Full wwPDB EM Validation Report ⓘ

Oct 24, 2026 – 10:49 am BST

PDB ID	:	9TRV / pdb_00009trv
EMDB ID	:	EMD-56198
Title	:	Structure of the Plant mitochondrial pre-initiation complex 1, (SSU,mtIF3)
Authors	:	Skaltsogiannis, V.; Giege, P.; Soufari, H.
Deposited on	:	2025-12-28
Resolution	:	2.28 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:

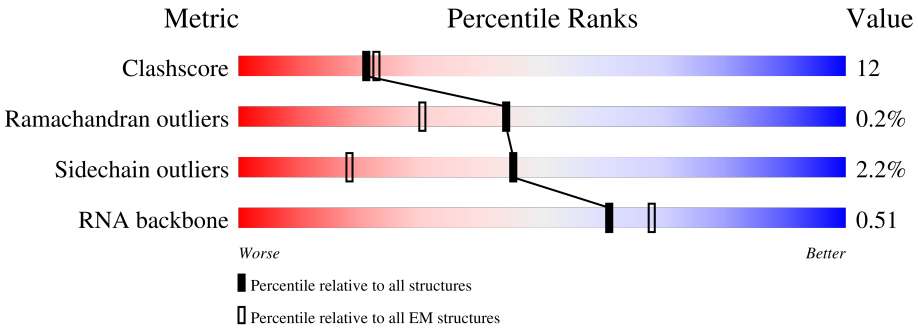
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

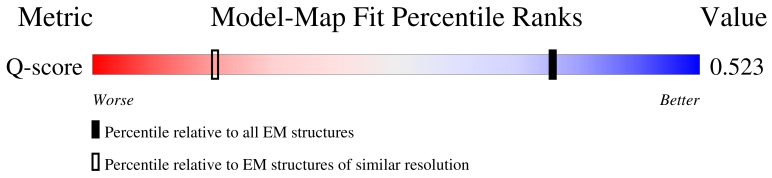
1 Overall quality at a glance

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

The reported resolution of this entry is 2.28 Å.

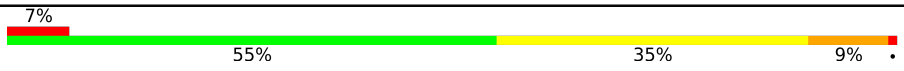
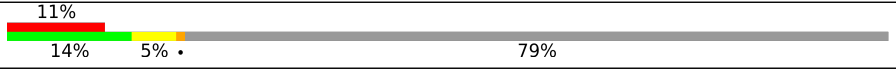
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3643 (1.78 - 2.78)

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 <=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	1611	
2	8	520	
3	A	212	

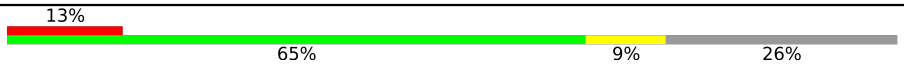
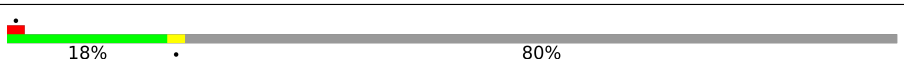
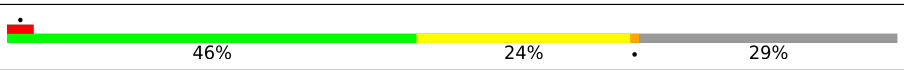
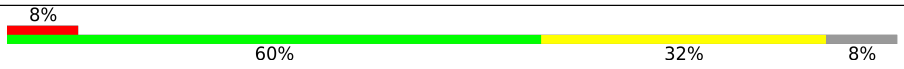
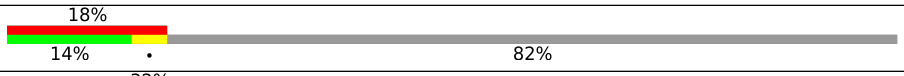
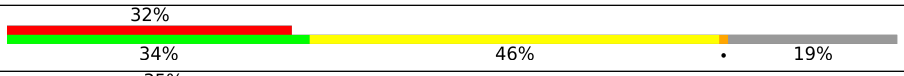
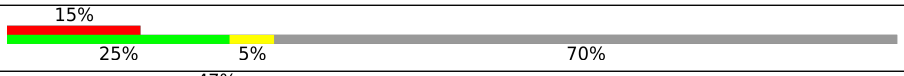
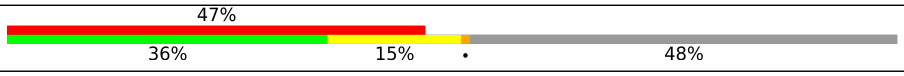
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Mol	Chain	Length	Quality of chain
4	B	554	12% 69% 14% 16%
5	C	362	6% 68% 24% 8%
6	D	501	15% 61% 22% 18%
7	E	138	59% 14% 27%
8	F	157	15% 86% 13%
9	G	129	81% 18%
10	H	383	10% 43% 12% 45%
11	I	228	46% 50%
12	J	304	6% 29% 12% 58%
13	K	125	78% 20%
14	L	154	61% 10% 29%
15	M	155	61% 35%
16	N	414	24% 72%
17	O	136	71% 10% 19%
18	P	110	7% 70% 13% 17%
19	Q	237	33% 62%
20	R	212	43% 66% 12% 22%
21	S	100	11% 55% 20% 25%
22	T	94	49% 47%
23	U	192	32% 41% 24% 34%
24	V	193	64% 20% 15%
25	W	483	73% 5% 21%
26	X	496	5% 36% 5% 59%
27	Y	102	6% 87% 9%
28	Z	153	30% 20% 48%

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Mol	Chain	Length	Quality of chain
29	a	424	
30	b	80	
31	c	128	
32	d	110	
33	e	383	
34	f	410	
35	g	668	
36	h	384	
37	i	725	
38	k	155	
39	l	576	

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 89547 atoms, of which 927 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1610	34484	15405	6287	11182	1610	0	0

- Molecule 2 is a protein called Translation initiation factor IF3-1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	8	109	1801	566	927	151	153	4	0	0

- Molecule 3 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	204	1611	1032	284	285	10	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	467	3877	2520	701	643	13	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	TRP	ARG	conflict	UNP A0A068BCX1
B	62	ILE	LEU	conflict	UNP A0A068BCX1
B	172	LEU	SER	conflict	UNP A0A068BCX1
B	202	LYS	ARG	conflict	UNP A0A068BCX1
B	296	LEU	SER	conflict	UNP A0A068BCX1
B	512	CYS	ARG	conflict	UNP A0A068BCX1
B	524	VAL	ALA	conflict	UNP A0A068BCX1
B	533	LEU	SER	conflict	UNP A0A068BCX1

- Molecule 5 is a protein called Ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	333	Total	C	N	O	S	0	0
			2806	1793	540	462	11		

- Molecule 6 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	413	Total	C	N	O	S	0	0
			3389	2125	596	656	12		

- Molecule 7 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	101	Total	C	N	O	S	0	0
			823	535	145	138	5		

- Molecule 8 is a protein called uS7m,Small ribosomal subunit protein uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	157	Total	C	N	O	S	0	0
			1254	793	244	213	4		

- Molecule 9 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	128	Total	C	N	O	S	0	0
			1037	652	193	189	3		

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	212	Total	C	N	O	S	0	0
			1671	1048	308	310	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	50	SER	PRO	conflict	UNP A0A3P6FWE0
H	94	SER	ASN	conflict	UNP A0A3P6FWE0

- Molecule 11 is a protein called Small ribosomal subunit protein uS10 domain-containing

protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	113	Total	C	N	O	S	0	0
			941	602	174	159	6		

- Molecule 12 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	127	Total	C	N	O	S	0	0
			988	608	195	181	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	124	Total	C	N	O	S	0	0
			993	614	209	166	4		

- Molecule 14 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	110	Total	C	N	O	S	0	0
			873	529	185	154	5		

- Molecule 15 is a protein called Small ribosomal subunit protein uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	101	Total	C	N	O	S	0	0
			843	524	174	140	5		

- Molecule 16 is a protein called Small ribosomal subunit protein uS15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	116	Total	C	N	O	S	0	0
			941	593	170	171	7		

- Molecule 17 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	110	Total	C	N	O	S	0	0
			869	550	169	144	6		

