	0.45
34:7:404:ARG:HD3	34:7:406:ARG:NH2	2.31	0.45
36:9:211:TYR:CE1	36:9:241:GLU:HB3	2.51	0.45
1:2:53:G:C2	1:2:54:C:C2	3.04	0.45
1:2:256:G:H2'	1:2:257:U:O4'	2.16	0.45
1:2:321:A:OP2	16:J:47:ARG:NH2	2.49	0.45
1:2:354:G:C2	1:2:355:C:C2	3.03	0.45
1:2:742:U:H3'	1:2:743:U:C6	2.51	0.45
1:2:1363:C:N4	31:5:821:G:OP1	2.46	0.45
1:2:1414:G:H21	14:G:79:HIS:CB	2.28	0.45
1:2:1467:U:O4	29:0:3:TRP:CH2	2.70	0.45
29:0:1:MET:O	29:0:4:LYS:N	2.49	0.45
1:2:4:C:N3	1:2:5:C:C5	2.84	0.45
1:2:43:A:O2'	1:2:302:A:H4'	2.15	0.45
1:2:1467:U:O4	29:0:3:TRP:CZ3	2.70	0.45
1:2:1489:A:O2'	1:2:1490:C:H5'	2.16	0.45
2:M:61:MET:HA	2:M:104:ALA:HB2	1.98	0.45
13:F:26:VAL:HG21	13:F:49:ILE:HG23	1.99	0.45
13:F:53:LEU:O	13:F:55:PRO:HD3	2.16	0.45
35:8:114:THR:HG22	35:8:127:CYS:HA	1.97	0.45
36:9:106:ILE:O	36:9:110:VAL:HG23	2.17	0.45
1:2:106:A:OP2	16:J:7:ARG:NH1	2.50	0.45
1:2:151:G:HO2'	14:G:64:ARG:HB3	1.80	0.45
1:2:672:G:N7	2:M:123:HIS:HA	2.31	0.45
1:2:836:G:OP2	15:I:76:LYS:HG3	2.16	0.45
1:2:945:G:H2'	1:2:946:G:O4'	2.17	0.45
1:2:1333:G:H5''	27:H:97:LYS:HD2	1.98	0.45
1:2:1334:A:OP2	27:H:48:HIS:HA	2.17	0.45
1:2:1347:U:C2'	1:2:1348:C:H5'	2.46	0.45
1:2:1409:G:C2	1:2:1410:G:C8	3.04	0.45
6:A:124:ILE:O	6:A:181:ARG:O	2.33	0.45
27:H:26:VAL:HG22	27:H:121:GLN:HB2	1.98	0.45
27:H:93:LEU:O	27:H:95:SER:N	2.48	0.45
1:2:414:G:C6	1:2:415:C:C4	3.05	0.45
1:2:474:G:C6	1:2:475:C:C4	3.04	0.45
1:2:973:U:H3'	1:2:974:G:H5''	1.98	0.45
17:C:6:UNK:O	17:C:10:UNK:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:64:TRP:HE3	21:P:52:PHE:HB3	1.81	0.45
20:O:134:ASN:O	20:O:135:PHE:CG	2.70	0.45
27:H:68:ILE:HG21	27:H:97:LYS:HG3	1.97	0.45
29:O:6:ILE:HG22	29:O:10:ILE:HD12	1.98	0.45
1:2:271:G:C5	1:2:272:C:C5	3.05	0.45
1:2:495:G:N3	1:2:496:C:C5	2.85	0.45
1:2:615:G:C6	1:2:698:A:C6	3.04	0.45
1:2:682:A:C8	4:Q:120:ARG:NH2	2.84	0.45
1:2:1032:A:OP1	13:F:84:ARG:NE	2.50	0.45
1:2:1344:U:H2'	1:2:1345:G:H8	1.80	0.45
1:2:1402:C:O3'	14:G:33:ARG:CZ	2.65	0.45
30:4:76:A:O3'	34:7:296:ALA:HB2	2.17	0.45
1:2:48:G:C2	1:2:49:C:C2	3.04	0.45
1:2:459:G:N3	1:2:459:G:C5'	2.80	0.45
1:2:949:G:H2'	1:2:950:C:OP2	2.16	0.45
7:B:104:PRO:HB3	7:B:109:PHE:CE2	2.52	0.45
23:T:24:LEU:HB3	23:T:28:PHE:CZ	2.52	0.45
1:2:643:G:C2	1:2:653:C:C4	3.05	0.45
1:2:740:G:C2	1:2:751:C:N3	2.85	0.45
1:2:788:C:C2	1:2:811:G:N2	2.85	0.45
1:2:878:U:C2	1:2:879:U:C5	3.05	0.45
1:2:1325:C:N4	1:2:1326:G:O6	2.50	0.45
1:2:1363:C:O5'	1:2:1363:C:C6	2.69	0.45
1:2:1483:U:O2'	1:2:1484:C:H3'	2.17	0.45
5:R:50:GLU:HA	5:R:69:LYS:HA	1.98	0.45
6:A:68:PHE:HB3	6:A:80:THR:HG22	1.98	0.45
21:P:20:ARG:HA	21:P:26:GLN:O	2.15	0.45
27:H:13:HIS:ND1	28:K:46:LEU:HG	2.32	0.45
27:H:63:ILE:HD13	27:H:124:VAL:HG22	1.98	0.45
30:4:2:G:N1	30:4:71:C:O2	2.45	0.45
1:2:62:G:C8	1:2:63:G:N7	2.83	0.45
1:2:150:G:H5'	14:G:73:PRO:HB3	1.98	0.45
1:2:462:A:N6	11:D:18:TRP:CZ2	2.84	0.45
1:2:677:U:O4	1:2:1493:C:H4'	2.16	0.45
1:2:745:G:H2'	1:2:746:A:H5'	1.99	0.45
1:2:797:U:H2'	1:2:799:C:C5	2.52	0.45
1:2:932:C:H6	1:2:932:C:O5'	1.99	0.45
1:2:992:G:C6	1:2:993:C:C4	3.04	0.45
1:2:1132:C:H2'	1:2:1133:C:H6	1.81	0.45
1:2:1262:U:O2'	1:2:1263:C:OP1	2.22	0.45
4:Q:33:ILE:HA	4:Q:36:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:78:ILE:O	4:Q:81:ILE:HB	2.17	0.45
6:A:130:GLN:NE2	6:A:178:TYR:OH	2.50	0.45
19:L:44:ARG:HG2	19:L:67:ARG:HG2	1.98	0.45
30:4:5:G:C6	30:4:6:G:C5	3.05	0.45
34:7:51:TYR:CD2	34:7:294:LEU:HD13	2.52	0.45
1:2:8:U:C2	1:2:873:A:C6	3.01	0.44
1:2:603:G:C2	1:2:604:C:C2	3.06	0.44
1:2:685:G:N1	1:2:686:C:C4	2.84	0.44
1:2:813:G:C2	1:2:814:C:C2	3.05	0.44
1:2:820:G:C5	1:2:821:G:N7	2.85	0.44
1:2:895:C:H2'	1:2:896:A:H8	1.82	0.44
1:2:1134:G:OP1	27:H:55:HIS:NE2	2.50	0.44
1:2:1402:C:H2'	1:2:1403:U:C1'	2.44	0.44
24:U:80:ARG:HE	27:H:81:VAL:CG1	2.30	0.44
27:H:132:PRO:N	27:H:204:LYS:HG2	2.32	0.44
1:2:168:G:C2	1:2:195:C:O2	2.71	0.44
1:2:264:C:H2'	1:2:265:C:H6	1.82	0.44
1:2:296:A:H1'	1:2:518:U:O2	2.17	0.44
1:2:542:G:C2	1:2:543:C:C2	3.06	0.44
1:2:908:G:H2'	1:2:909:U:O4'	2.17	0.44
1:2:955:G:C2	1:2:956:C:C2	3.05	0.44
1:2:1169:C:O2'	1:2:1174:A:N6	2.51	0.44
6:A:18:TRP:CH2	6:A:36:PRO:HB3	2.53	0.44
14:G:84:VAL:HG12	14:G:85:ARG:N	2.33	0.44
35:8:92:ILE:O	35:8:96:MET:HB2	2.17	0.44
35:8:118:LYS:HG2	35:8:123:TRP:CE2	2.52	0.44
36:9:93:LYS:HA	36:9:96:GLN:HB2	1.99	0.44
1:2:10:G:C5	1:2:1356:A:N1	2.86	0.44
1:2:57:G:N7	1:2:58:U:C5	2.86	0.44
1:2:157:A:H8	1:2:159:C:C5	2.34	0.44
1:2:568:C:C2	1:2:569:G:C8	3.04	0.44
1:2:685:G:N2	1:2:686:C:C2	2.86	0.44
1:2:722:G:C5	1:2:723:G:N7	2.85	0.44
1:2:813:G:C5	1:2:814:C:C5	3.06	0.44
1:2:1000:G:H2'	1:2:1002:G:C8	2.52	0.44
1:2:1414:G:C2'	1:2:1415:U:H5'	2.47	0.44
6:A:135:ARG:O	6:A:138:ARG:HB2	2.18	0.44
7:B:78:LYS:HE2	7:B:194:GLU:O	2.17	0.44
13:F:131:TRP:H	13:F:139:HIS:HE1	1.65	0.44
34:7:256:LEU:HB3	34:7:387:ALA:HB2	1.99	0.44
34:7:388:VAL:HG13	34:7:393:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:94:C:H2'	1:2:95:G:O4'	2.17	0.44
1:2:168:G:C6	1:2:169:C:C4	3.05	0.44
1:2:419:G:N1	1:2:420:C:C4	2.85	0.44
1:2:454:G:H2'	1:2:455:C:H6	1.82	0.44
1:2:472:C:OP1	33:6:52:PRO:HB3	2.17	0.44
1:2:647:G:O6	1:2:742:U:C5'	2.65	0.44
1:2:648:A:C2	1:2:649:A:H1'	2.52	0.44
1:2:707:A:C4'	1:2:708:C:C2	3.01	0.44
1:2:782:A:H2'	1:2:783:G:O5'	2.18	0.44
1:2:1044:A:C2	1:2:1045:A:C5	3.05	0.44
1:2:1143:G:H3'	1:2:1144:G:H5''	1.98	0.44
1:2:1404:C:O4'	14:G:76:PRO:HB2	2.17	0.44
1:2:1412:A:C2	14:G:77:ASP:OD2	2.69	0.44
1:2:1462:A:N7	1:2:1486:A:N6	2.65	0.44
1:2:1464:C:C2	1:2:1465:C:C6	3.04	0.44
11:D:14:PRO:HD3	11:D:22:ARG:NH2	2.33	0.44
30:4:75:C:H5''	30:4:76:A:H5'	2.00	0.44
31:5:809:G:N3	31:5:810:G:C8	2.85	0.44
33:6:75:GLN:HG3	33:6:79:ARG:NH2	2.32	0.44
1:2:57:G:N7	1:2:58:U:C4	2.85	0.44
1:2:157:A:OP2	1:2:159:C:N4	2.51	0.44
1:2:257:U:C5	16:J:116:GLN:NE2	2.85	0.44
1:2:372:G:H2'	1:2:373:C:H6	1.82	0.44
1:2:531:G:C2'	1:2:532:C:O5'	2.65	0.44
1:2:853:G:H2'	1:2:854:C:C6	2.53	0.44
1:2:978:G:H2'	1:2:979:U:C6	2.52	0.44
1:2:1404:C:C2	1:2:1405:C:C6	3.06	0.44
1:2:1454:A:N1	1:2:1455:A:C5	2.86	0.44
7:B:104:PRO:CG	13:F:19:LYS:HE2	2.47	0.44
13:F:178:ALA:HB2	13:F:205:LEU:HD23	2.00	0.44
24:U:12:LEU:HA	24:U:136:LEU:CD1	2.48	0.44
30:4:12:G:O6	30:4:13:C:C4	2.71	0.44
36:9:111:SER:HA	36:9:160:TRP:HZ3	1.83	0.44
1:2:299:G:OP1	3:N:30:TYR:OH	2.35	0.44
1:2:323:A:N1	1:2:325:A:C2	2.85	0.44
1:2:839:G:H2'	1:2:840:C:O4'	2.17	0.44
1:2:905:A:H2'	1:2:906:G:C8	2.53	0.44
1:2:1058:G:C2	1:2:1059:C:C2	3.05	0.44
1:2:1264:G:N1	1:2:1265:G:N2	2.66	0.44
6:A:11:ASP:HA	6:A:15:LEU:HD13	1.99	0.44
1:2:2:U:C5	13:F:184:TRP:CE3	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:4:C:HO2'	1:2:5:C:C5'	2.30	0.44
1:2:20:G:H4'	1:2:477:G:N2	2.32	0.44
1:2:63:G:O2'	1:2:64:G:C8	2.62	0.44
1:2:263:C:H2'	1:2:264:C:C6	2.53	0.44
1:2:1197:C:P	27:H:88:ARG:NH1	2.90	0.44
1:2:1240:A:H5''	19:L:41:PRO:HD3	2.00	0.44
1:2:1283:G:H2'	1:2:1284:C:C6	2.52	0.44
1:2:1493:C:O2'	1:2:1494:C:O5'	2.36	0.44
34:7:37:HIS:O	34:7:41:LEU:N	2.48	0.44
1:2:458:G:C2'	1:2:459:G:H5''	2.47	0.44
1:2:533:C:N4	1:2:534:G:H1	2.14	0.44
1:2:836:G:H5'	15:I:4:LEU:HD11	2.00	0.44
1:2:1193:G:H2'	1:2:1194:C:H6	1.82	0.44
1:2:1284:C:H2'	1:2:1285:C:H6	1.83	0.44
6:A:45:ASN:HB3	6:A:46:ARG:NH1	2.33	0.44
7:B:75:TYR:HA	7:B:197:MET:SD	2.58	0.44
7:B:167:ILE:HA	7:B:170:ILE:HG22	2.00	0.44
13:F:5:TRP:HA	13:F:55:PRO:HB2	1.99	0.44
27:H:173:CYS:HA	27:H:178:MET:O	2.18	0.44
30:4:12:G:C6	30:4:13:C:C4	3.06	0.44
32:1:86:ALA:O	32:1:90:VAL:HG23	2.18	0.44
34:7:207:ARG:HH21	34:7:291:PRO:C	2.21	0.44
34:7:323:VAL:HG13	34:7:389:TRP:HA	2.00	0.44
1:2:4:C:C2	1:2:5:C:C6	3.06	0.44
1:2:87:C:C4	1:2:88:G:C8	3.05	0.44
1:2:603:G:H2'	1:2:604:C:O4'	2.17	0.44
1:2:640:U:O2	1:2:641:A:N7	2.51	0.44
1:2:643:G:C2	1:2:644:G:C4	3.05	0.44
1:2:649:A:C2	1:2:740:G:O2'	2.66	0.44
1:2:772:G:O2'	1:2:774:U:OP2	2.25	0.44
1:2:878:U:N3	1:2:879:U:C5	2.86	0.44
1:2:901:G:N1	1:2:1302:C:C4	2.86	0.44
1:2:1178:C:C4	1:2:1179:C:N4	2.86	0.44
1:2:1269:G:C5	1:2:1270:C:C5	3.06	0.44
1:2:1481:G:C6	1:2:1482:C:C4	3.06	0.44
3:N:93:ALA:O	3:N:95:LYS:N	2.51	0.44
30:4:22:G:C2	30:4:23:C:C2	3.05	0.44
33:6:35:GLY:HA2	33:6:51:ILE:HD12	2.00	0.44
34:7:41:LEU:N	34:7:41:LEU:HD23	2.33	0.44
36:9:15:LEU:HD11	36:9:31:LEU:HD22	1.99	0.44
1:2:4:C:N3	1:2:5:C:C4	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:82:G:C5	1:2:83:C:C5	3.06	0.43
1:2:126:G:C2	1:2:219:C:N3	2.85	0.43
1:2:723:G:C6	1:2:724:C:C4	3.06	0.43
1:2:1013:G:H4'	19:L:58:SER:O	2.18	0.43
1:2:1313:G:C6	1:2:1314:C:C4	3.05	0.43
1:2:1327:C:O2'	19:L:48:THR:HB	2.18	0.43
1:2:1341:C:H1'	25:X:20:THR:CG2	2.48	0.43
1:2:1403:U:H2'	1:2:1403:U:O2	2.18	0.43
1:2:1454:A:C2	1:2:1455:A:C4	3.06	0.43
31:5:809:G:C4	31:5:810:G:N7	2.86	0.43
34:7:38:SER:C	34:7:40:GLU:H	2.20	0.43
1:2:13:C:C4	1:2:14:C:C5	3.05	0.43
1:2:90:C:O2'	1:2:375:G:OP1	2.36	0.43
1:2:152:G:C4'	14:G:64:ARG:HD2	2.45	0.43
1:2:441:U:N3	1:2:442:C:C4	2.86	0.43
1:2:884:G:H8	1:2:884:G:O5'	2.01	0.43
1:2:888:A:C2'	1:2:889:G:H5'	2.48	0.43
1:2:906:G:H2'	1:2:907:C:O4'	2.18	0.43
1:2:1024:G:C5	1:2:1025:U:C4	3.06	0.43
1:2:1236:G:H2'	1:2:1237:G:O4'	2.17	0.43
1:2:1312:C:P	27:H:78:HIS:O	2.76	0.43
1:2:1385:U:C2	1:2:1386:C:C5	3.06	0.43
34:7:59:CYS:HG	34:7:74:CYS:CB	2.31	0.43
1:2:72:C:H3'	1:2:73:U:H6	1.84	0.43
1:2:641:A:H4'	1:2:642:G:O5'	2.18	0.43
1:2:830:A:N7	1:2:832:G:C8	2.86	0.43
1:2:935:G:N1	1:2:1323:A:C6	2.86	0.43
1:2:1260:G:O2'	1:2:1261:U:OP2	2.35	0.43
1:2:1352:G:H2'	1:2:1353:C:C6	2.53	0.43
1:2:1391:U:H2'	1:2:1392:G:O4'	2.18	0.43
1:2:1414:G:C8	1:2:1414:G:O5'	2.72	0.43
1:2:1414:G:C5	1:2:1415:U:C4	3.06	0.43
1:2:1451:C:OP2	32:1:38:LYS:NZ	2.51	0.43
2:M:85:ALA:HB1	2:M:86:PRO:HD2	2.01	0.43
3:N:11:PHE:CZ	5:R:54:TYR:CZ	3.06	0.43
15:I:81:VAL:HG21	15:I:125:LEU:HD23	2.00	0.43
34:7:25:LEU:HD13	34:7:183:VAL:HG21	2.00	0.43
36:9:162:LYS:HB2	36:9:163:PRO:HD3	2.01	0.43
1:2:37:G:C2	1:2:397:C:C2	3.07	0.43
1:2:122:C:N3	1:2:223:G:C2	2.86	0.43
1:2:806:G:H2'	1:2:807:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:880:G:C6	1:2:881:G:C6	3.06	0.43
1:2:881:G:C2	1:2:882:C:C2	3.06	0.43
1:2:1193:G:C6	1:2:1194:C:C4	3.06	0.43
1:2:1372:C:H42	1:2:1443:G:H1	1.66	0.43
1:2:1472:G:C6	1:2:1473:A:C6	3.06	0.43
14:G:34:ILE:HG22	14:G:110:ASN:ND2	2.33	0.43
15:I:102:LEU:HB3	15:I:113:HIS:HB2	2.00	0.43
32:1:32:THR:HG22	32:1:40:MET:C	2.39	0.43
33:6:19:PRO:HD2	33:6:25:PHE:CZ	2.52	0.43
1:2:405:G:OP1	11:D:116:ARG:NH1	2.51	0.43
1:2:879:U:C4'	13:F:73:ARG:CZ	2.94	0.43
1:2:895:C:C2	1:2:896:A:C8	3.06	0.43
1:2:1028:C:C5'	7:B:128:ARG:NH2	2.81	0.43
1:2:1089:C:C4	1:2:1090:C:C5	3.06	0.43
1:2:1309:A:C2	1:2:1334:A:C4	3.06	0.43
1:2:1395:G:H5'	14:G:87:LEU:CD1	2.49	0.43
12:E:215:ILE:HG23	12:E:223:PHE:HB2	2.00	0.43
14:G:113:SER:HB3	14:G:114:PRO:CD	2.47	0.43
25:X:46:ARG:HH11	25:X:46:ARG:HB2	1.84	0.43
34:7:41:LEU:HD13	34:7:47:ILE:N	2.34	0.43
36:9:161:VAL:O	36:9:165:LEU:HG	2.19	0.43
1:2:106:A:C6	1:2:107:C:C2	3.06	0.43
1:2:434:A:C4	8:V:85:TYR:CD1	3.01	0.43
1:2:472:C:H2'	1:2:473:A:O4'	2.19	0.43
1:2:524:U:C5'	1:2:773:A:C5	3.02	0.43
1:2:921:G:H2'	1:2:922:G:O4'	2.18	0.43
1:2:1413:G:H5'	14:G:92:PRO:HG3	2.00	0.43
1:2:1468:A:H2'	1:2:1469:G:H8	1.82	0.43
1:2:1489:A:N1	1:2:1490:C:C4	2.87	0.43
2:M:15:GLY:O	2:M:79:VAL:HG13	2.18	0.43
3:N:72:ALA:CA	3:N:86:ALA:O	2.65	0.43
4:Q:149:ASP:H	4:Q:152:THR:HG22	1.84	0.43
8:V:28:GLU:CB	8:V:29:PRO:HD2	2.49	0.43
27:H:26:VAL:HG13	27:H:121:GLN:HG3	2.00	0.43
27:H:131:ALA:HB2	27:H:161:ALA:HB2	2.00	0.43
34:7:216:LEU:O	34:7:240:GLY:HA3	2.19	0.43
1:2:121:C:O2	1:2:122:C:C6	2.71	0.43
1:2:194:C:H4'	16:J:43:ARG:NH1	2.33	0.43
1:2:566:C:H4'	11:D:54:ARG:NH1	2.34	0.43
1:2:803:C:P	6:A:128:ARG:HH11	2.42	0.43
1:2:910:G:N7	20:O:132:ARG:NH1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1249:A:OP1	27:H:82:ALA:CB	2.66	0.43
2:M:31:THR:HG22	2:M:38:THR:HA	2.01	0.43
13:F:34:ILE:HD11	13:F:121:ILE:HD13	2.01	0.43
15:I:28:LYS:HB2	15:I:29:PRO:HD3	1.99	0.43
29:0:9:ARG:O	29:0:13:LEU:HG	2.19	0.43
30:4:4:G:C6	30:4:5:G:C5	3.07	0.43
30:4:76:A:O2'	34:7:296:ALA:HB3	2.19	0.43
34:7:257:PRO:HB3	34:7:325:VAL:HG13	2.00	0.43
1:2:1:A:P	13:F:166:VAL:CG1	3.07	0.43
1:2:6:G:C6	13:F:192:ARG:NH2	2.87	0.43
1:2:40:C:C2	1:2:41:C:C5	3.06	0.43
1:2:486:A:H2'	1:2:488:A:OP2	2.18	0.43
1:2:733:C:H2'	1:2:734:G:O4'	2.18	0.43
1:2:1036:G:C5	1:2:1037:U:C4	3.06	0.43
1:2:1394:G:H5''	14:G:104:LYS:HE3	2.00	0.43
1:2:1414:G:C4'	14:G:78:ILE:HG23	2.49	0.43
1:2:1475:C:H2'	1:2:1476:C:H6	1.82	0.43
6:A:121:ALA:HB3	6:A:141:MET:CE	2.49	0.43
7:B:173:ARG:HG2	7:B:184:SER:HA	2.01	0.43
12:E:195:ARG:HD3	12:E:195:ARG:N	2.34	0.43
13:F:214:SER:O	13:F:217:MET:HB2	2.19	0.43
24:U:136:LEU:O	24:U:140:LEU:HG	2.18	0.43
36:9:20:LYS:O	36:9:60:GLU:OE2	2.36	0.43
1:2:234:G:C5'	5:R:55:PHE:CZ	3.02	0.43
1:2:366:C:C2	1:2:388:G:N2	2.86	0.43
1:2:422:U:H5''	1:2:423:U:OP1	2.19	0.43
1:2:486:A:C6	1:2:489:C:C4	3.07	0.43
1:2:531:G:C5	1:2:532:C:C5	3.07	0.43
1:2:540:G:H4'	15:I:4:LEU:CB	2.47	0.43
1:2:605:C:H2'	1:2:606:U:C6	2.54	0.43
1:2:724:C:O3'	34:7:264:GLN:OE1	2.37	0.43
1:2:749:C:OP2	1:2:750:C:N4	2.51	0.43
1:2:798:U:O2	1:2:798:U:O4'	2.36	0.43
1:2:868:C:C4'	1:2:1373:A:O2'	2.66	0.43
1:2:1031:G:C2	1:2:1032:A:N1	2.87	0.43
1:2:1124:G:C6	1:2:1125:C:C4	3.07	0.43
1:2:1352:G:C2	1:2:1353:C:C2	3.07	0.43
1:2:1384:G:C2	1:2:1432:U:O2	2.72	0.43
1:2:1405:C:C4	1:2:1406:U:C5	3.06	0.43
1:2:1487:U:H3'	1:2:1487:U:H6	1.84	0.43
3:N:24:ARG:NE	3:N:30:TYR:CZ	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:104:PRO:HB3	7:B:109:PHE:CZ	2.53	0.43
13:F:196:ASN:O	13:F:199:LYS:N	2.51	0.43
25:X:7:TYR:CD2	25:X:60:THR:HG22	2.54	0.43
1:2:613:C:H2'	1:2:614:G:C8	2.54	0.43
1:2:642:G:C4	1:2:643:G:C8	3.07	0.43
1:2:677:U:N3	1:2:1493:C:C1'	2.81	0.43
1:2:811:G:C6	1:2:812:U:C4	3.06	0.43
1:2:1026:A:C6	1:2:1027:C:C4	3.07	0.43
1:2:1027:C:H4'	1:2:1053:A:N6	2.34	0.43
1:2:1179:C:H2'	1:2:1180:G:C8	2.53	0.43
1:2:1200:U:H5	27:H:92:SER:N	2.17	0.43
1:2:1267:U:H5''	20:O:125:PRO:HG3	2.01	0.43
1:2:1345:G:C5	1:2:1346:C:C5	3.07	0.43
1:2:1483:U:HO2'	1:2:1484:C:P	2.41	0.43
13:F:165:LEU:HD22	13:F:175:LEU:HD13	2.00	0.43
22:S:8:PHE:O	22:S:12:VAL:HG23	2.18	0.43
24:U:88:GLU:HG3	27:H:85:PHE:CE2	2.54	0.43
27:H:111:ILE:HG23	27:H:119:PRO:HB3	2.01	0.43
34:7:22:LYS:O	34:7:26:VAL:HG23	2.18	0.43
1:2:94:C:O2'	12:E:9:HIS:CE1	2.72	0.42
1:2:108:G:C6	1:2:109:U:C4	3.07	0.42
1:2:174:G:C2	1:2:189:C:C2	3.07	0.42
1:2:180:G:C2	1:2:184:G:C6	3.07	0.42
1:2:248:U:H2'	1:2:249:U:C5	2.54	0.42
1:2:419:G:C6	1:2:420:C:C4	3.07	0.42
1:2:531:G:C4	1:2:532:C:C6	3.07	0.42
1:2:1075:A:H2'	1:2:1076:G:O4'	2.18	0.42
1:2:1197:C:P	27:H:88:ARG:HH12	2.42	0.42
1:2:1307:G:HO2'	1:2:1333:G:H1	1.65	0.42
1:2:1312:C:H5'	27:H:80:LYS:HE3	2.01	0.42
13:F:143:PHE:CE2	15:I:96:ALA:HB3	2.54	0.42
14:G:94:PHE:HD2	14:G:105:LYS:HG2	1.84	0.42
30:4:58:A:C6	30:4:61:C:C2	3.06	0.42
34:7:38:SER:C	34:7:40:GLU:N	2.72	0.42
34:7:358:MET:HA	34:7:367:LEU:HD23	2.01	0.42
1:2:4:C:H2'	1:2:5:C:C6	2.54	0.42
1:2:323:A:C2	1:2:325:A:N3	2.87	0.42
1:2:766:G:O2'	1:2:767:U:OP2	2.30	0.42
1:2:786:G:H1	1:2:812:U:H3	1.67	0.42
1:2:839:G:C4	1:2:840:C:C6	3.07	0.42
1:2:1120:G:N1	1:2:1121:C:C4	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1203:G:C2	1:2:1255:C:C2	3.07	0.42
4:Q:4:MET:HA	4:Q:7:ARG:CG	2.49	0.42
4:Q:115:ASP:O	4:Q:119:MET:HB2	2.18	0.42
16:J:11:LYS:C	16:J:13:SER:H	2.22	0.42
25:X:58:ARG:NH2	27:H:134:GLU:OE2	2.52	0.42
34:7:38:SER:HB2	34:7:41:LEU:HD21	2.00	0.42
34:7:92:ILE:CD1	34:7:294:LEU:HD12	2.49	0.42
36:9:175:ARG:HA	36:9:175:ARG:HE	1.83	0.42
1:2:105:C:H4'	1:2:106:A:OP1	2.19	0.42
1:2:350:G:C6	1:2:351:C:C4	3.07	0.42
1:2:354:G:H2'	1:2:355:C:C6	2.54	0.42
1:2:540:G:C4'	15:I:4:LEU:HB2	2.45	0.42
1:2:641:A:C2	1:2:642:G:C4	3.05	0.42
1:2:898:G:H2'	1:2:899:G:C8	2.53	0.42
1:2:974:G:C8	1:2:974:G:O5'	2.73	0.42
1:2:1142:G:H5''	1:2:1143:G:OP1	2.19	0.42
1:2:1184:U:H4'	1:2:1185:A:OP1	2.19	0.42
1:2:1275:U:C2	1:2:1279:A:N6	2.87	0.42
1:2:1283:G:C6	1:2:1284:C:N4	2.87	0.42
1:2:1317:G:OP1	1:2:1319:C:N4	2.52	0.42
1:2:1348:C:O5'	1:2:1348:C:H6	2.00	0.42