- Molecule 18 is a protein called Small ribosomal subunit protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	91	Total	C	N	O	S	0	0
			717	455	135	124	3		

- Molecule 19 is a protein called Small ribosomal subunit protein bS18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	90	Total	C	N	O	S	0	0
			724	460	127	134	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	250	ILE	VAL	conflict	UNP A0A078FCZ9

- Molecule 20 is a protein called Small ribosomal subunit protein uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	166	Total	C	N	O	S	0	0
			1299	819	236	237	7		

- Molecule 21 is a protein called Ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	75	Total	C	N	O	S	0	0
			611	386	120	103	2		

- Molecule 22 is a protein called 30S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	50	Total	C	N	O	S	0	0
			408	260	79	68	1		

- Molecule 23 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	127	Total	C	N	O	S	0	0
			1014	647	184	178	5		

- Molecule 24 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	164	Total	C	N	O	S	0	0
			1399	874	266	255	4		

- Molecule 25 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	380	Total	C	N	O	S	0	0
			3062	1955	535	559	13		

- Molecule 26 is a protein called BnaC06g06470D protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	204	Total	C	N	O	S	0	0
			1613	1011	262	329	11		

- Molecule 27 is a protein called MOSC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	98	Total	C	N	O	S	0	0
			793	495	159	137	2		

- Molecule 28 is a protein called Mitochondrial 28S ribosomal protein S34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	80	Total	C	N	O	S	0	0
			649	422	121	104	2		

- Molecule 29 is a protein called Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	315	Total	C	N	O	S	0	0
			2486	1546	448	482	10		

- Molecule 30 is a protein called IMS import disulfide relay-system CHCH-CHCH-like Cx9C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	77	Total	C	N	O	S	0	0
			610	378	116	108	8		

- Molecule 31 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	26	Total	C	N	O	S	0	0
			232	145	54	32	1		

- Molecule 32 is a protein called IGR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	78	Total	C	N	O	S	0	0
			616	403	110	102	1		

- Molecule 33 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	246	Total	C	N	O	S	0	0
			2074	1310	374	380	10		

- Molecule 34 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	377	Total	C	N	O	S	0	0
			2922	1843	486	573	20		

- Molecule 35 is a protein called Small ribosomal subunit protein mS81 (rPPR8).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	119	Total	C	N	O	S	0	0
			946	608	157	174	7		

- Molecule 36 is a protein called (rape) hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	310	Total	C	N	O	S	0	0
			2463	1557	438	455	13		

- Molecule 37 is a protein called PROP1-like PPR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	370	Total	C	N	O	S	0	0
			2993	1890	503	582	18		

- Molecule 38 is a protein called Small ribosomal subunit protein mS86.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	47	Total	C	N	O	S	0	0
			313	194	61	54	4		

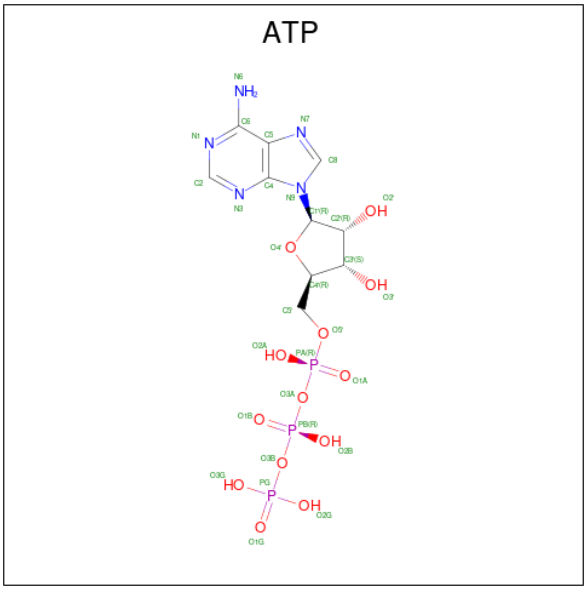
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	9	LYS	ARG	conflict	UNP Q9FZ84
k	20	MET	LEU	conflict	UNP Q9FZ84

- Molecule 39 is a protein called Small ribosomal subunit protein mS80 (rPPR6).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	302	Total	C	N	O	S	0	0
			2371	1506	397	447	21		

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

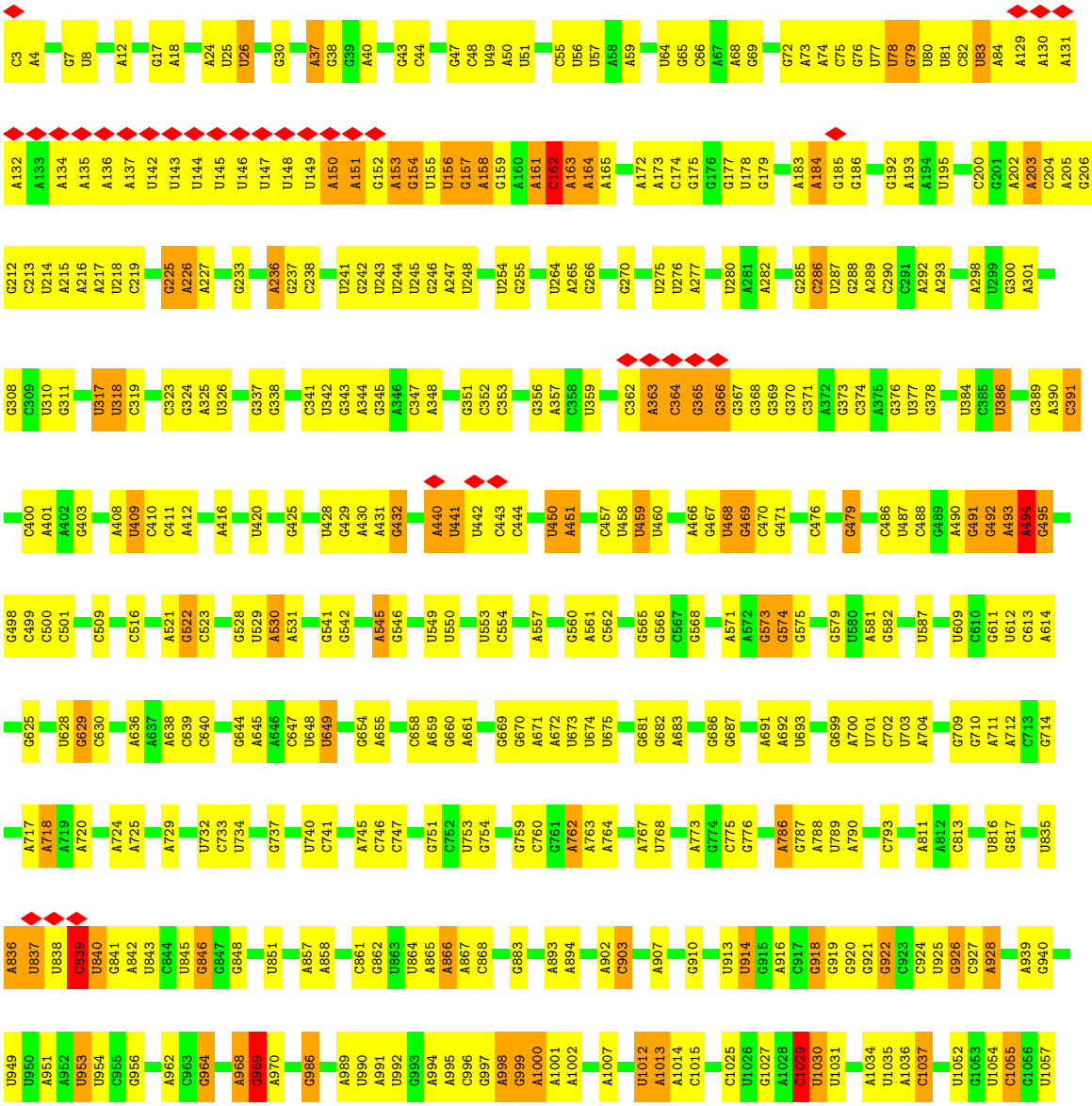
3 Residue-property plots (i)