5:R:91:THR:OG1	5:R:92:ARG:N	2.52	0.42
12:E:19:TRP:CD1	12:E:19:TRP:N	2.87	0.42
13:F:123:GLU:O	13:F:209:ASN:ND2	2.52	0.42
19:L:16:LEU:CD2	19:L:69:HIS:HB2	2.49	0.42
23:T:44:GLN:HE22	23:T:47:LEU:HD23	1.85	0.42
27:H:21:TRP:CD1	27:H:119:PRO:CD	3.01	0.42
27:H:79:TYR:O	27:H:88:ARG:HG2	2.19	0.42
30:4:76:A:H1'	34:7:296:ALA:HB3	2.00	0.42
34:7:305:LEU:HD23	36:9:186:ARG:NH1	2.33	0.42
1:2:22:G:H2'	1:2:23:G:O5'	2.19	0.42
1:2:262:G:O2'	1:2:264:C:OP2	2.38	0.42
1:2:426:C:C2	1:2:445:G:N2	2.87	0.42
1:2:457:G:H1'	1:2:488:A:C6	2.54	0.42
1:2:495:G:N3	1:2:496:C:C6	2.87	0.42
1:2:744:A:O2'	32:1:34:ARG:NE	2.52	0.42
1:2:898:G:C2	1:2:899:G:C6	3.07	0.42
3:N:51:ARG:HA	3:N:104:ILE:HA	2.01	0.42
6:A:57:GLY:O	6:A:61:LYS:HG2	2.19	0.42
11:D:136:ILE:HG22	11:D:137:ILE:N	2.35	0.42
15:I:95:PRO:HD3	15:I:130:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:30:ALA:HA	23:T:33:ARG:HD3	2.02	0.42
34:7:159:ALA:HB3	35:8:15:TYR:OH	2.19	0.42
1:2:4:C:O2'	1:2:5:C:O5'	2.37	0.42
1:2:152:G:C1'	14:G:64:ARG:NH1	2.83	0.42
1:2:597:C:C4	1:2:598:U:C5	3.08	0.42
1:2:787:U:H2'	1:2:788:C:C6	2.54	0.42
1:2:901:G:C2	1:2:1302:C:C2	3.07	0.42
1:2:977:G:O2'	1:2:978:G:OP2	2.34	0.42
3:N:30:TYR:CE2	3:N:34:VAL:HG21	2.55	0.42
25:X:18:THR:C	25:X:24:VAL:HG13	2.39	0.42
34:7:41:LEU:HD22	34:7:47:ILE:CG1	2.49	0.42
34:7:48:LYS:HB3	34:7:48:LYS:HE2	1.91	0.42
34:7:274:THR:HG22	34:7:275:LYS:N	2.34	0.42
35:8:69:LEU:CD1	35:8:83:ILE:HD13	2.50	0.42
1:2:265:C:H2'	1:2:266:A:C8	2.55	0.42
1:2:276:A:C5	5:R:67:ARG:HD2	2.54	0.42
1:2:314:G:H1'	1:2:1424:G:H5'	2.01	0.42
1:2:354:G:C6	1:2:355:C:C4	3.07	0.42
1:2:457:G:C4	1:2:488:A:C2	3.07	0.42
1:2:523:C:O4'	1:2:774:U:C2	2.73	0.42
1:2:649:A:C6	1:2:650:A:C6	3.08	0.42
1:2:732:G:H2'	1:2:733:C:O4'	2.20	0.42
1:2:853:G:C2	1:2:854:C:C2	3.08	0.42
1:2:889:G:N2	1:2:890:C:C2	2.88	0.42
1:2:984:C:H1'	26:Y:32:ALA:HB2	2.01	0.42
13:F:153:ARG:HD2	13:F:153:ARG:N	2.34	0.42
15:I:89:TRP:CZ3	15:I:93:PHE:CE1	3.08	0.42
27:H:108:PHE:HA	27:H:111:ILE:HG22	2.02	0.42
1:2:22:G:H5'	11:D:15:PRO:O	2.20	0.42
1:2:97:C:H2'	1:2:98:U:C6	2.55	0.42
1:2:649:A:C2	1:2:741:A:O4'	2.72	0.42
1:2:869:U:O2'	1:2:1444:G:O2'	2.22	0.42
1:2:888:A:H2'	1:2:889:G:H5'	2.01	0.42
1:2:1115:G:C6	1:2:1116:G:C5	3.08	0.42
1:2:1401:U:N3	1:2:1402:C:C4	2.88	0.42
3:N:24:ARG:HG2	3:N:30:TYR:CD2	2.55	0.42
4:Q:108:HIS:CE1	4:Q:112:HIS:CD2	3.07	0.42
7:B:104:PRO:HG2	13:F:19:LYS:CE	2.49	0.42
8:V:32:SER:O	8:V:35:ASP:N	2.52	0.42
13:F:46:GLU:HB2	13:F:49:ILE:CD1	2.49	0.42
30:4:9:G:O4'	30:4:46:A:N3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:5:812:G:C2'	31:5:813:A:O4'	2.67	0.42
34:7:98:GLU:HG3	34:7:99:VAL:HG23	2.00	0.42
1:2:185:G:H2'	1:2:186:U:O4'	2.19	0.42
1:2:229:G:H2'	1:2:230:C:C6	2.54	0.42
1:2:238:G:H8	1:2:238:G:O5'	2.03	0.42
1:2:253:G:C6	1:2:254:G:C5	3.08	0.42
1:2:372:G:H2'	1:2:373:C:O4'	2.19	0.42
1:2:458:G:H3'	1:2:459:G:H5''	2.00	0.42
1:2:643:G:N1	1:2:653:C:C4	2.87	0.42
1:2:858:A:H2'	1:2:859:A:C8	2.55	0.42
1:2:1031:G:C6	1:2:1032:A:N6	2.88	0.42
1:2:1120:G:N3	1:2:1121:C:C6	2.88	0.42
1:2:1253:G:C2	1:2:1254:C:C2	3.08	0.42
1:2:1414:G:H5''	14:G:86:VAL:CG2	2.49	0.42
1:2:1479:C:C4	1:2:1480:G:N7	2.88	0.42
5:R:43:PRO:HB2	5:R:46:THR:HB	2.01	0.42
13:F:143:PHE:CE1	13:F:213:ILE:HD11	2.53	0.42
16:J:113:ARG:O	16:J:117:ASP:OD2	2.38	0.42
24:U:5:TYR:O	28:K:32:PRO:HD2	2.20	0.42
27:H:61:VAL:CG1	27:H:66:ARG:HG2	2.49	0.42
30:4:62:C:H2'	30:4:63:G:C8	2.55	0.42
34:7:186:LEU:HD11	35:8:124:TYR:CE2	2.54	0.42
36:9:9:PRO:O	36:9:71:VAL:HG21	2.19	0.42
1:2:29:G:C2	1:2:30:C:C2	3.08	0.42
1:2:387:G:C2	1:2:388:G:C4	3.08	0.42
1:2:552:C:H4'	15:I:122:GLY:C	2.40	0.42
1:2:563:U:C4	1:2:564:C:C5	3.08	0.42
1:2:695:G:H2'	1:2:696:G:O4'	2.20	0.42
1:2:889:G:C6	1:2:890:C:C4	3.08	0.42
1:2:985:C:H1'	26:Y:41:GLY:HA3	2.01	0.42
1:2:1200:U:OP1	27:H:179:SER:HA	2.19	0.42
14:G:40:ALA:HB3	14:G:59:VAL:CG1	2.42	0.42
27:H:48:HIS:HB3	28:K:10:ARG:NH2	2.34	0.42
1:2:239:A:C2	1:2:241:U:H2'	2.55	0.42
1:2:297:G:C5	1:2:298:C:C5	3.08	0.42
1:2:412:U:C5	1:2:413:G:H1'	2.54	0.42
1:2:535:U:C2	1:2:536:A:C8	3.07	0.42
1:2:647:G:C6	1:2:648:A:C5	3.08	0.42
1:2:707:A:O4'	1:2:708:C:N3	2.52	0.42
1:2:846:G:H3'	1:2:847:A:H2'	2.01	0.42
1:2:932:C:H3'	1:2:933:G:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:128:LYS:HE2	3:N:131:ARG:HA	2.02	0.42
7:B:57:LYS:HB3	17:C:26:UNK:CB	2.50	0.42
19:L:45:ILE:HG23	19:L:66:LEU:O	2.20	0.42
1:2:81:C:N3	1:2:82:G:N7	2.68	0.41
1:2:130:G:C2	1:2:163:C:C2	3.08	0.41
1:2:330:U:O4	1:2:331:C:N4	2.53	0.41
1:2:521:G:N2	1:2:522:C:C2	2.88	0.41
1:2:531:G:N2	1:2:532:C:C2	2.88	0.41
1:2:566:C:C4'	11:D:54:ARG:CZ	2.98	0.41
1:2:574:A:H2'	1:2:575:A:C8	2.55	0.41
1:2:599:G:C4	1:2:600:C:C6	3.08	0.41
1:2:616:G:N2	1:2:697:A:C2	2.89	0.41
1:2:853:G:C6	1:2:854:C:C4	3.08	0.41
1:2:867:A:H2'	1:2:1374:C:H4'	2.01	0.41
1:2:1117:A:O4'	1:2:1118:C:C2	2.73	0.41
1:2:1341:C:C1'	25:X:20:THR:HG1	2.33	0.41
1:2:1447:A:H1'	33:6:34:ALA:HB2	2.01	0.41
1:2:1470:G:N2	1:2:1476:C:C2	2.87	0.41
6:A:12:LYS:N	6:A:13:TRP:HA	2.35	0.41
6:A:70:VAL:O	6:A:70:VAL:HG23	2.19	0.41
11:D:111:LYS:HA	11:D:177:GLY:CA	2.51	0.41
13:F:165:LEU:HG	13:F:181:GLN:O	2.19	0.41
30:4:73:A:N3	30:4:74:C:H5	2.17	0.41
30:4:76:A:HO3'	37:7:501:MET:HA	1.78	0.41
34:7:273:PHE:O	36:9:190:PRO:HA	2.20	0.41
1:2:432:G:C6	1:2:433:U:C5	3.08	0.41
1:2:498:C:C2	1:2:499:G:C8	3.08	0.41
1:2:1307:G:C2'	1:2:1308:U:OP2	2.68	0.41
1:2:1313:G:N2	1:2:1314:C:C2	2.88	0.41
1:2:1334:A:H1'	27:H:69:ASN:ND2	2.35	0.41
1:2:1345:G:C2	1:2:1346:C:C2	3.08	0.41
1:2:1390:G:H2'	1:2:1391:U:O4'	2.20	0.41
19:L:45:ILE:HD12	19:L:66:LEU:HB3	2.01	0.41
20:O:78:ALA:CB	24:U:35:VAL:HG21	2.50	0.41
30:4:15:G:C5	30:4:16:C:H5	2.36	0.41
30:4:22:G:C6	30:4:23:C:C4	3.08	0.41
35:8:33:MET:CG	35:8:44:ILE:HG23	2.50	0.41
36:9:114:LEU:HD21	36:9:163:PRO:HG2	2.02	0.41
36:9:114:LEU:HD13	36:9:159:ILE:HG22	2.01	0.41
1:2:234:G:O2'	1:2:235:G:H5'	2.20	0.41
1:2:318:C:H2'	1:2:319:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:355:C:H2'	1:2:356:G:H8	1.85	0.41
1:2:528:G:HO2'	1:2:529:C:P	2.43	0.41
1:2:832:G:C6	1:2:833:C:C4	3.08	0.41
1:2:861:G:C2	1:2:862:C:C2	3.08	0.41
1:2:955:G:C5	1:2:956:C:C4	3.08	0.41
1:2:1112:G:H5''	19:L:13:VAL:HG13	2.01	0.41
1:2:1161:A:H1'	1:2:1162:G:OP2	2.20	0.41
1:2:1193:G:C4	1:2:1194:C:C5	3.09	0.41
1:2:1291:G:C2'	1:2:1292:A:OP2	2.68	0.41
1:2:1379:G:C6	1:2:1380:C:N3	2.88	0.41
1:2:1466:G:H2'	1:2:1467:U:O4'	2.21	0.41
13:F:173:LYS:O	13:F:177:LEU:HG	2.20	0.41
35:8:47:PHE:CE2	35:8:81:LEU:HD22	2.56	0.41
1:2:66:G:H2'	1:2:67:C:O4'	2.21	0.41
1:2:779:G:C2	1:2:780:C:C2	3.09	0.41
1:2:782:A:C2'	1:2:783:G:O5'	2.69	0.41
1:2:837:C:P	3:N:7:PRO:HA	2.61	0.41
1:2:874:G:N2	1:2:875:G:C4	2.89	0.41
1:2:1275:U:O4	1:2:1276:G:C6	2.73	0.41
1:2:1275:U:C4	1:2:1276:G:N1	2.88	0.41
1:2:1395:G:H8	1:2:1395:G:O5'	2.02	0.41
3:N:19:LYS:O	3:N:23:PHE:CD2	2.74	0.41
8:V:57:ARG:HH21	8:V:58:SER:C	2.23	0.41
10:Z:25:LEU:HD12	10:Z:30:TYR:CE1	2.56	0.41
13:F:119:LEU:H	13:F:119:LEU:HD22	1.84	0.41
14:G:67:THR:HG23	14:G:118:GLN:HE22	1.85	0.41
18:3:58:ASP:HA	18:3:59:PRO:C	2.40	0.41
30:4:43:A:H2'	30:4:44:A:C8	2.55	0.41
32:1:23:GLU:HB2	32:1:50:VAL:HG11	2.02	0.41
1:2:10:G:C8	1:2:1356:A:C4	3.08	0.41
1:2:87:C:H2'	1:2:88:G:C5'	2.51	0.41
1:2:459:G:C2	1:2:460:C:C2	3.08	0.41
1:2:1317:G:C6	1:2:1318:U:N3	2.89	0.41
1:2:1414:G:H5''	14:G:86:VAL:HG22	2.03	0.41
1:2:1451:C:O2'	32:1:67:GLY:N	2.50	0.41
8:V:54:GLN:O	8:V:55:TYR:C	2.58	0.41
11:D:105:LEU:HA	11:D:144:VAL:HG21	2.00	0.41
12:E:179:PHE:HB3	12:E:232:VAL:HG21	2.03	0.41
14:G:103:ARG:HG2	14:G:105:LYS:HD3	2.03	0.41
14:G:108:ARG:HH11	14:G:109:GLY:N	2.18	0.41
1:2:164:A:H2'	1:2:165:U:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:246:A:O2'	1:2:247:G:OP2	2.33	0.41
1:2:480:G:C2	1:2:481:C:C2	3.08	0.41
1:2:1189:G:OP1	20:O:137:ARG:HA	2.20	0.41
1:2:1312:C:C5'	27:H:80:LYS:HB3	2.51	0.41
1:2:1370:U:O2	1:2:1370:U:H2'	2.20	0.41
2:M:124:ASP:CG	2:M:125:GLY:N	2.74	0.41
7:B:52:LEU:O	7:B:52:LEU:HD13	2.20	0.41
14:G:52:GLY:HA2	14:G:54:GLU:HB2	2.02	0.41
28:K:13:ALA:HA	28:K:68:GLY:HA3	2.01	0.41
34:7:22:LYS:N	39:7:503:GNP:O1B	2.54	0.41
34:7:163:TYR:CG	35:8:7:TYR:CE2	3.08	0.41
1:2:14:C:H2'	1:2:15:U:C6	2.55	0.41
1:2:502:U:C2	1:2:503:G:C8	3.09	0.41
1:2:895:C:H2'	1:2:896:A:C8	2.56	0.41
1:2:944:C:C2	1:2:1181:G:N2	2.89	0.41
1:2:1344:U:H2'	1:2:1345:G:C8	2.55	0.41
1:2:1394:G:H5''	14:G:104:LYS:HE2	2.03	0.41
13:F:196:ASN:O	13:F:197:PHE:C	2.59	0.41
15:I:36:GLU:O	15:I:39:ARG:HB3	2.21	0.41
22:S:3:LYS:HD3	22:S:3:LYS:C	2.41	0.41
25:X:11:VAL:HA	25:X:29:VAL:HA	2.01	0.41
36:9:114:LEU:HD21	36:9:163:PRO:CG	2.50	0.41
1:2:314:G:N2	1:2:332:C:C2	2.88	0.41
1:2:368:C:N4	1:2:384:G:OP2	2.53	0.41
1:2:457:G:C2	1:2:458:G:C4	3.09	0.41
1:2:641:A:C5'	2:M:46:MET:HE3	2.51	0.41
1:2:1041:C:C4'	25:X:71:ARG:NH2	2.84	0.41
1:2:1372:C:O2'	3:N:121:GLY:HA2	2.21	0.41
1:2:1457:A:N3	1:2:1457:A:C2'	2.84	0.41
12:E:45:LEU:HD12	12:E:83:PHE:CB	2.49	0.41
13:F:175:LEU:O	13:F:178:ALA:HB3	2.20	0.41
13:F:191:THR:HG23	13:F:197:PHE:CG	2.55	0.41
13:F:201:VAL:HG22	13:F:205:LEU:HD13	2.02	0.41
14:G:10:ASP:HA	14:G:123:LEU:HB2	2.02	0.41
18:3:26:ALA:HB2	18:3:101:ILE:HD12	2.02	0.41
27:H:26:VAL:CG2	27:H:120:ILE:HG23	2.50	0.41
30:4:12:G:C6	30:4:13:C:C2	3.09	0.41
30:4:21:A:C5	30:4:48:C:C4	3.09	0.41
1:2:127:G:O2'	1:2:198:A:N1	2.49	0.41
1:2:387:G:C6	1:2:388:G:C5	3.08	0.41
1:2:605:C:O2'	1:2:606:U:O5'	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:610:G:C4	1:2:611:A:C8	3.09	0.41
1:2:677:U:C2	1:2:1493:C:O2'	2.58	0.41
1:2:732:G:C5	1:2:733:C:C5	3.09	0.41
1:2:766:G:O2'	1:2:767:U:P	2.79	0.41
1:2:1072:C:N3	1:2:1114:G:C2	2.89	0.41
12:E:158:TYR:O	12:E:162:TYR:HE1	2.04	0.41
13:F:40:ARG:HB3	13:F:42:TYR:CD1	2.56	0.41
13:F:108:ILE:HG23	13:F:109:ALA:N	2.36	0.41
16:J:4:TRP:HB2	16:J:5:GLN:HA	2.03	0.41
27:H:88:ARG:O	27:H:95:SER:OG	2.39	0.41
28:K:19:ILE:HG23	28:K:19:ILE:O	2.20	0.41
34:7:51:TYR:CD2	34:7:294:LEU:CD1	3.04	0.41
34:7:133:PHE:O	34:7:136:LEU:HB2	2.21	0.41
34:7:151:VAL:HG21	35:8:14:LEU:HD13	2.03	0.41
34:7:235:GLY:HA3	34:7:299:THR:O	2.21	0.41
35:8:40:ASN:HA	35:8:86:LYS:HB2	2.03	0.41
36:9:17:ALA:HB1	36:9:29:VAL:HG22	2.02	0.41
1:2:62:G:N7	1:2:63:G:C8	2.89	0.41
1:2:258:A:H2'	1:2:259:A:C8	2.56	0.41
1:2:330:U:C4	1:2:331:C:C4	3.09	0.41
1:2:556:G:N2	1:2:590:G:C4	2.89	0.41
1:2:649:A:N3	1:2:741:A:H4'	2.36	0.41
1:2:703:U:O2'	4:Q:51:GLY:HA3	2.21	0.41
1:2:710:G:H2'	1:2:711:U:O4'	2.22	0.41
1:2:1175:C:O2	1:2:1175:C:H2'	2.20	0.41
1:2:1383:A:C2	1:2:1384:G:C4	3.09	0.41
1:2:1428:G:C6	1:2:1429:G:C5	3.09	0.41
13:F:48:GLU:O	13:F:49:ILE:C	2.59	0.41
13:F:86:LEU:HD21	13:F:195:VAL:HG22	2.03	0.41
13:F:128:CYS:SG	13:F:138:PRO:HG3	2.60	0.41
19:L:50:ARG:HB2	21:P:40:ARG:HD2	2.03	0.41
19:L:51:LYS:HA	21:P:44:ARG:HD2	2.02	0.41
34:7:20:HIS:O	34:7:149:ASN:ND2	2.50	0.41
1:2:276:A:C4'	3:N:14:ARG:NH2	2.80	0.40
1:2:298:C:H4'	3:N:24:ARG:HH22	1.86	0.40
1:2:451:A:C6	1:2:500:A:C8	3.09	0.40
1:2:455:C:H2'	1:2:456:U:H6	1.86	0.40
1:2:612:C:H2'	1:2:613:C:H6	1.86	0.40
1:2:690:C:C2	1:2:691:G:C8	3.09	0.40
1:2:841:C:O2'	1:2:842:U:H5'	2.20	0.40
1:2:1169:C:HO2'	1:2:1174:A:N6	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1195:U:P	27:H:78:HIS:HA	2.61	0.40
1:2:1413:G:N2	14:G:77:ASP:OD1	2.51	0.40
10:Z:151:LEU:HG	10:Z:152:ALA:N	2.36	0.40
13:F:54:LEU:HD23	13:F:54:LEU:HA	1.93	0.40
13:F:163:LEU:HD11	13:F:184:TRP:CZ2	2.56	0.40
24:U:7:VAL:HG11	24:U:136:LEU:HD13	2.04	0.40
27:H:174:TYR:CD2	27:H:175:ARG:HD2	2.56	0.40
1:2:239:A:H4'	1:2:240:U:H5'	2.02	0.40
1:2:329:G:C3'	14:G:103:ARG:HH12	2.34	0.40
1:2:540:G:H5'	15:I:4:LEU:HB2	2.02	0.40
1:2:621:G:C2	1:2:622:C:C2	3.08	0.40
1:2:643:G:N1	1:2:644:G:C4	2.89	0.40
1:2:822:A:H2'	1:2:823:A:N9	2.32	0.40
1:2:832:G:C2	1:2:833:C:C2	3.09	0.40
1:2:1128:U:O2	1:2:1128:U:O4'	2.38	0.40
1:2:1269:G:C2	1:2:1270:C:C2	3.09	0.40
1:2:1344:U:C2	1:2:1345:G:C8	3.09	0.40
1:2:1379:G:C2	1:2:1380:C:C2	3.09	0.40
1:2:1413:G:N2	14:G:77:ASP:OD2	2.54	0.40
3:N:42:ASP:HB3	3:N:123:ARG:NH2	2.36	0.40
6:A:10:ARG:CZ	36:9:92:LYS:HB2	2.52	0.40
34:7:214:VAL:HB	34:7:244:GLN:HG2	2.03	0.40
35:8:69:LEU:HD22	35:8:87:PHE:CD2	2.56	0.40
36:9:140:ILE:HA	36:9:143:ALA:HB3	2.03	0.40
1:2:271:G:C2	1:2:272:C:C6	3.10	0.40
1:2:358:G:H5'	3:N:79:LYS:HB2	2.03	0.40
1:2:389:G:C2	1:2:390:G:C8	3.10	0.40
1:2:430:G:C6	1:2:431:U:H1'	2.56	0.40
1:2:486:A:C2	1:2:489:C:C5	3.09	0.40
1:2:1034:G:OP1	13:F:73:ARG:NH1	2.53	0.40
1:2:1186:C:C4	20:O:132:ARG:HA	2.56	0.40
1:2:1205:G:OP1	24:U:54:ARG:NH2	2.54	0.40
1:2:1386:C:C2	1:2:1387:C:C5	3.09	0.40
1:2:1403:U:N1	14:G:77:ASP:OD1	2.54	0.40
6:A:11:ASP:C	6:A:13:TRP:HA	2.42	0.40
6:A:135:ARG:HA	6:A:138:ARG:CG	2.51	0.40
11:D:160:PHE:CZ	11:D:168:ARG:HG2	2.56	0.40
30:4:9:G:C5	30:4:46:A:C6	3.09	0.40
35:8:36:LEU:HD11	35:8:45:ARG:CZ	2.52	0.40
1:2:1:A:P	13:F:166:VAL:HG11	2.62	0.40
1:2:375:G:O2'	1:2:376:G:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:430:G:O6	1:2:440:C:N4	2.51	0.40
1:2:608:G:C2	1:2:707:A:C4	3.09	0.40
1:2:732:G:C2	1:2:733:C:C2	3.09	0.40
1:2:811:G:C5	1:2:812:U:C5	3.10	0.40
1:2:897:A:N6	1:2:898:G:N1	2.70	0.40
1:2:1195:U:O4'	24:U:85:HIS:O	2.40	0.40
1:2:1306:A:H1'	1:2:1308:U:C5	2.57	0.40
3:N:93:ALA:O	3:N:96:PHE:N	2.55	0.40
10:Z:8:ILE:O	10:Z:12:VAL:HG23	2.21	0.40
11:D:14:PRO:HD3	11:D:22:ARG:CZ	2.51	0.40
15:I:30:ALA:HB3	15:I:59:GLY:C	2.42	0.40
18:3:41:LYS:HG2	26:Y:15:VAL:HG11	2.04	0.40
19:L:50:ARG:HA	19:L:61:PHE:CD1	2.57	0.40
21:P:17:GLY:HA2	21:P:27:TYR:HB3	2.04	0.40
1:2:57:G:C8	1:2:58:U:C5	3.09	0.40
1:2:93:A:C2'	1:2:322:G:N2	2.84	0.40
1:2:389:G:C6	1:2:390:G:N7	2.89	0.40
1:2:419:G:C6	1:2:420:C:C5	3.09	0.40
1:2:461:A:HO2'	1:2:462:A:H8	1.67	0.40
1:2:509:C:OP2	3:N:33:ARG:NH1	2.54	0.40
1:2:531:G:C2	1:2:532:C:N1	2.90	0.40
1:2:897:A:N6	1:2:898:G:C6	2.90	0.40
1:2:998:A:H61	1:2:1173:A:H61	1.68	0.40
1:2:1290:U:O4	1:2:1291:G:N1	2.55	0.40
1:2:1307:G:O2'	1:2:1333:G:N1	2.47	0.40
1:2:1483:U:O2'	1:2:1484:C:O5'	2.31	0.40
2:M:54:GLU:HB3	2:M:55:PRO:HD3	2.03	0.40
3:N:106:GLU:O	3:N:124:TYR:HB3	2.21	0.40
13:F:127:GLY:O	13:F:138:PRO:HA	2.22	0.40
14:G:52:GLY:HA2	14:G:53:LYS:HA	1.85	0.40
27:H:67:LEU:O	27:H:71:ILE:CG1	2.69	0.40
30:4:24:U:C4	30:4:25:C:C4	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	131/137 (96%)	116 (88%)	12 (9%)	3 (2%)	5	27
3	N	143/147 (97%)	119 (83%)	12 (8%)	12 (8%)	0	9
4	Q	156/158 (99%)	140 (90%)	12 (8%)	4 (3%)	4	25
5	R	111/113 (98%)	104 (94%)	6 (5%)	1 (1%)	14	51
6	A	188/198 (95%)	163 (87%)	15 (8%)	10 (5%)	1	15
7	B	200/202 (99%)	170 (85%)	28 (14%)	2 (1%)	13	49
8	V	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	1	15
9	W	61/63 (97%)	52 (85%)	8 (13%)	1 (2%)	8	37
10	Z	184/210 (88%)	167 (91%)	15 (8%)	2 (1%)	12	46
11	D	170/180 (94%)	148 (87%)	15 (9%)	7 (4%)	2	17
12	E	239/243 (98%)	209 (87%)	21 (9%)	9 (4%)	2	19
13	F	215/236 (91%)	176 (82%)	32 (15%)	7 (3%)	3	20
14	G	123/125 (98%)	97 (79%)	15 (12%)	11 (9%)	0	8
15	I	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	8	37
16	J	125/127 (98%)	106 (85%)	13 (10%)	6 (5%)	2	16
18	3	121/123 (98%)	102 (84%)	14 (12%)	5 (4%)	2	17
19	L	100/102 (98%)	90 (90%)	3 (3%)	7 (7%)	1	11
20	O	146/148 (99%)	122 (84%)	18 (12%)	6 (4%)	2	17
21	P	54/56 (96%)	43 (80%)	10 (18%)	1 (2%)	6	31
22	S	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
23	T	109/132 (83%)	97 (89%)	9 (8%)	3 (3%)	4	24
24	U	142/150 (95%)	129 (91%)	10 (7%)	3 (2%)	5	29
25	X	69/71 (97%)	56 (81%)	11 (16%)	2 (3%)	3	23
26	Y	48/50 (96%)	40 (83%)	8 (17%)	0	100	100
27	H	212/215 (99%)	161 (76%)	32 (15%)	19 (9%)	0	8
28	K	133/135 (98%)	117 (88%)	13 (10%)	3 (2%)	5	27
29	0	20/22 (91%)	20 (100%)	0	0	100	100
32	1	81/102 (79%)	71 (88%)	8 (10%)	2 (2%)	4	26
33	6	89/113 (79%)	88 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	7	407/415 (98%)	337 (83%)	50 (12%)	20 (5%)	2	16
35	8	125/139 (90%)	98 (78%)	25 (20%)	2 (2%)	8	37
36	9	247/266 (93%)	204 (83%)	35 (14%)	8 (3%)	3	21
All	All	4438/4674 (95%)	3797 (86%)	478 (11%)	163 (4%)	4	19