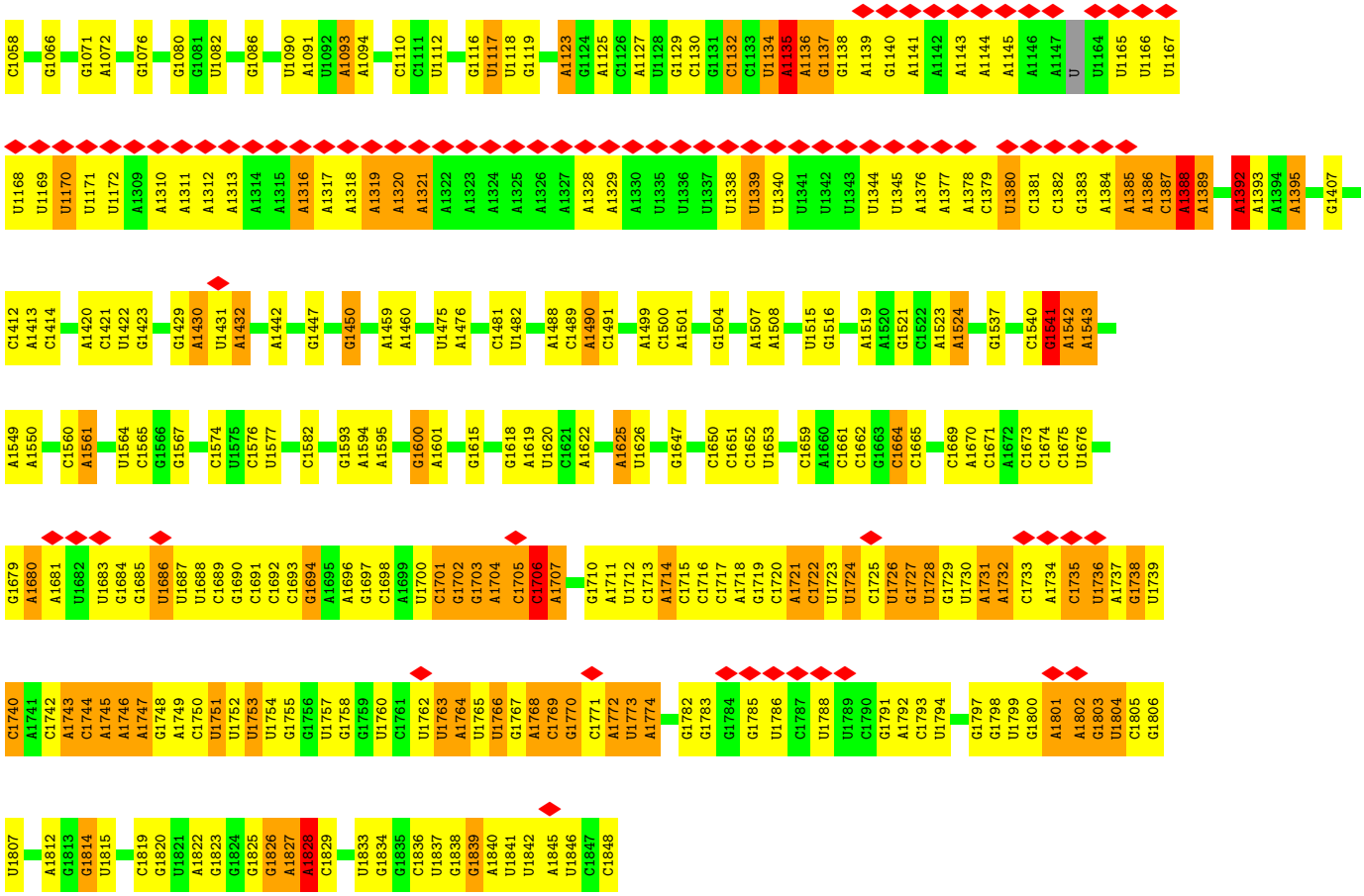
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 18S rRNA

Chain 2:



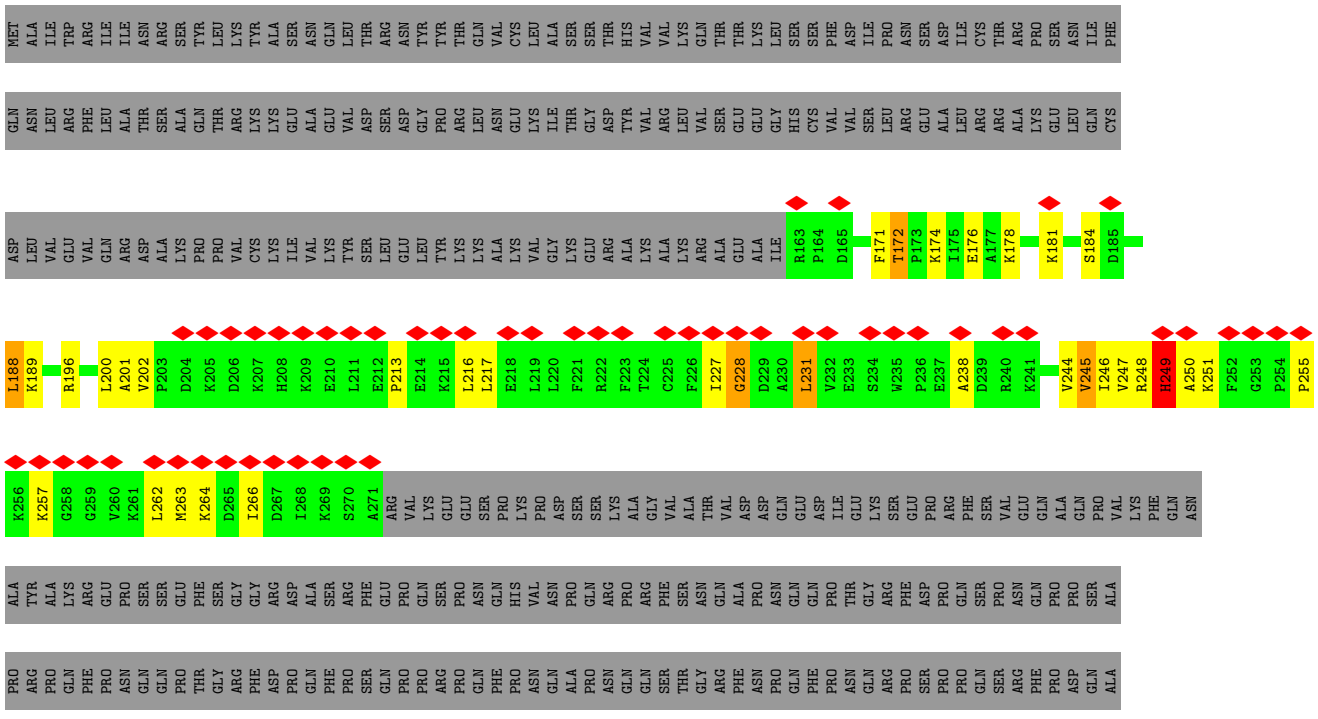


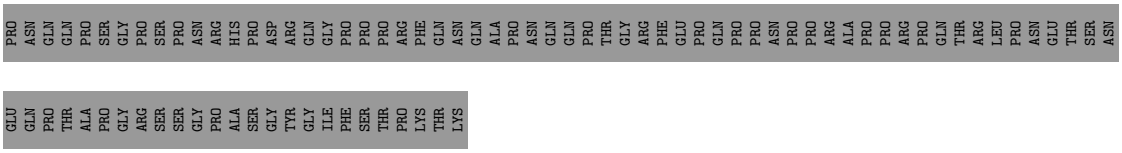


• Molecule 2: Translation initiation factor IF3-1, mitochondrial

Chain 8:



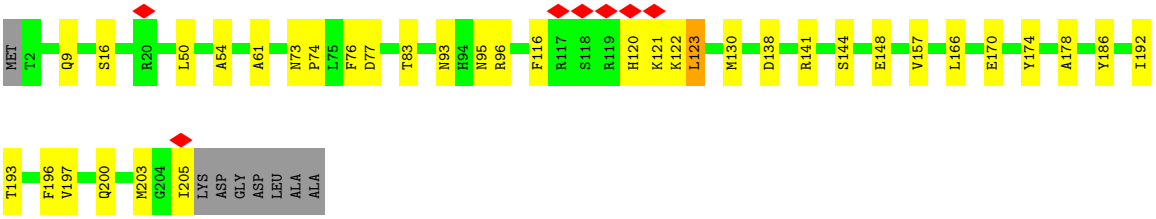




• Molecule 3: Ribosomal protein S2

Chain A:

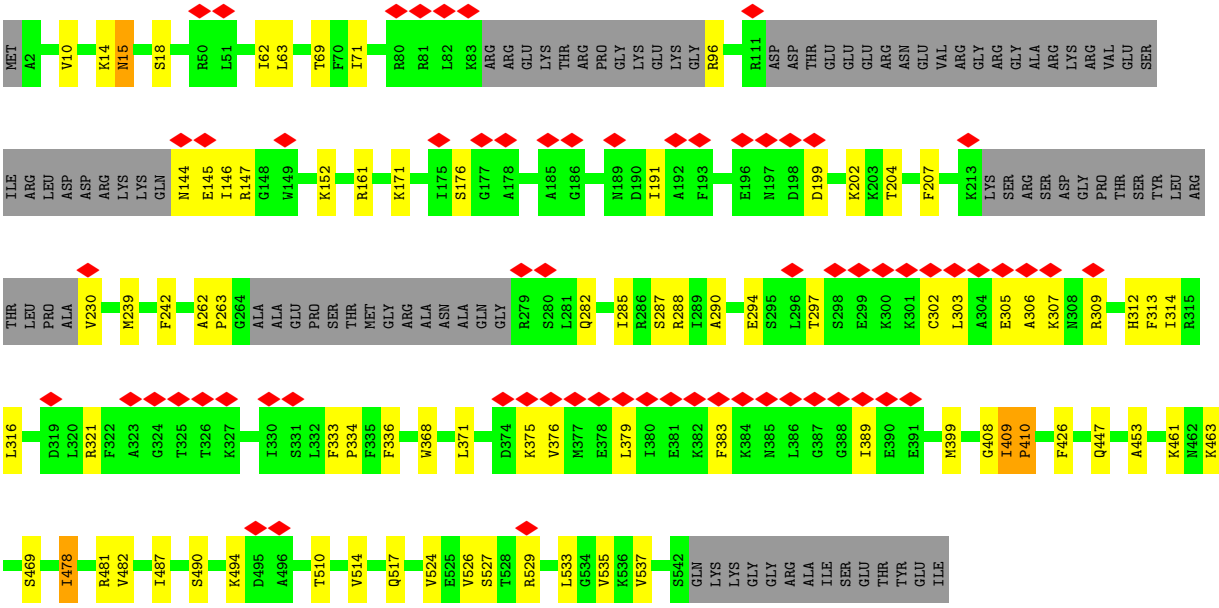




• Molecule 4: Small ribosomal subunit protein uS3m

Chain B:

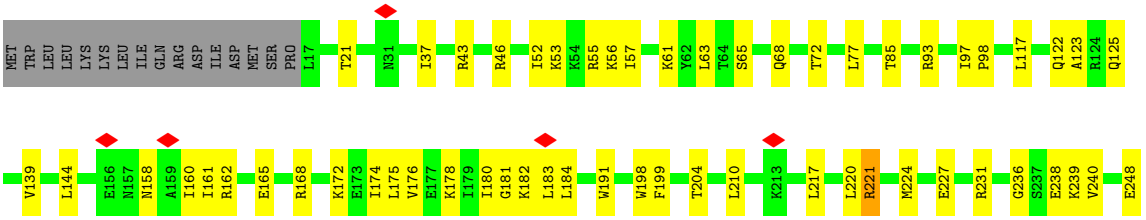


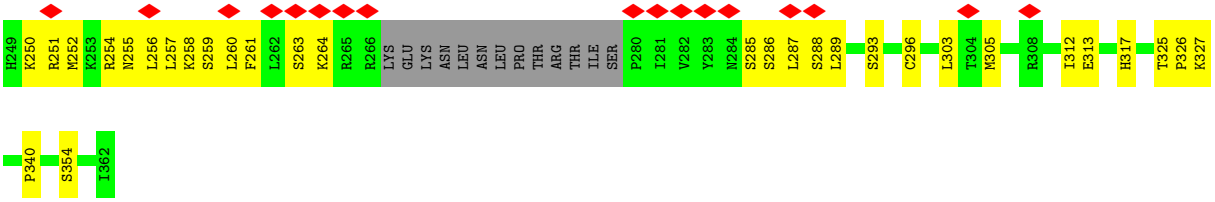


• Molecule 5: Ribosomal protein S4

Chain C:

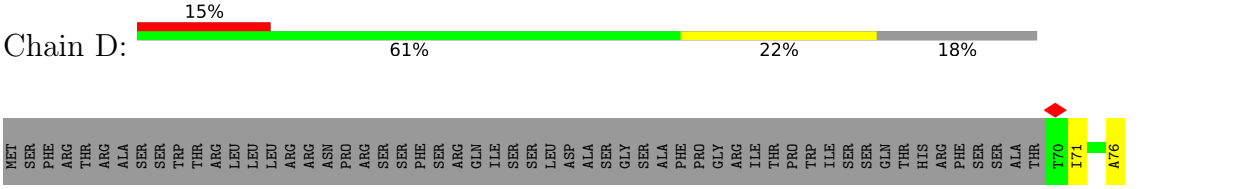


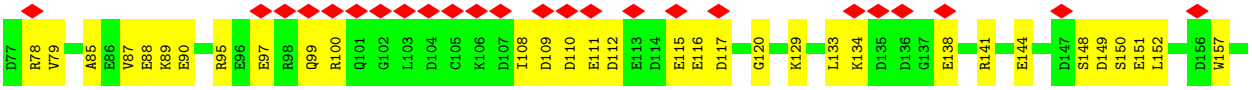


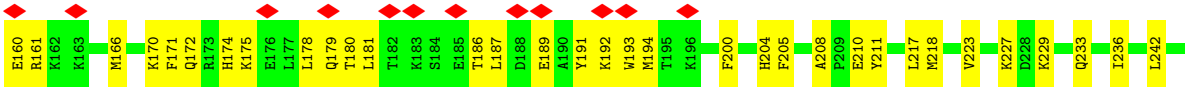


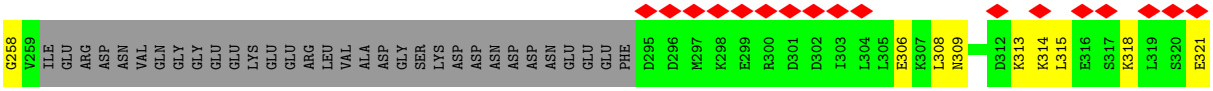
• Molecule 6: S5 DRBM domain-containing protein

Chain D:









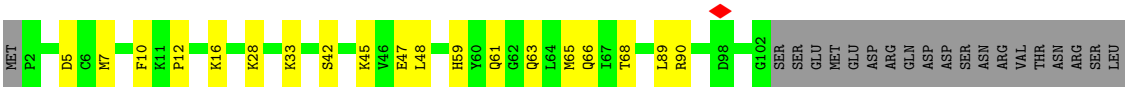


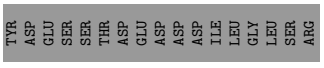


• Molecule 7: bS6m

Chain E:



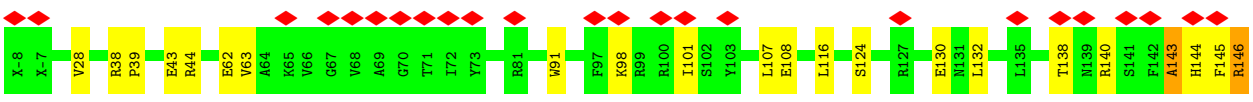




• Molecule 8: uS7m,Small ribosomal subunit protein uS7m

Chain F:







• Molecule 9: 40S ribosomal protein S15a

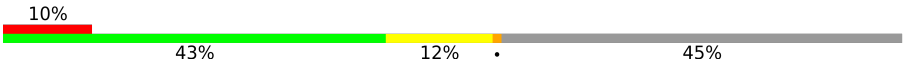
Chain G:

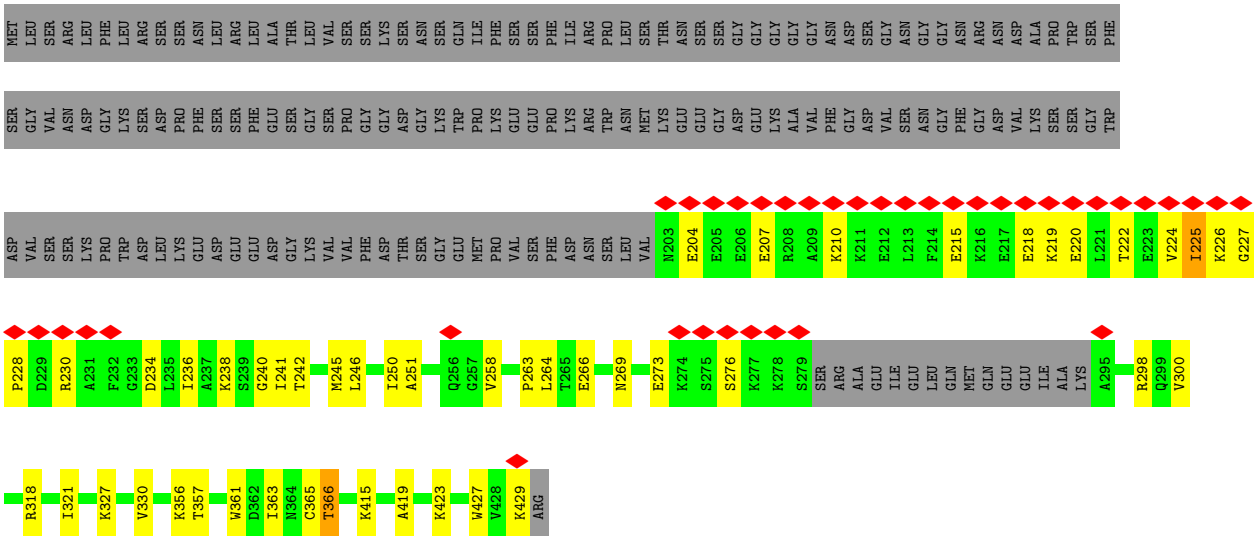




• Molecule 10: 30S ribosomal protein S9

Chain H:

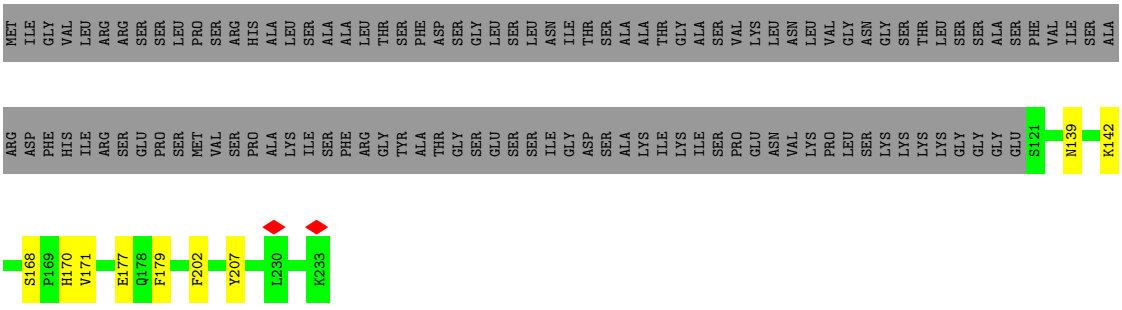




• Molecule 11: Small ribosomal subunit protein uS10 domain-containing protein

Chain I:



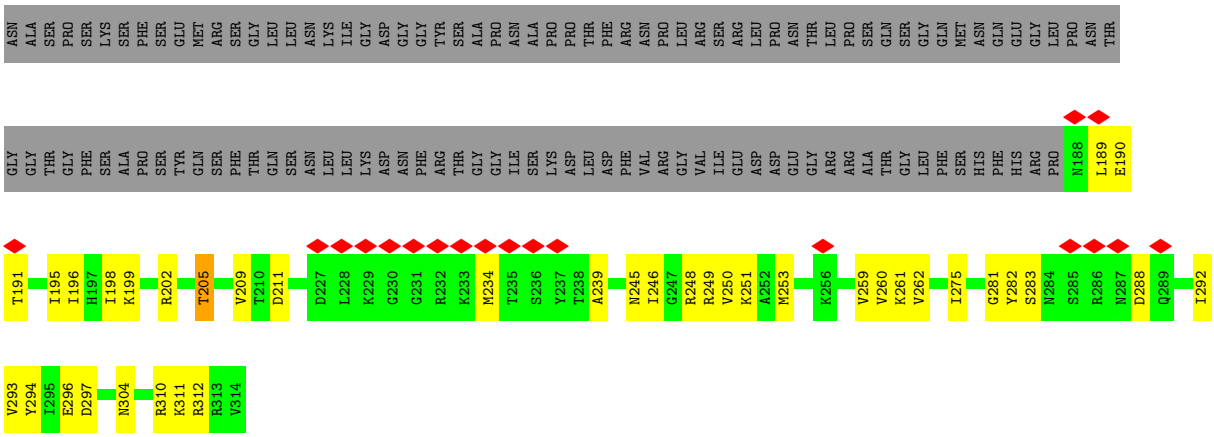


• Molecule 12: Ribosomal protein S11

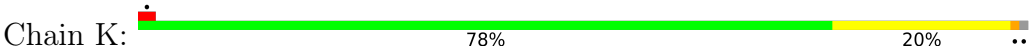
Chain J:







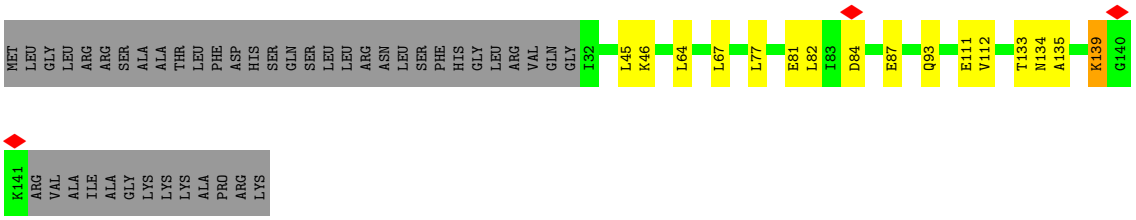
• Molecule 13: Small ribosomal subunit protein uS12m





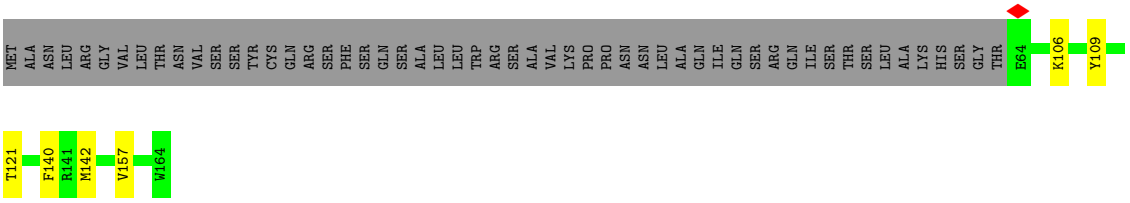
• Molecule 14: uS13m





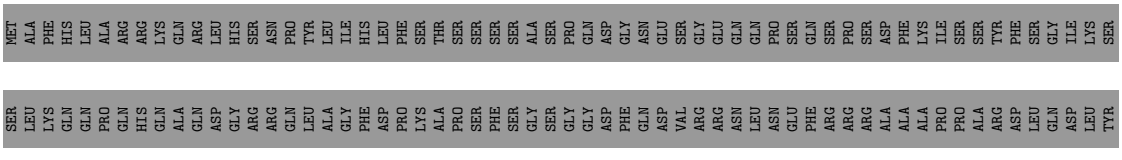
• Molecule 15: Small ribosomal subunit protein uS14m