All (163) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	36	ARG
3	N	42	ASP
3	N	43	PRO
3	N	44	LEU
3	N	63	LYS
3	N	93	ALA
3	N	112	LYS
4	Q	71	ASN
4	Q	78	ILE
6	A	45	ASN
6	A	194	PRO
8	V	61	GLY
8	V	84	GLU
8	V	95	LYS
10	Z	158	ALA
11	D	84	PRO
11	D	163	PRO
12	E	153	ALA
13	F	92	ARG
13	F	130	SER
14	G	48	ASN
14	G	50	LEU
14	G	56	PRO
14	G	77	ASP
19	L	30	THR
19	L	92	GLU
25	X	4	ASP
27	H	13	HIS
27	H	47	THR
27	H	50	ARG
27	H	78	HIS
27	H	81	VAL
27	H	89	GLU

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Mol	Chain	Res	Type
27	H	92	SER
27	H	94	ASN
27	H	95	SER
32	1	35	ARG
34	7	39	GLU
34	7	98	GLU
34	7	124	PHE
34	7	176	GLU
34	7	222	ASP
34	7	307	LYS
34	7	309	ASP
35	8	76	ASP
36	9	133	TYR
36	9	210	ASP
36	9	213	SER
36	9	241	GLU
2	M	55	PRO
3	N	114	GLY
4	Q	4	MET
6	A	65	LYS
6	A	193	GLU
7	B	29	LYS
8	V	55	TYR
12	E	150	VAL
12	E	160	THR
12	E	161	SER
13	F	32	THR
13	F	49	ILE
13	F	61	GLU
14	G	43	LEU
14	G	54	GLU
14	G	60	LYS
14	G	99	LYS
15	I	22	LYS
16	J	3	ILE
16	J	4	TRP
16	J	64	ASN
16	J	105	ILE
18	3	95	ALA
19	L	40	LEU
19	L	88	ILE
20	O	129	GLN

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Mol	Chain	Res	Type
24	U	35	VAL
27	H	60	ASN
27	H	77	SER
27	H	179	SER
28	K	89	TRP
28	K	133	SER
34	7	75	LYS
36	9	44	SER
36	9	212	GLU
3	N	120	PRO
6	A	100	THR
6	A	129	ILE
7	B	23	GLN
11	D	155	ALA
12	E	237	LYS
13	F	132	GLU
18	3	122	MET
19	L	90	VAL
20	O	83	LYS
20	O	85	TYR
20	O	143	VAL
23	T	41	THR
24	U	67	PRO
27	H	20	ARG
27	H	158	LEU
28	K	11	LYS
34	7	170	THR
34	7	308	ALA
2	M	123	HIS
5	R	16	CYS
6	A	29	GLY
6	A	127	ARG
9	W	6	ILE
11	D	10	LYS
11	D	66	ALA
13	F	39	ARG
16	J	23	LYS
23	T	8	TYR
23	T	20	SER
24	U	117	LYS
25	X	37	LYS
27	H	49	GLY

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Mol	Chain	Res	Type
27	H	82	ALA
27	H	91	ARG
32	1	23	GLU
34	7	44	GLY
34	7	81	ASP
34	7	220	SER
3	N	95	LYS
3	N	110	GLY
8	V	28	GLU
11	D	174	ALA
12	E	152	ILE
12	E	175	GLU
14	G	27	GLU
14	G	96	PRO
15	I	57	ARG
16	J	82	GLU
18	3	96	ALA
18	3	103	GLU
19	L	93	ASP
20	O	74	ILE
21	P	8	LYS
27	H	90	HIS
34	7	36	LYS
34	7	100	LEU
35	8	120	LYS
36	9	153	ASP
2	M	7	ASN
12	E	79	LYS
12	E	157	ASN
19	L	91	PRO
34	7	123	PRO
34	7	292	GLY
36	9	224	ALA
14	G	55	PHE
4	Q	112	HIS
18	3	58	ASP
20	O	123	GLY
3	N	108	ILE
6	A	39	ASP
11	D	15	PRO
34	7	127	PRO
34	7	340	VAL