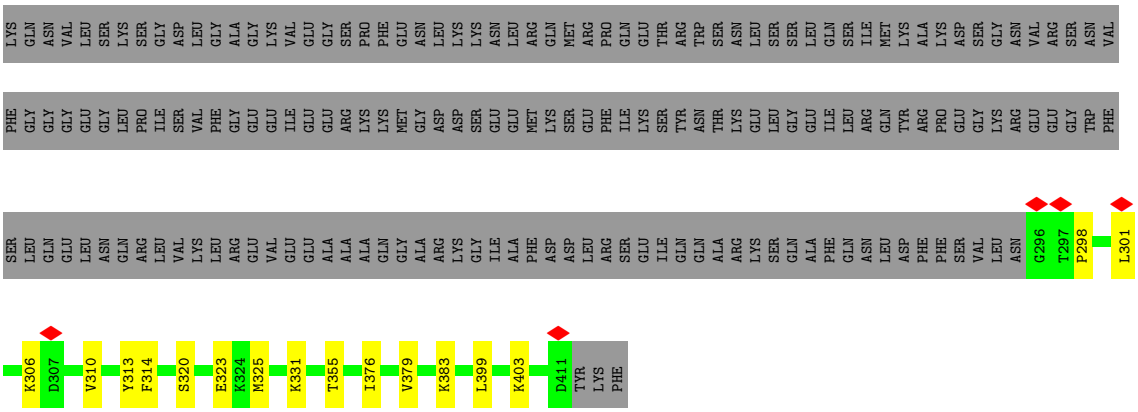




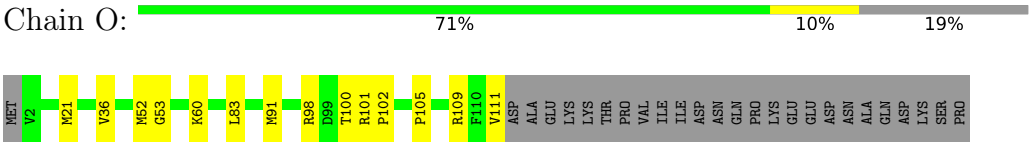
• Molecule 16: Small ribosomal subunit protein uS15c



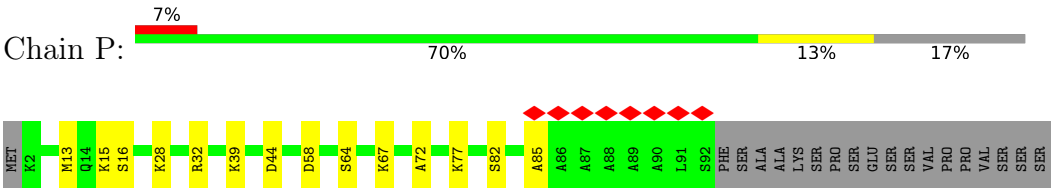




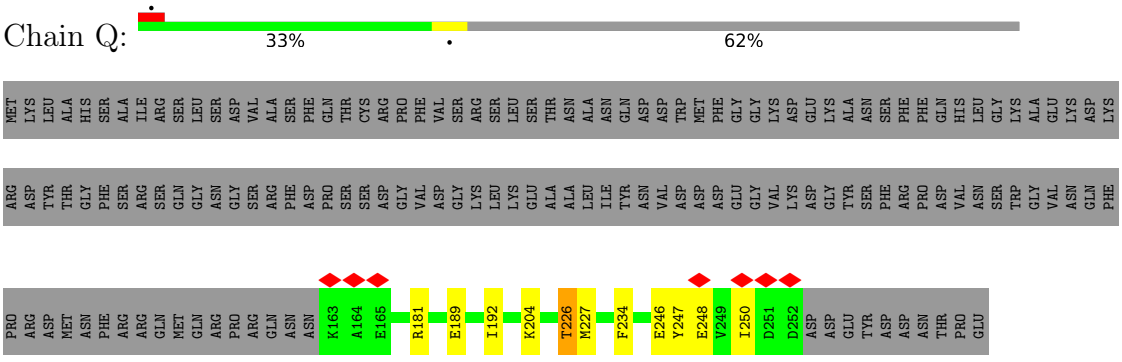
• Molecule 17: 30S ribosomal protein S16



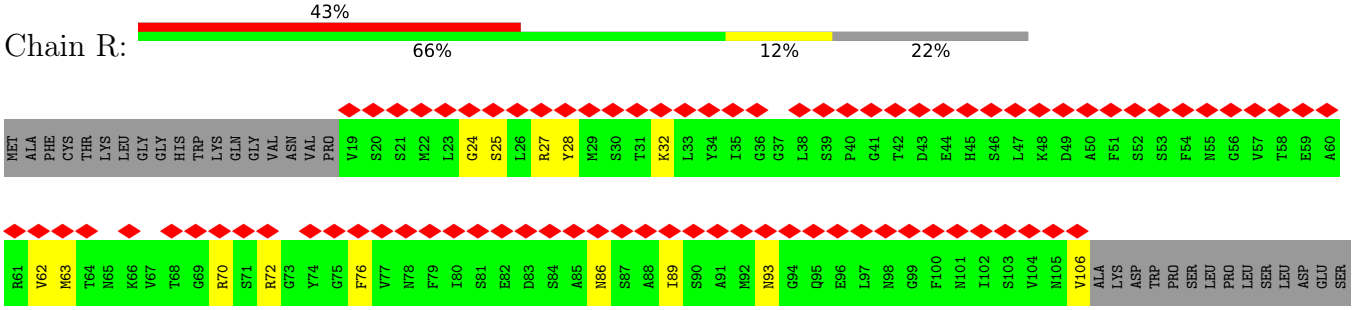
• Molecule 18: Small ribosomal subunit protein uS17c

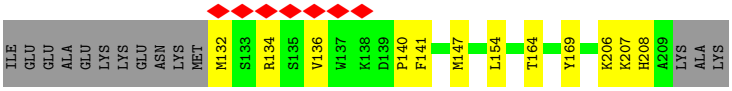


• Molecule 19: Small ribosomal subunit protein bS18c



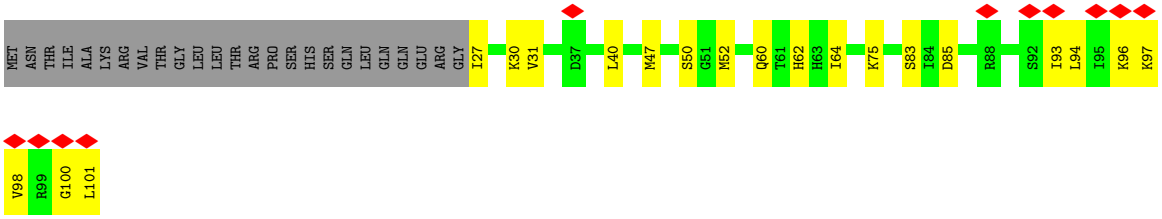
• Molecule 20: Small ribosomal subunit protein uS19m



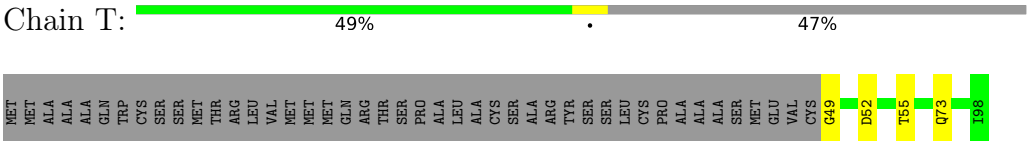


• Molecule 21: Ribosomal protein S21

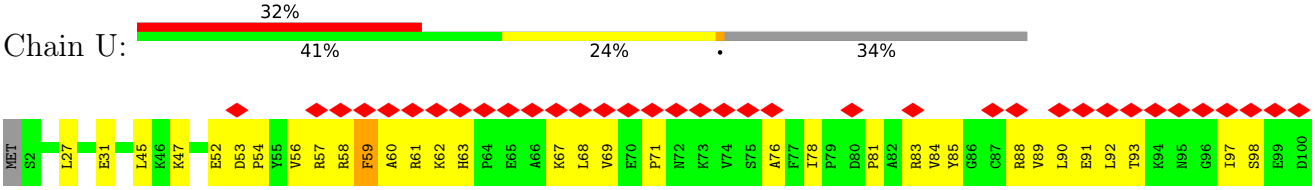




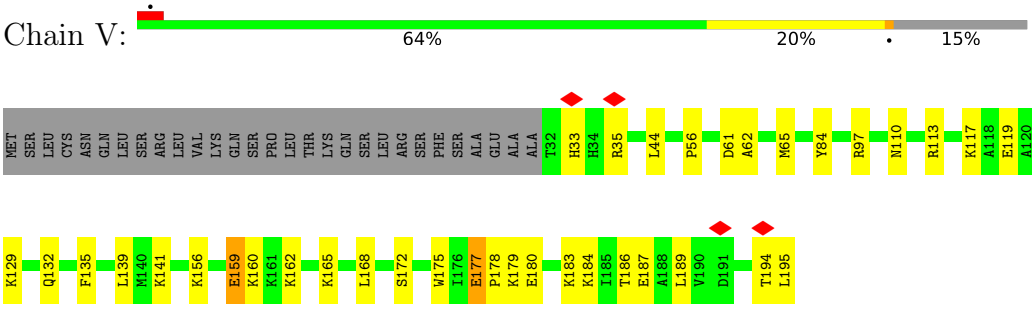
• Molecule 22: 30S ribosomal protein S31, mitochondrial