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Mol	Chain	Res	Type
6	A	57	GLY
10	Z	58	GLY
27	H	83	GLY
34	7	226	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	
2	M	100/104 (96%)	91 (91%)	9 (9%)	8	24
3	N	118/121 (98%)	105 (89%)	13 (11%)	5	18
4	Q	143/143 (100%)	131 (92%)	12 (8%)	9	28
5	R	102/102 (100%)	99 (97%)	3 (3%)	37	57
6	A	166/171 (97%)	160 (96%)	6 (4%)	30	51
7	B	173/173 (100%)	161 (93%)	12 (7%)	13	33
8	V	89/89 (100%)	81 (91%)	8 (9%)	8	24
9	W	54/54 (100%)	52 (96%)	2 (4%)	29	50
10	Z	145/167 (87%)	142 (98%)	3 (2%)	48	67
11	D	153/160 (96%)	145 (95%)	8 (5%)	19	41
12	E	212/213 (100%)	194 (92%)	18 (8%)	8	27
13	F	181/197 (92%)	173 (96%)	8 (4%)	24	45
14	G	108/108 (100%)	93 (86%)	15 (14%)	3	13
15	I	107/108 (99%)	96 (90%)	11 (10%)	6	20
16	J	103/103 (100%)	99 (96%)	4 (4%)	27	48
18	3	99/99 (100%)	93 (94%)	6 (6%)	15	37
19	L	91/91 (100%)	85 (93%)	6 (7%)	14	35
20	O	122/122 (100%)	118 (97%)	4 (3%)	33	53
21	P	46/46 (100%)	41 (89%)	5 (11%)	5	18
22	S	61/61 (100%)	58 (95%)	3 (5%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	T	99/114 (87%)	95 (96%)	4 (4%)	27	47
24	U	121/127 (95%)	114 (94%)	7 (6%)	17	38
25	X	60/60 (100%)	53 (88%)	7 (12%)	4	16
26	Y	41/41 (100%)	38 (93%)	3 (7%)	11	31
27	H	183/184 (100%)	167 (91%)	16 (9%)	8	25
28	K	111/111 (100%)	102 (92%)	9 (8%)	9	29
29	0	21/21 (100%)	21 (100%)	0	100	100
32	1	73/91 (80%)	66 (90%)	7 (10%)	7	22
33	6	83/99 (84%)	76 (92%)	7 (8%)	9	28
34	7	352/357 (99%)	315 (90%)	37 (10%)	5	19
35	8	118/126 (94%)	106 (90%)	12 (10%)	6	20
36	9	227/239 (95%)	198 (87%)	29 (13%)	3	14
All	All	3862/4002 (96%)	3568 (92%)	294 (8%)	13	30

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	13	LYS
2	M	20	TYR
2	M	22	SER
2	M	31	THR
2	M	41	ARG
2	M	56	SER
2	M	89	SER
2	M	92	LYS
2	M	124	ASP
3	N	16	LEU
3	N	20	ARG
3	N	57	LYS
3	N	61	GLU
3	N	64	GLN
3	N	66	ASN
3	N	69	MET
3	N	80	ASN
3	N	97	ILE
3	N	132	VAL
3	N	135	LYS
3	N	136	GLU

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Mol	Chain	Res	Type
3	N	144	LYS
4	Q	1	MET
4	Q	9	ARG
4	Q	15	LYS
4	Q	46	SER
4	Q	70	ASP
4	Q	97	PHE
4	Q	115	ASP
4	Q	117	HIS
4	Q	118	SER
4	Q	127	SER
4	Q	132	LEU
4	Q	152	THR
5	R	62	ARG
5	R	65	LEU
5	R	84	ASP
6	A	31	GLU
6	A	44	LEU
6	A	72	ASP
6	A	85	MET
6	A	101	THR
6	A	113	ASP
7	B	13	LEU
7	B	26	LYS
7	B	27	ASP
7	B	33	TYR
7	B	38	ASP
7	B	52	LEU
7	B	59	LEU
7	B	66	SER
7	B	114	VAL
7	B	128	ARG
7	B	174	GLU
7	B	188	PHE
8	V	12	LYS
8	V	14	ILE
8	V	50	THR
8	V	57	ARG
8	V	60	PHE
8	V	65	SER
8	V	85	TYR
8	V	88	ILE

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Mol	Chain	Res	Type
9	W	11	SER
9	W	14	LEU
10	Z	133	SER
10	Z	172	LYS
10	Z	175	VAL
11	D	34	GLU
11	D	46	THR
11	D	94	SER
11	D	118	MET
11	D	125	ILE
11	D	137	ILE
11	D	141	SER
11	D	151	THR
12	E	4	LYS
12	E	17	THR
12	E	42	SER
12	E	98	GLU
12	E	122	ILE
12	E	137	ARG
12	E	143	HIS
12	E	151	SER
12	E	160	THR
12	E	179	PHE
12	E	185	VAL
12	E	195	ARG
12	E	198	ARG
12	E	211	ASP
12	E	212	VAL
12	E	217	ASP
12	E	237	LYS
12	E	242	LEU
13	F	5	TRP
13	F	13	LEU
13	F	45	LYS
13	F	64	GLU
13	F	112	LYS
13	F	128	CYS
13	F	153	ARG
13	F	185	SER
14	G	8	ILE
14	G	13	SER
14	G	15	ILE

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Mol	Chain	Res	Type
14	G	44	ASN
14	G	51	PHE
14	G	57	GLU
14	G	64	ARG
14	G	70	ASP
14	G	86	VAL
14	G	87	LEU
14	G	89	SER
14	G	99	LYS
14	G	102	ARG
14	G	104	LYS
14	G	118	GLN
15	I	3	LEU
15	I	12	SER
15	I	17	SER
15	I	18	GLU
15	I	22	LYS
15	I	24	GLU
15	I	27	ILE
15	I	36	GLU
15	I	77	PRO
15	I	98	GLU
15	I	125	LEU
16	J	34	ASN
16	J	65	VAL
16	J	67	ASP
16	J	112	SER
18	3	1	MET
18	3	51	VAL
18	3	62	ILE
18	3	66	LEU
18	3	82	SER
18	3	84	LYS
19	L	5	ARG
19	L	45	ILE
19	L	46	ARG
19	L	68	VAL
19	L	69	HIS
19	L	84	GLN
20	O	4	PHE
20	O	7	ILE
20	O	139	GLN

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Mol	Chain	Res	Type
20	O	144	SER
21	P	3	LYS
21	P	7	ASN
21	P	14	PHE
21	P	36	LEU
21	P	55	TYR
22	S	6	GLN
22	S	27	ASP
22	S	43	SER
23	T	9	ARG
23	T	34	ARG
23	T	35	SER
23	T	71	ILE
24	U	10	ASP
24	U	15	ARG
24	U	76	TYR
24	U	77	TYR
24	U	81	LYS
24	U	103	GLN
24	U	121	ILE
25	X	17	ARG
25	X	20	THR
25	X	24	VAL
25	X	29	VAL
25	X	36	ASP
25	X	46	ARG
25	X	65	ARG
26	Y	5	TRP
26	Y	15	VAL
26	Y	22	CYS
27	H	9	PHE
27	H	32	SER
27	H	44	LEU
27	H	48	HIS
27	H	50	ARG
27	H	72	MET
27	H	73	ARG
27	H	78	HIS
27	H	86	MET
27	H	87	ARG
27	H	88	ARG
27	H	97	LYS

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Mol	Chain	Res	Type
27	H	98	VAL
27	H	102	GLU
27	H	174	TYR
27	H	175	ARG
28	K	3	ILE
28	K	10	ARG
28	K	16	ARG
28	K	23	LYS
28	K	31	LYS
28	K	55	GLU
28	K	71	PHE
28	K	112	ARG
28	K	119	PRO
32	1	33	LYS
32	1	35	ARG
32	1	36	PHE
32	1	38	LYS
32	1	71	LYS
32	1	80	ASP
32	1	84	LYS
33	6	38	ASP
33	6	49	CYS
33	6	60	TRP
33	6	62	ARG
33	6	81	ASP
33	6	85	ARG
33	6	96	ARG
34	7	19	ASP
34	7	35	SER
34	7	38	SER
34	7	39	GLU
34	7	41	LEU
34	7	45	MET
34	7	62	CYS
34	7	75	LYS
34	7	87	ARG
34	7	90	SER
34	7	104	MET
34	7	105	LEU
34	7	106	SER
34	7	111	MET
34	7	116	LEU

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Mol	Chain	Res	Type
34	7	134	VAL
34	7	171	LYS
34	7	176	GLU
34	7	192	ASP
34	7	203	LYS
34	7	219	ARG
34	7	221	PHE
34	7	229	GLN
34	7	231	ASN
34	7	232	GLU
34	7	246	LEU
34	7	248	LYS
34	7	260	ARG
34	7	266	LYS
34	7	277	SER
34	7	306	THR
34	7	307	LYS
34	7	347	LYS
34	7	366	THR
34	7	384	ARG
34	7	404	ARG
34	7	415	ILE
35	8	36	LEU
35	8	45	ARG
35	8	53	ARG
35	8	58	ASP
35	8	66	LEU
35	8	74	ASN
35	8	76	ASP
35	8	98	ARG
35	8	109	CYS
35	8	111	SER
35	8	127	CYS
35	8	130	CYS
36	9	4	SER
36	9	27	SER
36	9	29	VAL
36	9	30	SER
36	9	43	TRP
36	9	55	ARG
36	9	60	GLU
36	9	62	ARG

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Mol	Chain	Res	Type
36	9	65	ILE
36	9	74	ARG
36	9	82	LEU
36	9	88	ASP
36	9	91	ARG
36	9	100	ILE
36	9	101	GLN
36	9	103	LEU
36	9	130	GLU
36	9	175	ARG
36	9	187	THR
36	9	204	LEU
36	9	208	GLU
36	9	213	SER
36	9	214	LEU
36	9	215	LEU
36	9	222	ILE
36	9	230	ASP
36	9	235	ASN
36	9	256	GLU
36	9	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	29	HIS
3	N	66	ASN
4	Q	85	HIS
4	Q	104	ASN
4	Q	112	HIS
6	A	130	GLN
7	B	11	GLN
7	B	22	GLN
7	B	23	GLN
11	D	72	GLN
12	E	37	HIS
12	E	38	ASN
12	E	113	HIS
12	E	139	GLN
12	E	143	HIS
12	E	147	ASN
12	E	157	ASN

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Mol	Chain	Res	Type
13	F	30	GLN
13	F	196	ASN
13	F	207	ASN
14	G	44	ASN
14	G	48	ASN
14	G	110	ASN
14	G	118	GLN
14	G	120	ASN
15	I	13	HIS
15	I	16	ASN
16	J	34	ASN
16	J	52	ASN
16	J	121	ASN
22	S	48	ASN
23	T	44	GLN
24	U	103	GLN
26	Y	19	ASN
27	H	129	ASN
27	H	193	ASN
28	K	117	HIS
34	7	37	HIS
34	7	190	ASN
34	7	244	GLN
35	8	84	GLN
36	9	245	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1493/1519 (98%)	335 (22%)	113 (7%)
30	4	75/76 (98%)	28 (37%)	3 (4%)
31	5	17/26 (65%)	10 (58%)	3 (17%)
All	All	1585/1621 (97%)	373 (23%)	119 (7%)

All (373) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	4	C
1	2	14	C
1	2	25	C

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Mol	Chain	Res	Type
1	2	38	G
1	2	39	U
1	2	42	G
1	2	43	A
1	2	44	C
1	2	45	U
1	2	46	A
1	2	47	A
1	2	48	G
1	2	49	C
1	2	57	G
1	2	64	G
1	2	71	C
1	2	72	C
1	2	73	U
1	2	74	U
1	2	75	C
1	2	85	A
1	2	100	A
1	2	102	U
1	2	104	A
1	2	105	C
1	2	106	A
1	2	112	G
1	2	114	A
1	2	115	A
1	2	116	C
1	2	151	G
1	2	158	U
1	2	177	A
1	2	184	G
1	2	197	A
1	2	199	A
1	2	200	G
1	2	211	G
1	2	236	C
1	2	240	U
1	2	241	U
1	2	243	G
1	2	247	G
1	2	248	U
1	2	249	U

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Mol	Chain	Res	Type
1	2	262	G
1	2	263	C
1	2	268	C
1	2	275	A
1	2	276	A
1	2	277	G
1	2	278	A
1	2	285	C
1	2	286	G
1	2	297	G
1	2	301	G
1	2	308	G
1	2	315	A
1	2	317	A
1	2	318	C
1	2	323	A
1	2	324	C
1	2	325	A
1	2	326	C
1	2	328	G
1	2	340	A
1	2	341	C
1	2	343	G
1	2	348	C
1	2	349	A
1	2	350	G
1	2	363	C
1	2	369	A
1	2	370	A
1	2	380	C
1	2	389	G
1	2	393	A
1	2	394	C
1	2	402	G
1	2	409	C
1	2	410	U
1	2	411	C
1	2	412	U
1	2	413	G
1	2	423	U
1	2	425	C
1	2	430	G

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Mol	Chain	Res	Type
1	2	431	U
1	2	432	G
1	2	434	A
1	2	435	A
1	2	436	A
1	2	438	A
1	2	439	G
1	2	440	C
1	2	449	U
1	2	450	A
1	2	459	G
1	2	460	C
1	2	461	A
1	2	462	A
1	2	463	G
1	2	464	G
1	2	466	C
1	2	471	G
1	2	472	C
1	2	480	G
1	2	485	A
1	2	486	A
1	2	487	U
1	2	494	G
1	2	500	A
1	2	503	G
1	2	509	C
1	2	512	U
1	2	513	A
1	2	514	U
1	2	520	G
1	2	523	C
1	2	525	A
1	2	526	A
1	2	528	G
1	2	529	C
1	2	530	G
1	2	531	G
1	2	532	C
1	2	540	G
1	2	541	G
1	2	574	A

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Mol	Chain	Res	Type
1	2	580	G
1	2	581	G
1	2	585	U
1	2	586	C
1	2	587	G
1	2	588	C
1	2	598	U
1	2	607	U
1	2	619	A
1	2	640	U
1	2	641	A
1	2	642	G
1	2	647	G
1	2	649	A
1	2	652	C
1	2	655	A
1	2	656	U
1	2	657	A
1	2	670	C
1	2	672	G
1	2	673	C
1	2	677	U
1	2	678	G
1	2	685	G
1	2	687	G
1	2	702	G
1	2	703	U
1	2	709	G
1	2	718	G
1	2	729	G
1	2	731	A
1	2	735	A
1	2	736	A
1	2	746	A
1	2	747	U
1	2	748	A
1	2	766	G
1	2	767	U
1	2	769	A
1	2	771	G
1	2	772	G
1	2	775	G

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Mol	Chain	Res	Type
1	2	782	A
1	2	801	A
1	2	816	G
1	2	832	G
1	2	847	A
1	2	860	G
1	2	863	U
1	2	872	A
1	2	884	G
1	2	885	G
1	2	892	C
1	2	893	U
1	2	904	G
1	2	905	A
1	2	919	U
1	2	920	U
1	2	925	U
1	2	928	A
1	2	931	C
1	2	933	G
1	2	934	G
1	2	935	G
1	2	936	A
1	2	937	A
1	2	948	G
1	2	949	G
1	2	950	C
1	2	951	G
1	2	953	C
1	2	960	A
1	2	961	U
1	2	962	G
1	2	964	A
1	2	965	G
1	2	970	G
1	2	973	U
1	2	974	G
1	2	975	A
1	2	976	A
1	2	977	G
1	2	978	G
1	2	985	C

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Mol	Chain	Res	Type
1	2	986	G
1	2	988	A
1	2	989	C
1	2	993	C
1	2	1001	A
1	2	1002	G
1	2	1005	G
1	2	1006	C
1	2	1017	U
1	2	1018	C
1	2	1020	G
1	2	1032	A
1	2	1037	U
1	2	1038	C
1	2	1041	C
1	2	1043	U
1	2	1046	G
1	2	1047	U
1	2	1048	G
1	2	1053	A
1	2	1054	A
1	2	1064	C
1	2	1077	U
1	2	1078	U
1	2	1079	G
1	2	1081	C
1	2	1082	A
1	2	1083	G
1	2	1096	G
1	2	1102	A
1	2	1105	C
1	2	1112	G
1	2	1115	G
1	2	1119	U
1	2	1128	U
1	2	1143	G
1	2	1144	G
1	2	1151	A
1	2	1156	A
1	2	1157	G
1	2	1161	A
1	2	1162	G

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Mol	Chain	Res	Type
1	2	1171	G
1	2	1172	A
1	2	1175	C
1	2	1184	U
1	2	1185	A
1	2	1186	C
1	2	1187	A
1	2	1198	A
1	2	1200	U
1	2	1201	G
1	2	1209	C
1	2	1216	A
1	2	1218	C
1	2	1221	A
1	2	1227	A
1	2	1239	A
1	2	1240	A
1	2	1242	C
1	2	1245	C
1	2	1246	U
1	2	1247	A
1	2	1258	C
1	2	1260	G
1	2	1261	U
1	2	1262	U
1	2	1263	C
1	2	1265	G
1	2	1268	C
1	2	1280	C
1	2	1292	A
1	2	1307	G
1	2	1308	U
1	2	1313	G
1	2	1321	U
1	2	1323	A
1	2	1324	U
1	2	1325	C
1	2	1330	G
1	2	1332	C
1	2	1336	U
1	2	1338	C
1	2	1339	G

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Mol	Chain	Res	Type
1	2	1340	U
1	2	1341	C
1	2	1354	A
1	2	1358	A
1	2	1361	G
1	2	1375	C
1	2	1389	G
1	2	1402	C
1	2	1403	U
1	2	1404	C
1	2	1409	G
1	2	1410	G
1	2	1413	G
1	2	1414	G
1	2	1415	U
1	2	1424	G
1	2	1434	C
1	2	1436	U
1	2	1437	G
1	2	1445	A
1	2	1447	A
1	2	1448	A
1	2	1454	A
1	2	1457	A
1	2	1458	A
1	2	1459	G
1	2	1460	G
1	2	1461	U
1	2	1472	G
1	2	1475	C
1	2	1484	C
1	2	1485	G
1	2	1486	A
1	2	1487	U
1	2	1488	C
1	2	1490	C
1	2	1494	C
30	4	3	C
30	4	4	G
30	4	5	G
30	4	7	G
30	4	8	U

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Mol	Chain	Res	Type
30	4	9	G
30	4	13	C
30	4	17	C
30	4	17(A)	U
30	4	18	G
30	4	20	H2U
30	4	21	A
30	4	25	C
30	4	32	OMC
30	4	33	U
30	4	37	A
30	4	38	A
30	4	44	A
30	4	45	G
30	4	49	G
30	4	52	G
30	4	59	A
30	4	60	U
30	4	64	G
30	4	73	A
30	4	74	C
30	4	75	C
30	4	76	A
31	5	808	A
31	5	812	G
31	5	813	A
31	5	814	U
31	5	815	U
31	5	816	U
31	5	817	A
31	5	818	A
31	5	819	A
31	5	821	G

All (119) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1	A
1	2	3	U
1	2	8	U
1	2	42	G
1	2	45	U

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Mol	Chain	Res	Type
1	2	47	A
1	2	56	A
1	2	99	C
1	2	103	A
1	2	111	G
1	2	114	A
1	2	115	A
1	2	176	U
1	2	199	A
1	2	239	A
1	2	246	A
1	2	247	G
1	2	262	G
1	2	270	A
1	2	275	A
1	2	277	G
1	2	323	A
1	2	324	C
1	2	325	A
1	2	347	G
1	2	362	C
1	2	368	C
1	2	399	A
1	2	408	C
1	2	422	U
1	2	434	A
1	2	439	G
1	2	448	A
1	2	462	A
1	2	471	G
1	2	486	A
1	2	512	U
1	2	513	A
1	2	528	G
1	2	529	C
1	2	540	G
1	2	584	C
1	2	598	U
1	2	641	A
1	2	655	A
1	2	687	G
1	2	746	A

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Mol	Chain	Res	Type
1	2	747	U
1	2	766	G
1	2	790	G
1	2	847	A
1	2	856	G
1	2	871	A
1	2	884	G
1	2	891	A
1	2	892	C
1	2	904	G
1	2	919	U
1	2	924	U
1	2	934	G
1	2	941	C
1	2	959	G
1	2	960	A
1	2	961	U
1	2	963	A
1	2	964	A
1	2	974	G
1	2	975	A
1	2	977	G
1	2	985	C
1	2	1001	A
1	2	1017	U
1	2	1037	U
1	2	1053	A
1	2	1081	C
1	2	1089	C
1	2	1098	G
1	2	1142	G
1	2	1150	G
1	2	1156	A
1	2	1161	A
1	2	1171	G
1	2	1174	A
1	2	1184	U
1	2	1186	C
1	2	1200	U
1	2	1217	C
1	2	1241	U
1	2	1245	C

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Mol	Chain	Res	Type
1	2	1260	G
1	2	1261	U
1	2	1262	U
1	2	1289	G
1	2	1291	G
1	2	1306	A
1	2	1307	G
1	2	1323	A
1	2	1324	U
1	2	1337	A
1	2	1340	U
1	2	1367	C
1	2	1368	A
1	2	1370	U
1	2	1423	A
1	2	1436	U
1	2	1448	A
1	2	1453	U
1	2	1457	A
1	2	1458	A
1	2	1459	G
1	2	1460	G
1	2	1483	U
1	2	1486	A
30	4	52	G
30	4	73	A
30	4	74	C
31	5	811	U
31	5	813	A
31	5	818	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	H2U	4	20	30	18,21,22	1.00	1 (5%)	21,30,33	1.90	6 (28%)
30	5MU	4	54	30	19,22,23	1.45	4 (21%)	28,32,35	1.83	8 (28%)
30	PSU	4	55	30	18,21,22	1.47	2 (11%)	22,30,33	2.11	5 (22%)
30	OMC	4	32	30	19,22,23	1.13	1 (5%)	26,31,34	1.31	3 (11%)

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
30	H2U	4	20	30	-	3/7/38/39	0/2/2/2
30	5MU	4	54	30	-	0/7/25/26	0/2/2/2
30	PSU	4	55	30	-	0/7/25/26	0/2/2/2
30	OMC	4	32	30	-	2/9/27/28	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	55	PSU	C6-C5	4.92	1.41	1.35
30	4	54	5MU	C6-C5	3.45	1.40	1.34
30	4	32	OMC	C6-C5	2.65	1.41	1.35
30	4	54	5MU	C4-C5	2.53	1.49	1.44
30	4	54	5MU	C2-N1	2.44	1.42	1.38
30	4	20	H2U	C1'-N1	2.30	1.51	1.46
30	4	55	PSU	C4-C5	2.04	1.50	1.44
30	4	54	5MU	C4-N3	-2.00	1.35	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	55	PSU	C6-C5-C4	-5.28	114.51	118.20
30	4	20	H2U	O4'-C1'-N1	4.91	115.98	109.30
30	4	54	5MU	N3-C2-N1	4.70	121.12	114.89
30	4	55	PSU	N1-C2-N3	4.69	120.44	115.13
30	4	20	H2U	C5-C4-N3	3.92	121.05	116.65
30	4	55	PSU	C4-N3-C2	-3.80	120.87	126.34
30	4	54	5MU	C4-N3-C2	-3.61	122.68	127.35
30	4	54	5MU	O4-C4-C5	-3.34	121.03	124.90
30	4	20	H2U	C3'-C2'-C1'	3.10	107.31	101.43
30	4	54	5MU	C5-C4-N3	2.94	117.82	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	54	5MU	O5'-C5'-C4'	2.49	117.47	108.99
30	4	54	5MU	C6-N1-C2	-2.48	118.78	121.30
30	4	32	OMC	C6-N1-C2	-2.45	116.25	120.49
30	4	20	H2U	N3-C2-N1	2.42	119.21	116.65
30	4	32	OMC	N4-C4-N3	2.34	122.07	117.97
30	4	55	PSU	O2-C2-N1	-2.30	120.26	122.79
30	4	55	PSU	C2'-C3'-C4'	-2.26	98.25	102.64
30	4	20	H2U	O4-C4-C5	-2.26	117.35	122.17
30	4	20	H2U	O2-C2-N3	-2.24	117.32	121.50
30	4	32	OMC	C5-C4-N3	-2.19	117.59	121.33
30	4	54	5MU	C5M-C5-C4	2.08	121.05	118.77
30	4	54	5MU	O2-C2-N1	-2.05	120.06	122.79

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	4	20	H2U	C4'-C5'-O5'-P
30	4	20	H2U	O4'-C1'-N1-C2
30	4	20	H2U	O4'-C1'-N1-C6
30	4	32	OMC	O4'-C4'-C5'-O5'
30	4	32	OMC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	GNP	7	503	38	29,34,34	2.66	8 (27%)	33,54,54	2.46	8 (24%)
37	MET	7	501	-	6,7,8	0.95	1 (16%)	2,7,9	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
39	GNP	7	503	38	-	3/14/38/38	0/3/3/3
37	MET	7	501	-	-	4/5/6/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	503	GNP	PB-O1B	9.32	1.61	1.46
39	7	503	GNP	C5-C6	5.14	1.50	1.41
39	7	503	GNP	PG-N3B	4.65	1.75	1.63
39	7	503	GNP	PB-N3B	4.59	1.75	1.63
39	7	503	GNP	PB-O2B	-3.17	1.48	1.56
39	7	503	GNP	C5-C4	2.77	1.48	1.40
39	7	503	GNP	O4'-C1'	2.73	1.44	1.41
37	7	501	MET	O-C	2.27	1.29	1.19
39	7	503	GNP	PG-O3G	2.13	1.62	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	7	503	GNP	C2-N3-C4	7.52	123.95	115.36
39	7	503	GNP	PB-O3A-PA	-5.29	114.00	132.62
39	7	503	GNP	C4-C5-C6	-4.86	116.16	120.80
39	7	503	GNP	N3-C2-N1	-4.69	120.97	127.22
39	7	503	GNP	C2-N1-C6	3.97	122.24	115.93
39	7	503	GNP	C3'-C2'-C1'	3.97	106.95	100.98
39	7	503	GNP	C5-C6-N1	-2.49	120.03	123.43
39	7	503	GNP	C4-C5-N7	-2.49	106.81	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

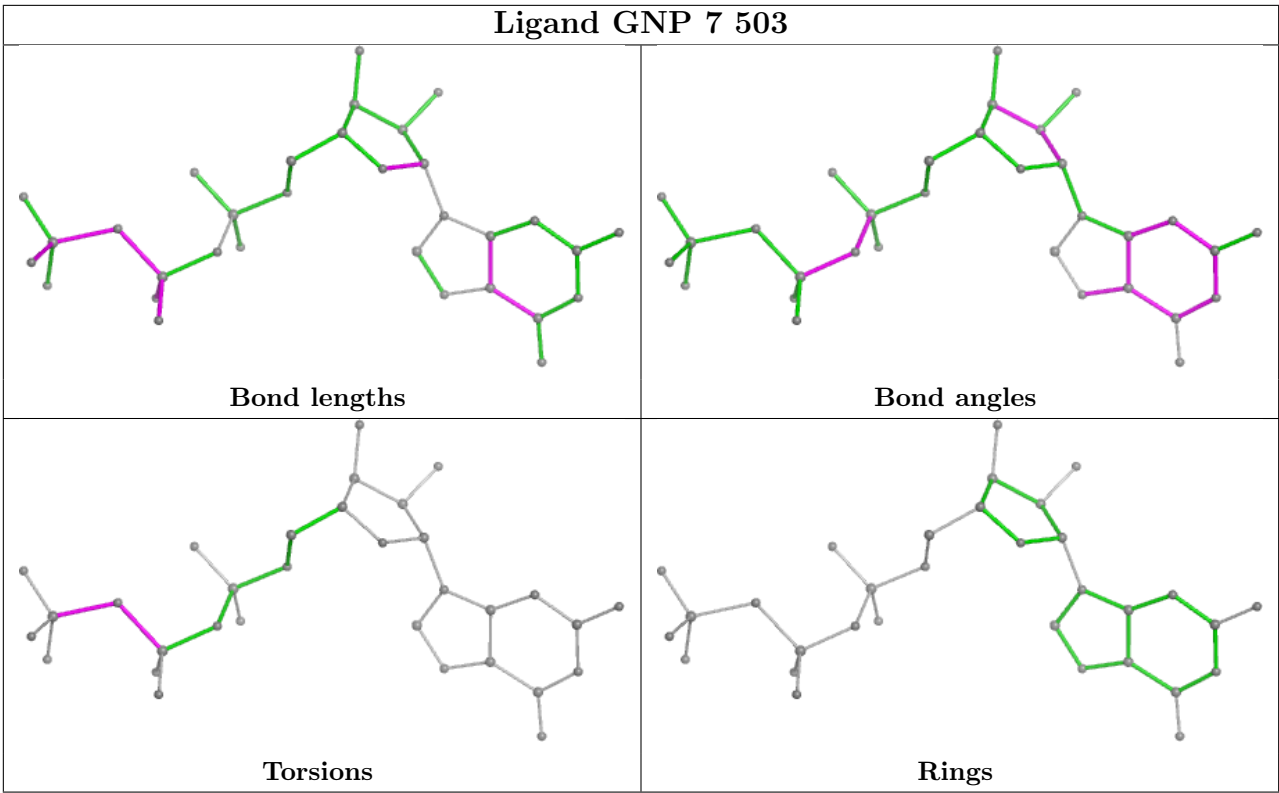
Mol	Chain	Res	Type	Atoms
37	7	501	MET	O-C-CA-CB
37	7	501	MET	N-CA-CB-CG
39	7	503	GNP	PB-N3B-PG-O1G
39	7	503	GNP	PG-N3B-PB-O1B
39	7	503	GNP	PG-N3B-PB-O3A
37	7	501	MET	CA-CB-CG-SD
37	7	501	MET	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	7	503	GNP	1	0
37	7	501	MET	11	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	3
33	6	2
36	9	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1342:C	O3'	1343:C	P	3.20
1	9	1:MET	C	2:ILE	N	3.16
1	6	76:SER	C	77:ASP	N	3.11
1	2	1060:G	O3'	1061:A	P	2.56
1	6	89:THR	C	90:GLN	N	2.54
1	2	1019:A	O3'	1020:G	P	2.00

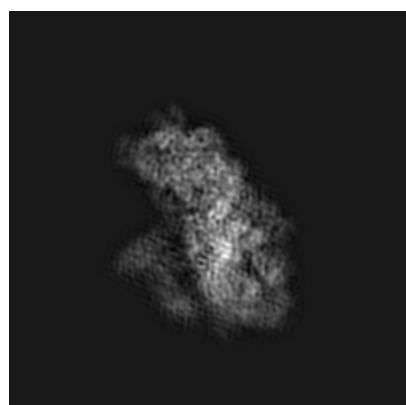
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8148. These allow visual inspection of the internal detail of the map and identification of artifacts.