• Molecule 23: mS23

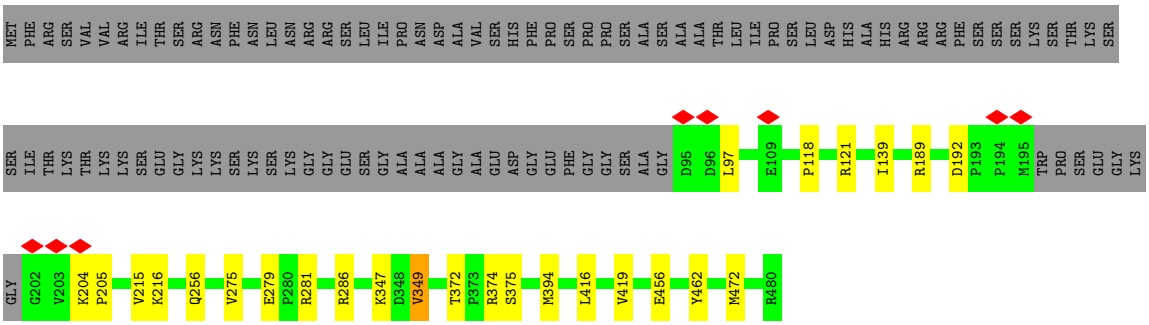


• Molecule 24: mS26



• Molecule 25: Small ribosomal subunit protein mS29

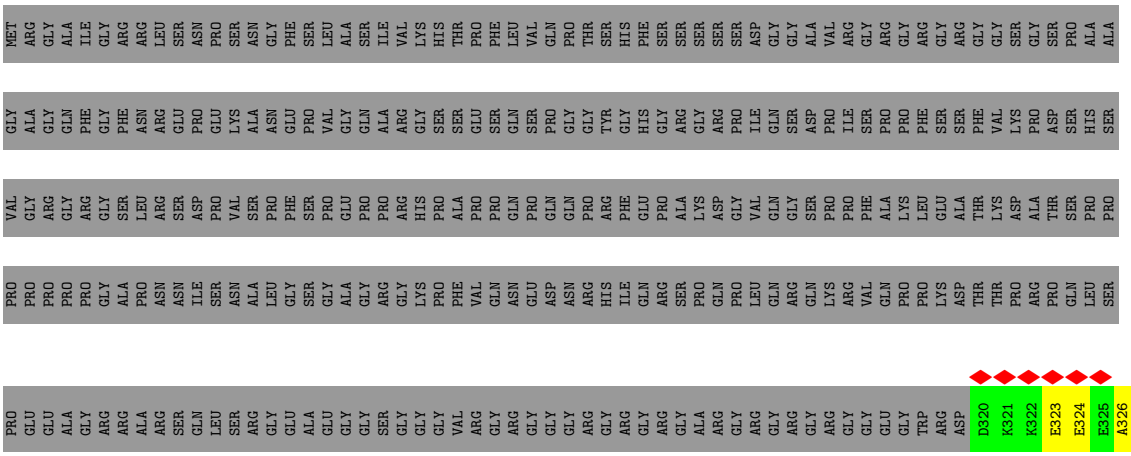




• Molecule 26: BnaC06g06470D protein

Chain X:

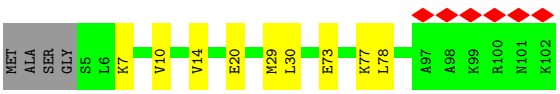




• Molecule 27: MOSC domain-containing protein

Chain Y:

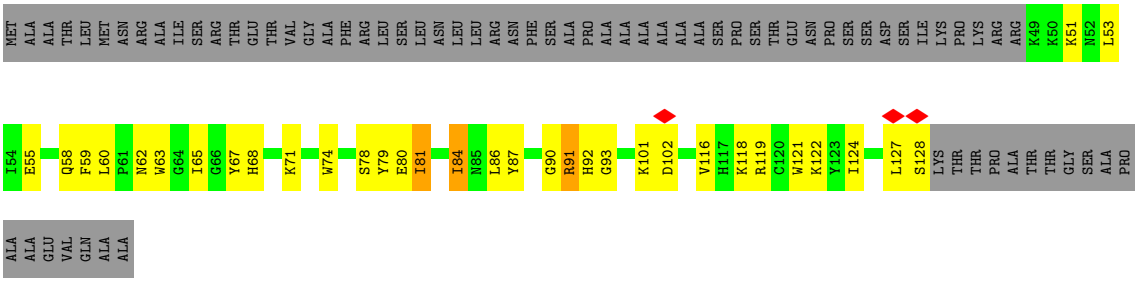




• Molecule 28: Mitochondrial 28S ribosomal protein S34

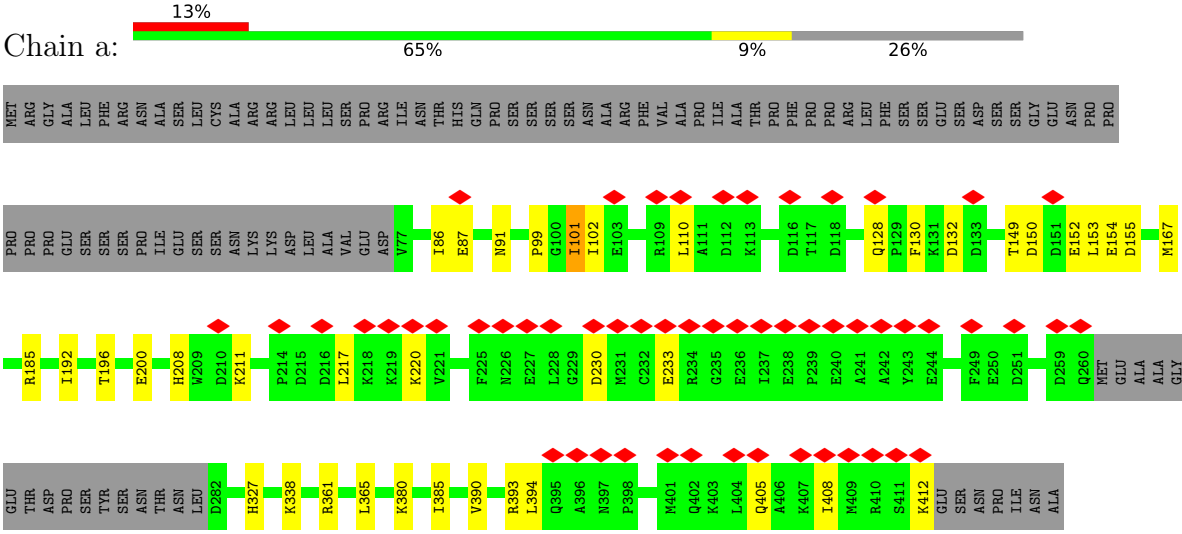
Chain Z:





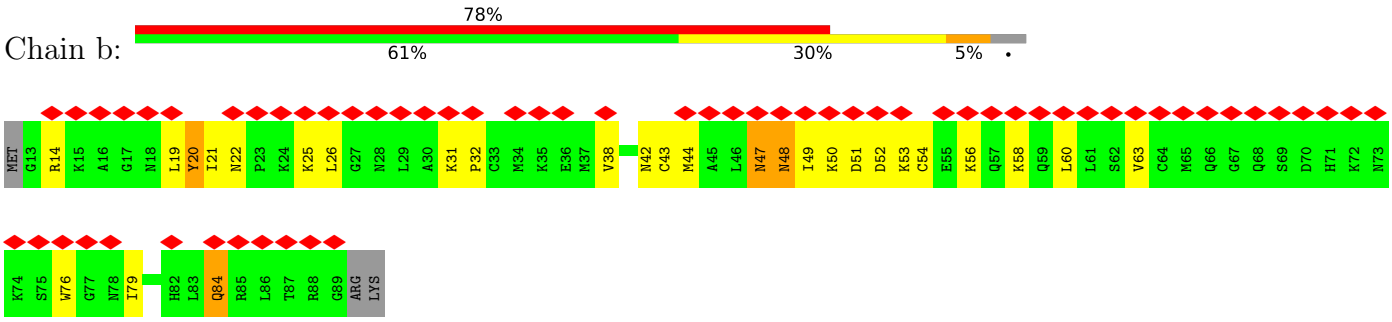
• Molecule 29: Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein