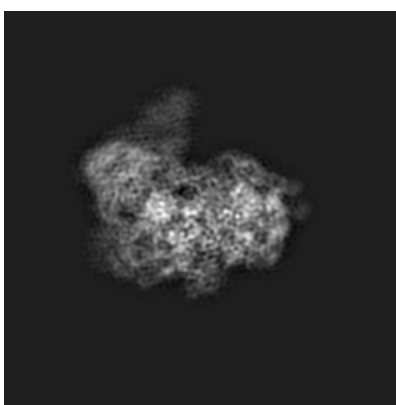
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

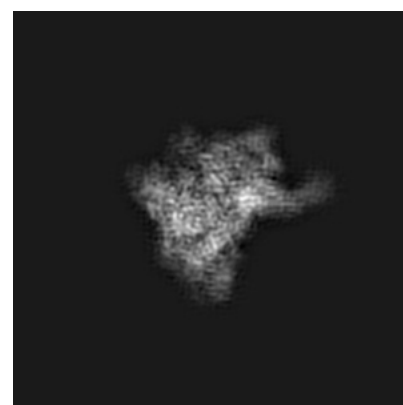
6.1.1 Primary map



X



Y

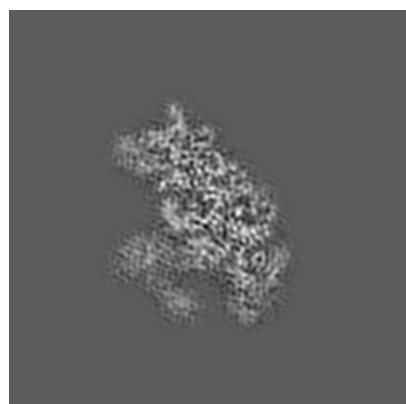


Z

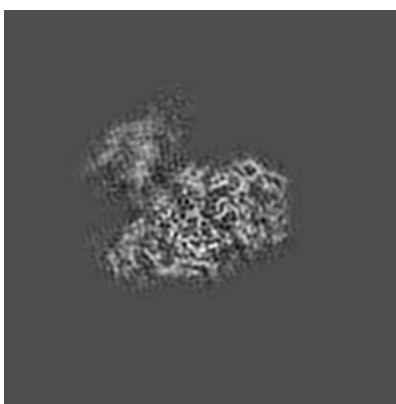
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

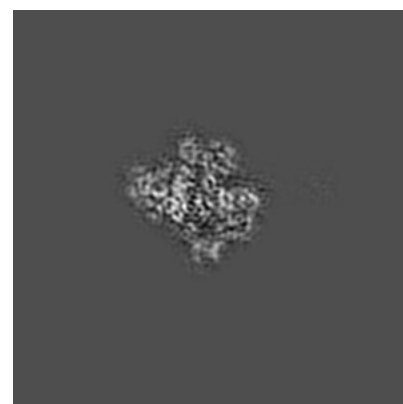
6.2.1 Primary map



X Index: 174



Y Index: 174

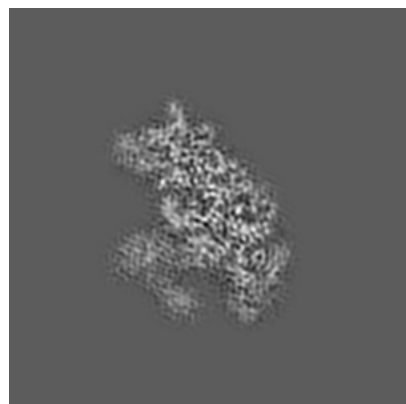


Z Index: 174

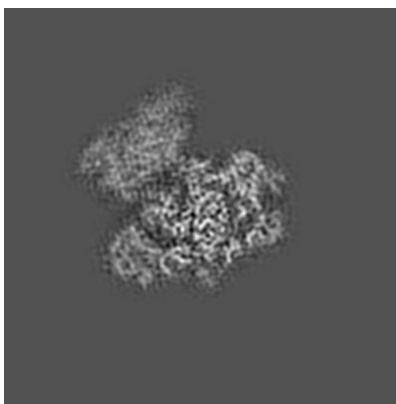
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 174



Y Index: 181

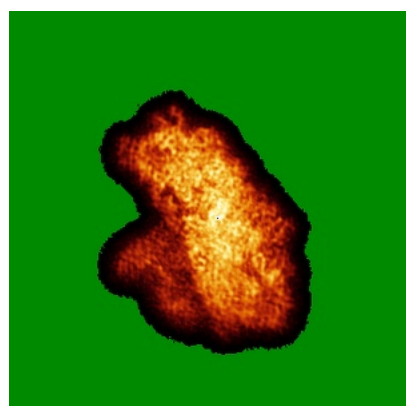


Z Index: 203

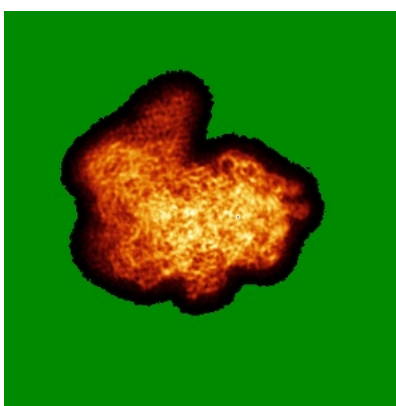
The images above show the largest variance slices of the map in three orthogonal directions.

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

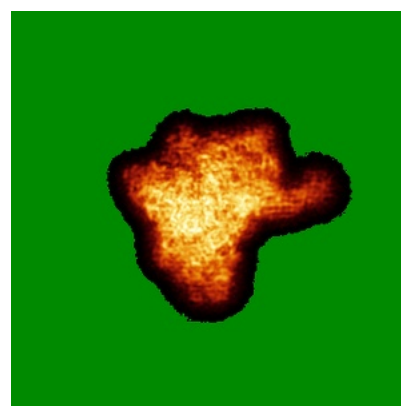
6.4.1 Primary map



X



Y

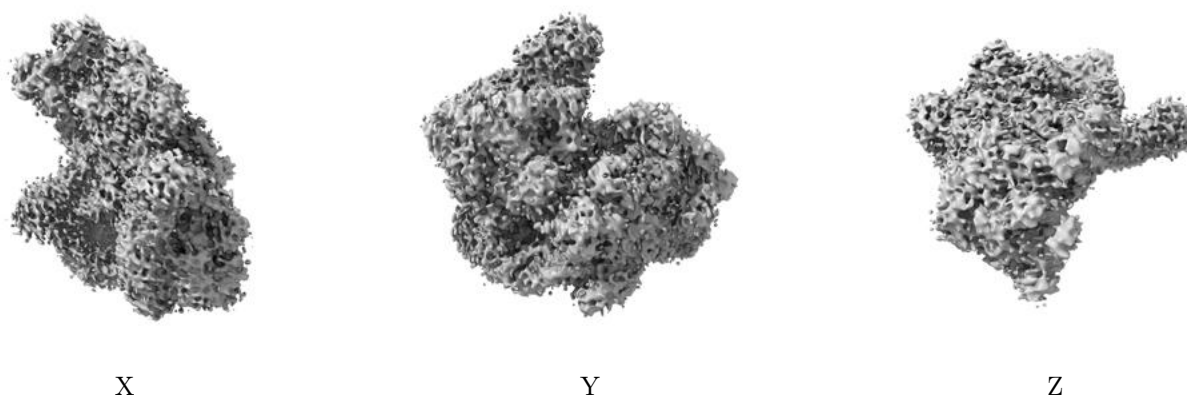


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

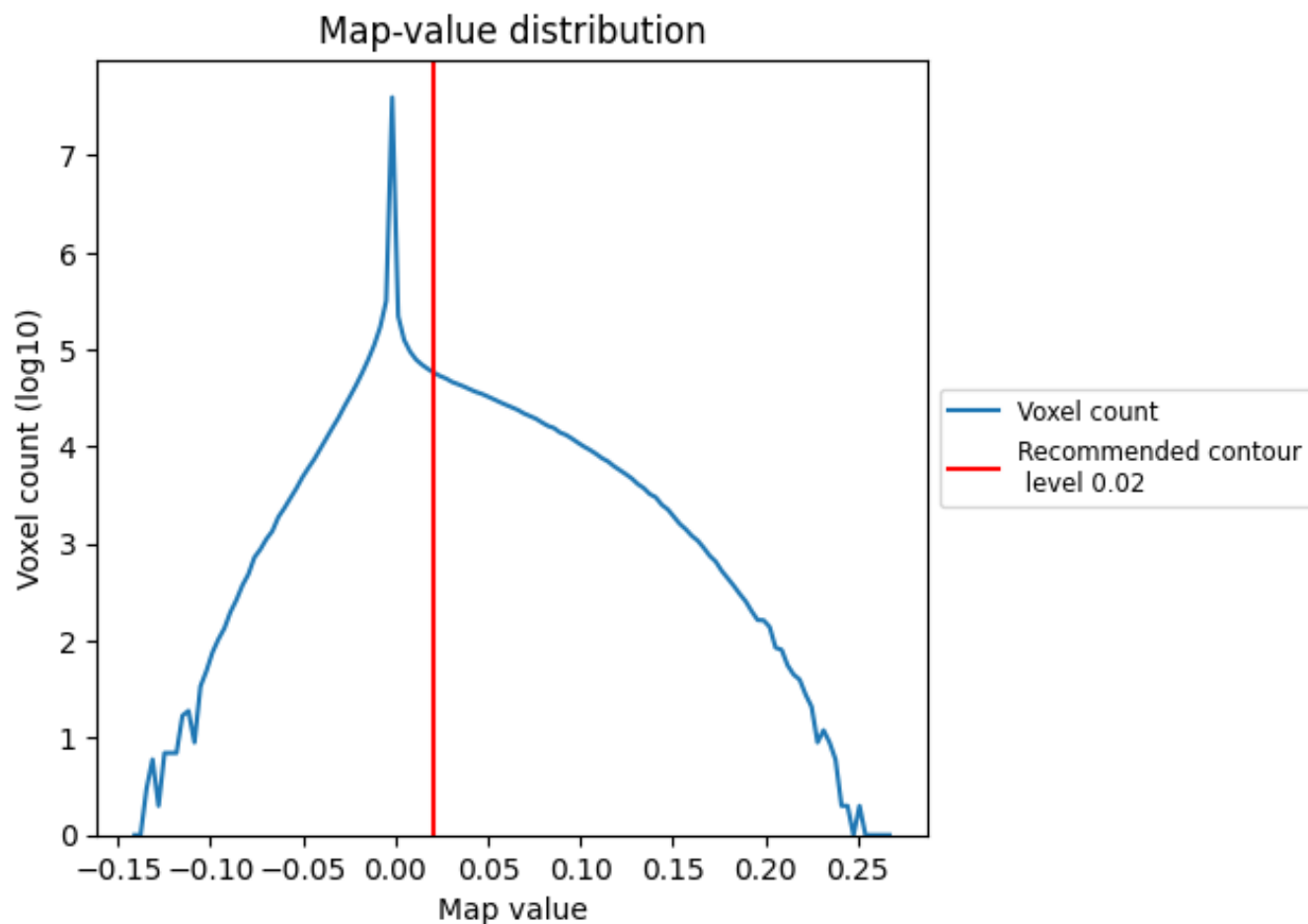
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

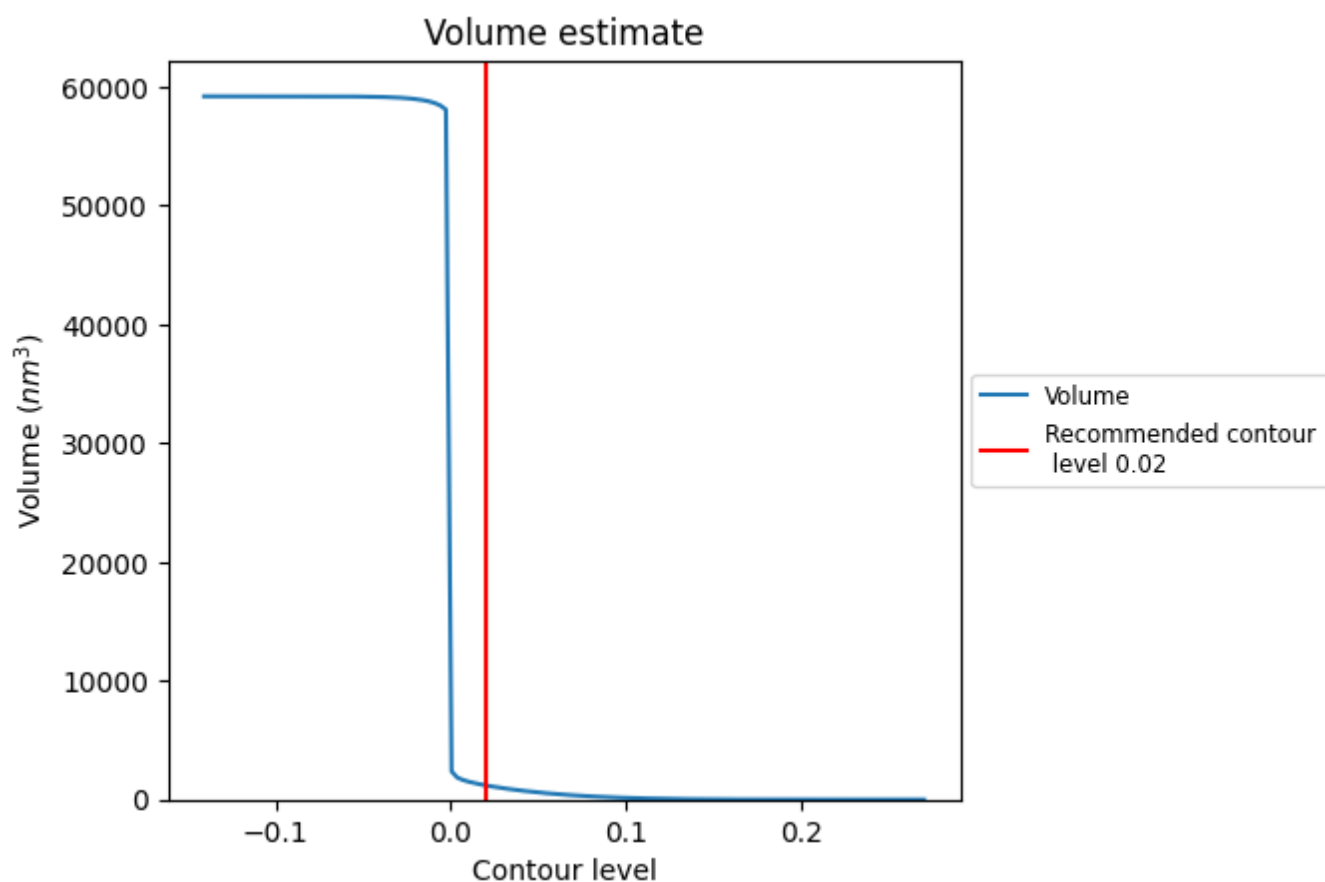
This section contains the results of statistical analysis of the map.

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.

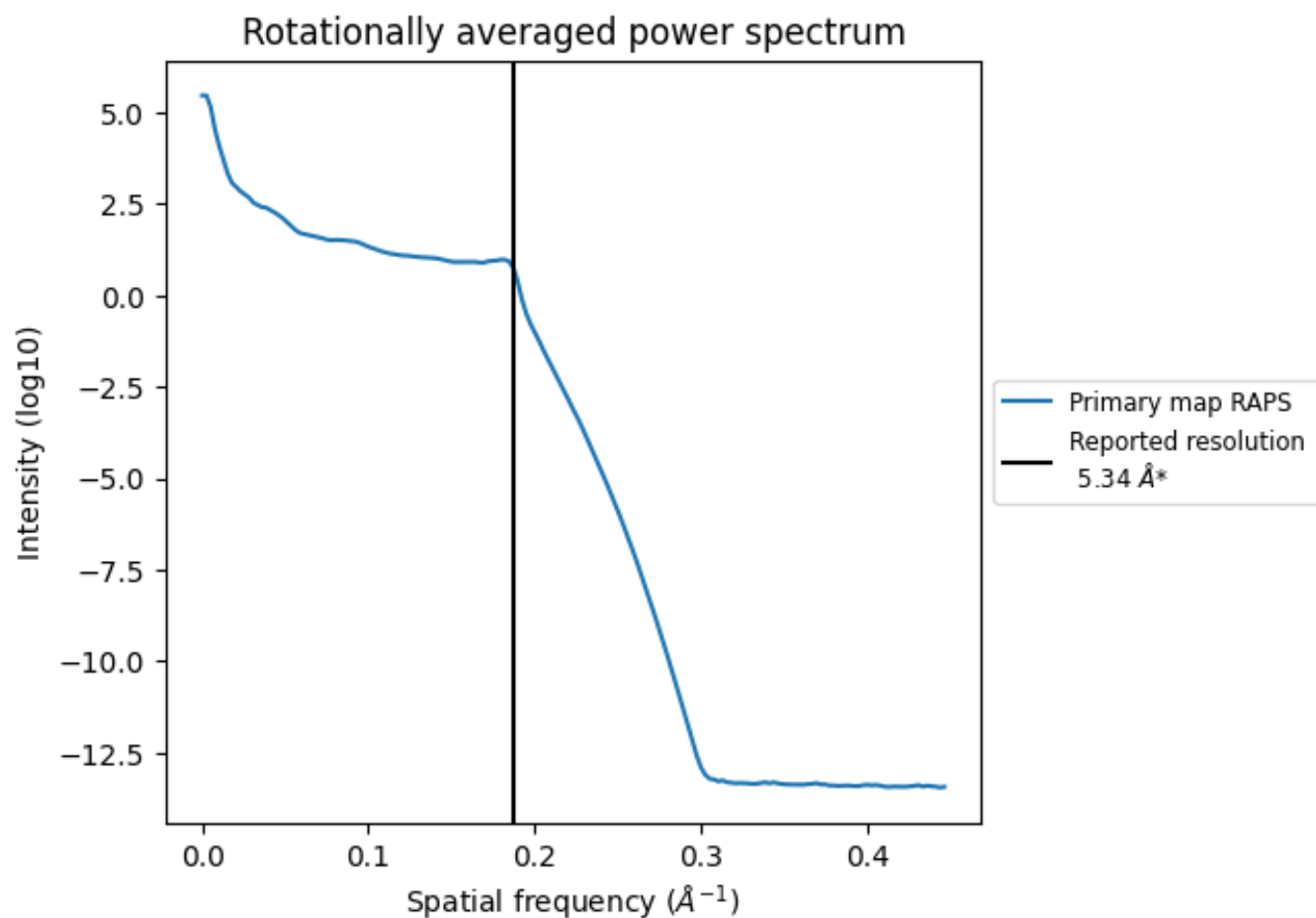
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1191 nm^3 ; this corresponds to an approximate mass of 1076 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 ⓘ

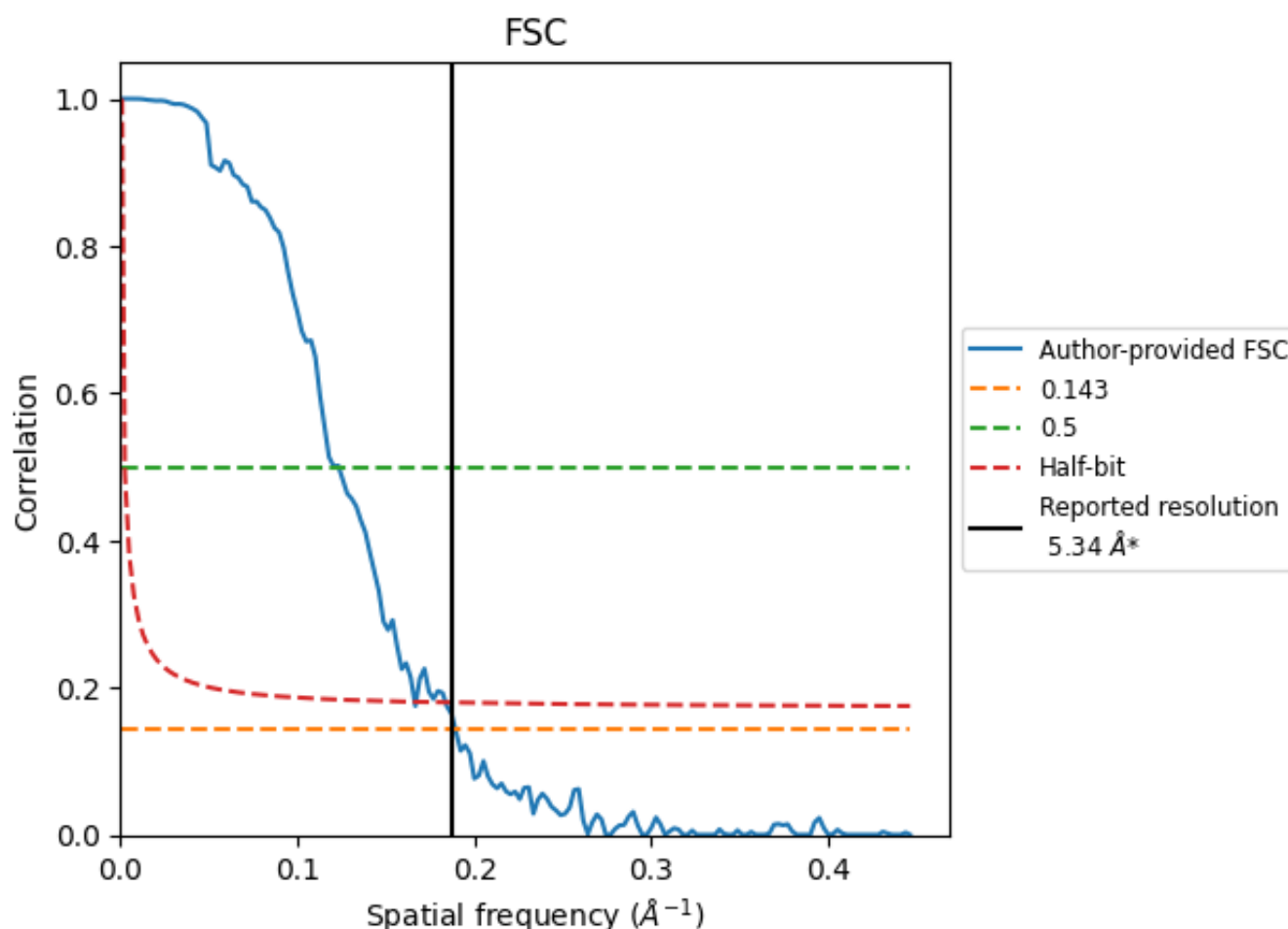


*Reported resolution corresponds to spatial frequency of 0.187 Å⁻¹

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 0.187 Å⁻¹

8.2 Resolution estimates [i](#)

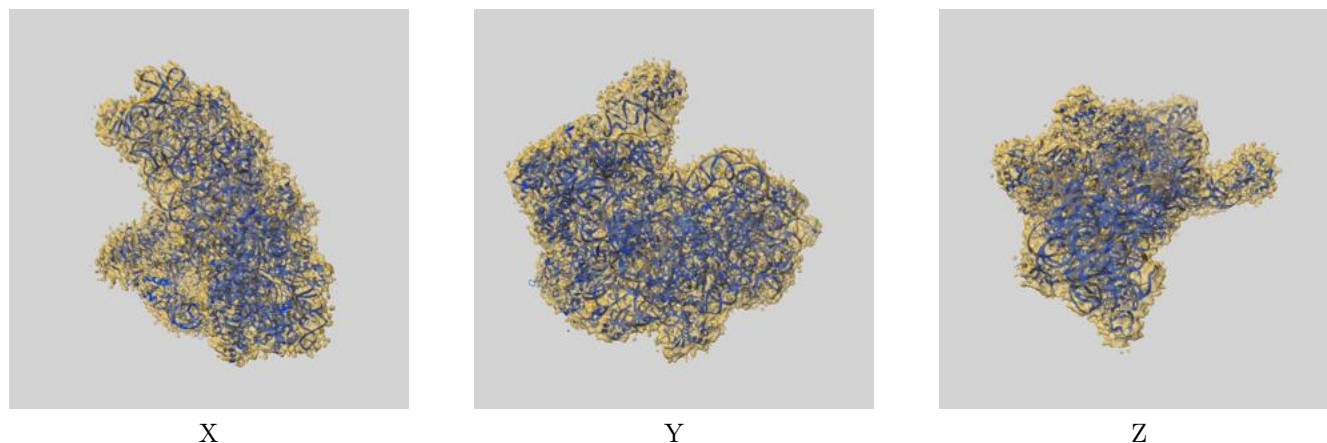
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.34	-	-
Author-provided FSC curve	5.28	8.10	6.01
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

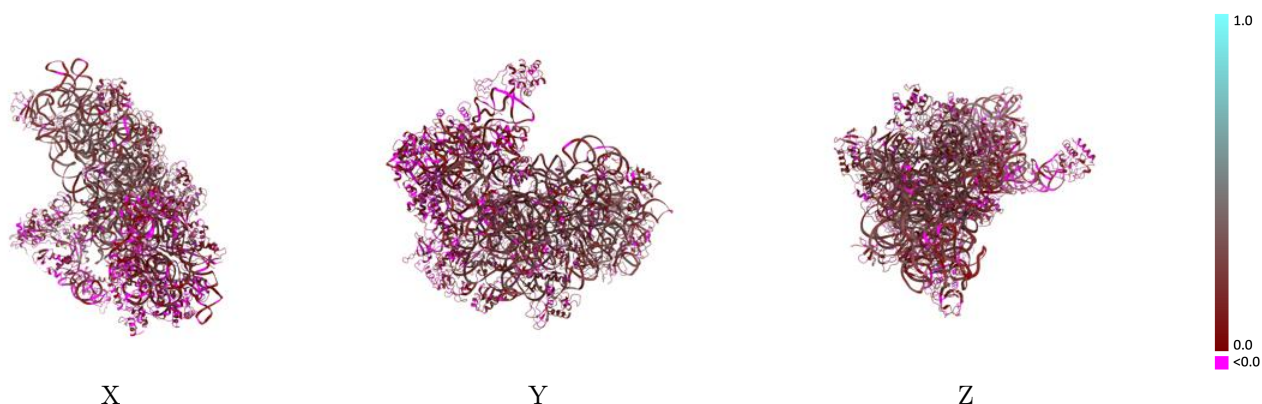
This section contains information regarding the fit between EMDB map EMD-8148 and PDB model 5JB3. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



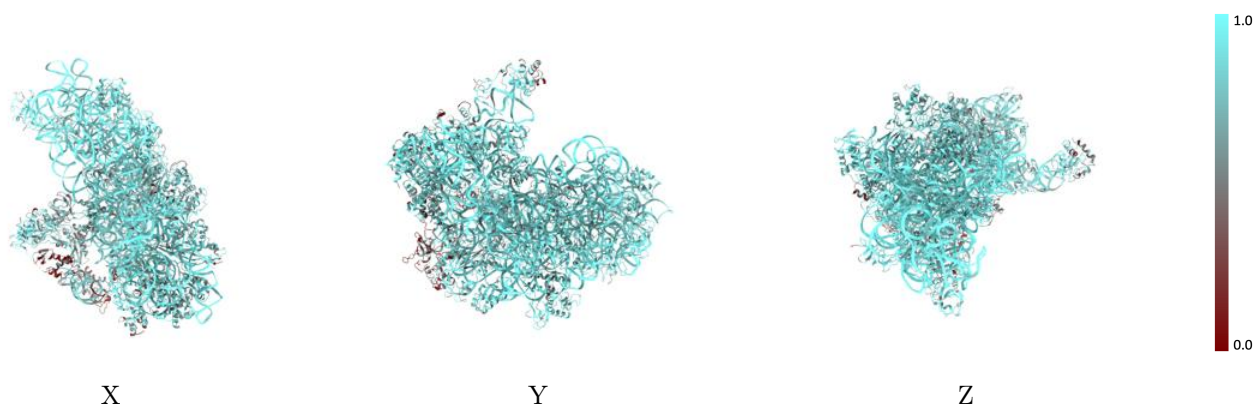
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



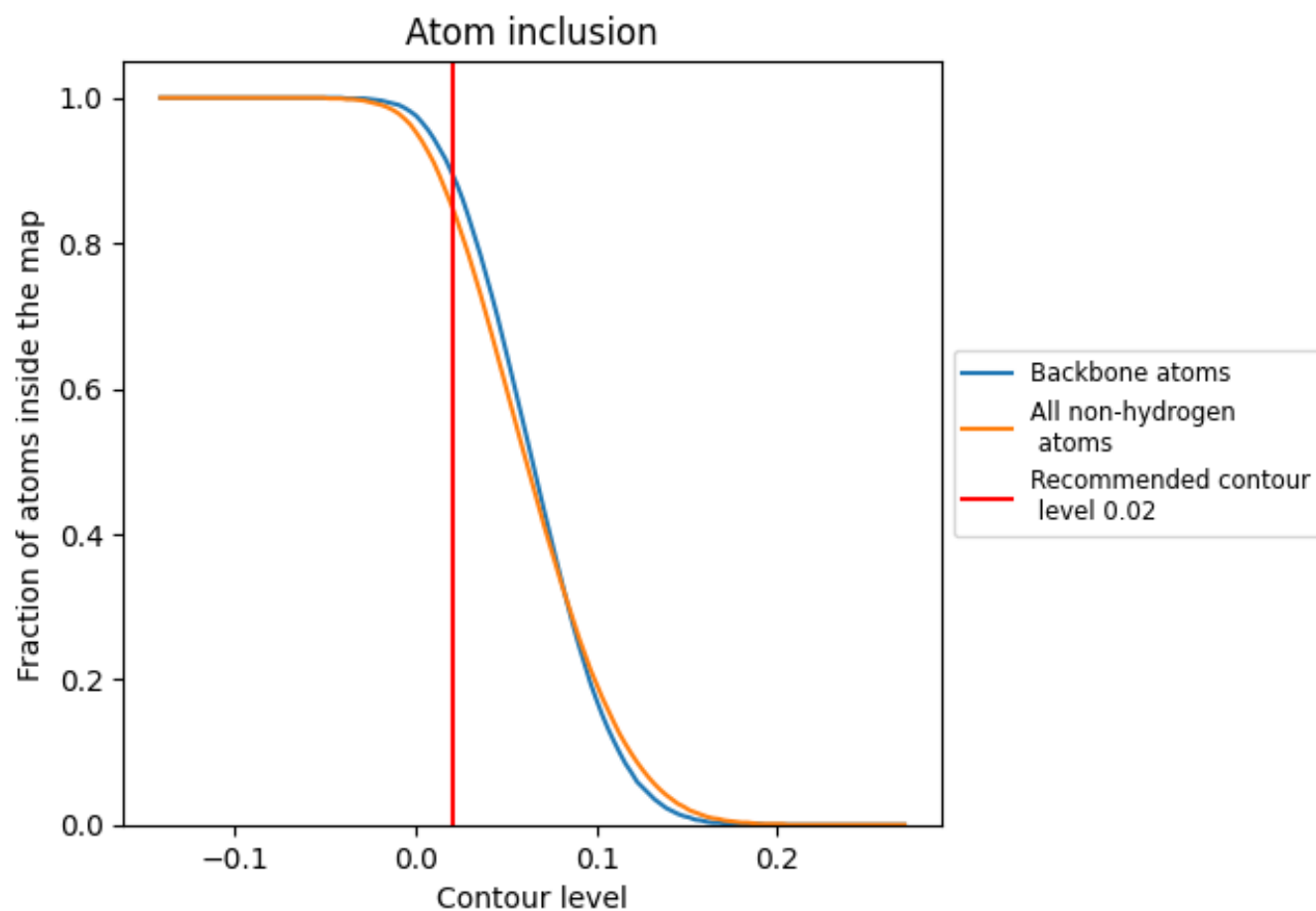
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.1640
0	 0.7410	 0.1450
1	 0.7570	 0.1550
2	 0.9600	 0.2130
3	 0.7200	 0.0750
4	 0.7440	 0.0520
5	 0.9120	 0.2470
6	 0.7240	 0.1540
7	 0.7380	 0.1050
8	 0.3580	 0.0590
9	 0.4690	 0.0670
A	 0.8270	 0.1490
B	 0.8040	 0.1500
C	 0.9370	 0.2270
D	 0.8390	 0.1770
E	 0.8340	 0.1640
F	 0.8000	 0.1810
G	 0.8390	 0.1000
H	 0.7230	 0.0680
I	 0.8330	 0.1900
J	 0.8390	 0.1680
K	 0.7620	 0.1080
L	 0.8060	 0.1300
M	 0.7710	 0.1370
N	 0.7800	 0.1730
O	 0.7760	 0.0720
P	 0.8280	 0.1520
Q	 0.7920	 0.1600
R	 0.8440	 0.1820
S	 0.7600	 0.0970
T	 0.6990	 0.0480
U	 0.8100	 0.0690
V	 0.8140	 0.1550
W	 0.8470	 0.1280
X	 0.6490	 0.0890



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Chain	Atom inclusion	Q-score
Y	 0.7460	 0.0750
Z	 0.7750	 0.1120