Chain a:



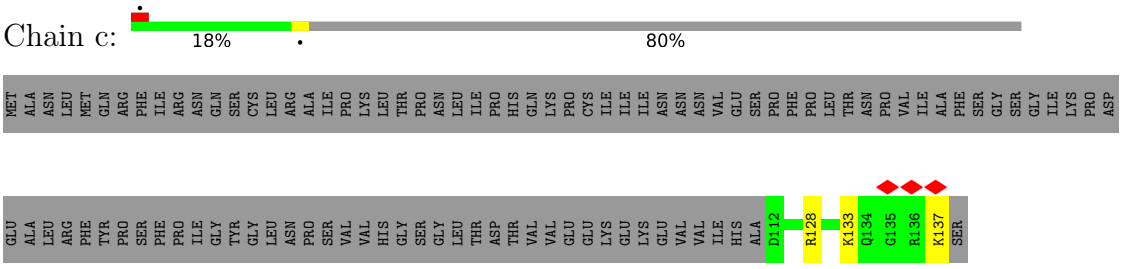
• Molecule 30: IMS import disulfide relay-system CHCH-CHCH-like Cx9C domain-containing protein

Chain b:



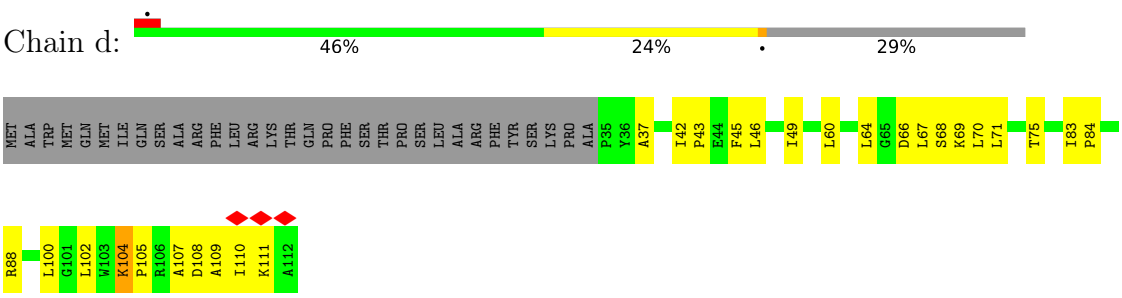
• Molecule 31: Small ribosomal subunit protein mS38

Chain c:



• Molecule 32: IGR domain-containing protein

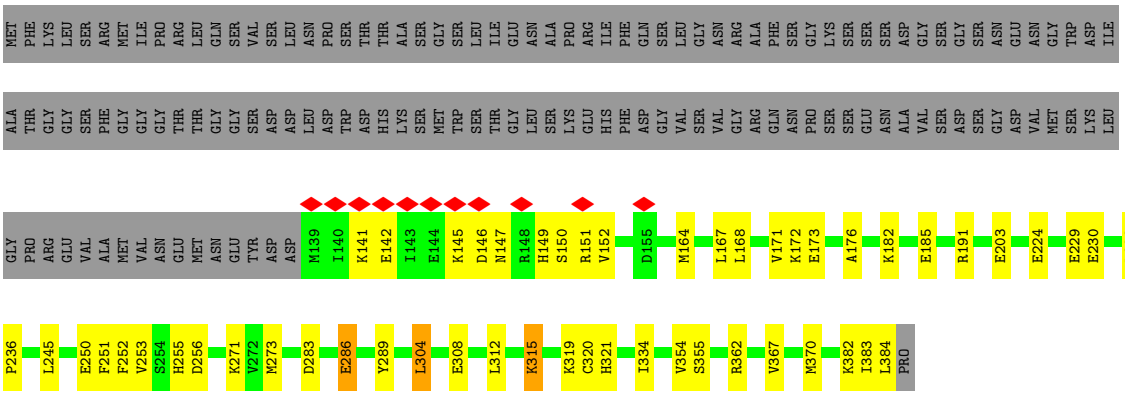
Chain d:



• Molecule 33: mS45

Chain e:

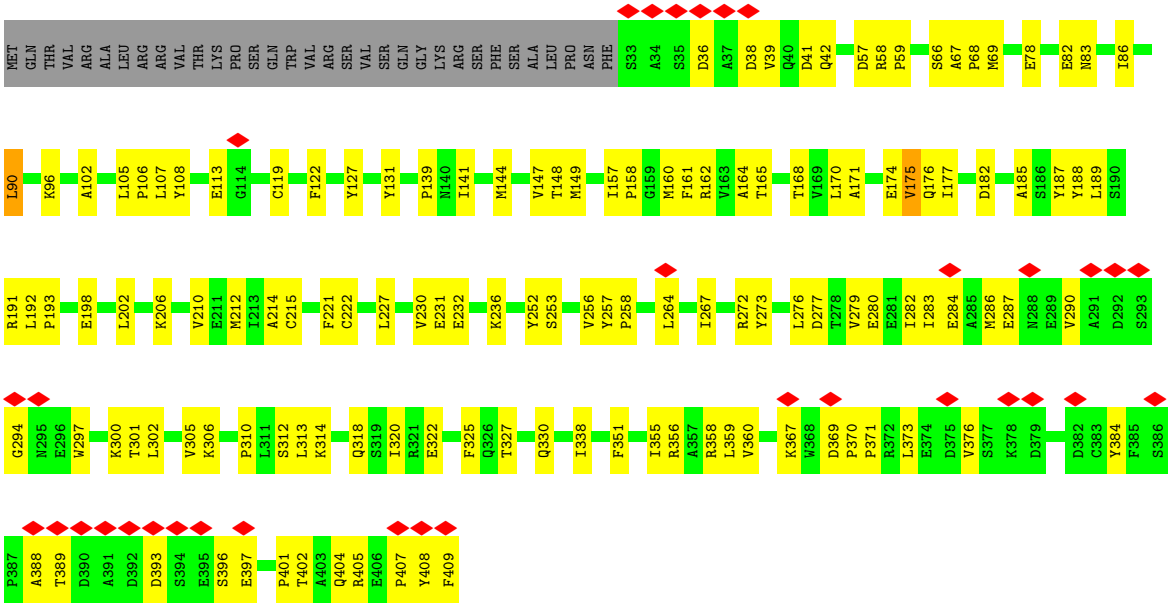




• Molecule 34: mS47

Chain f:

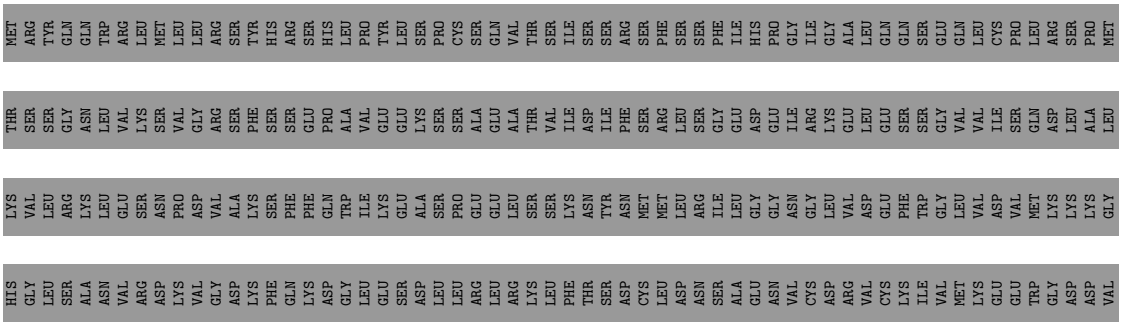


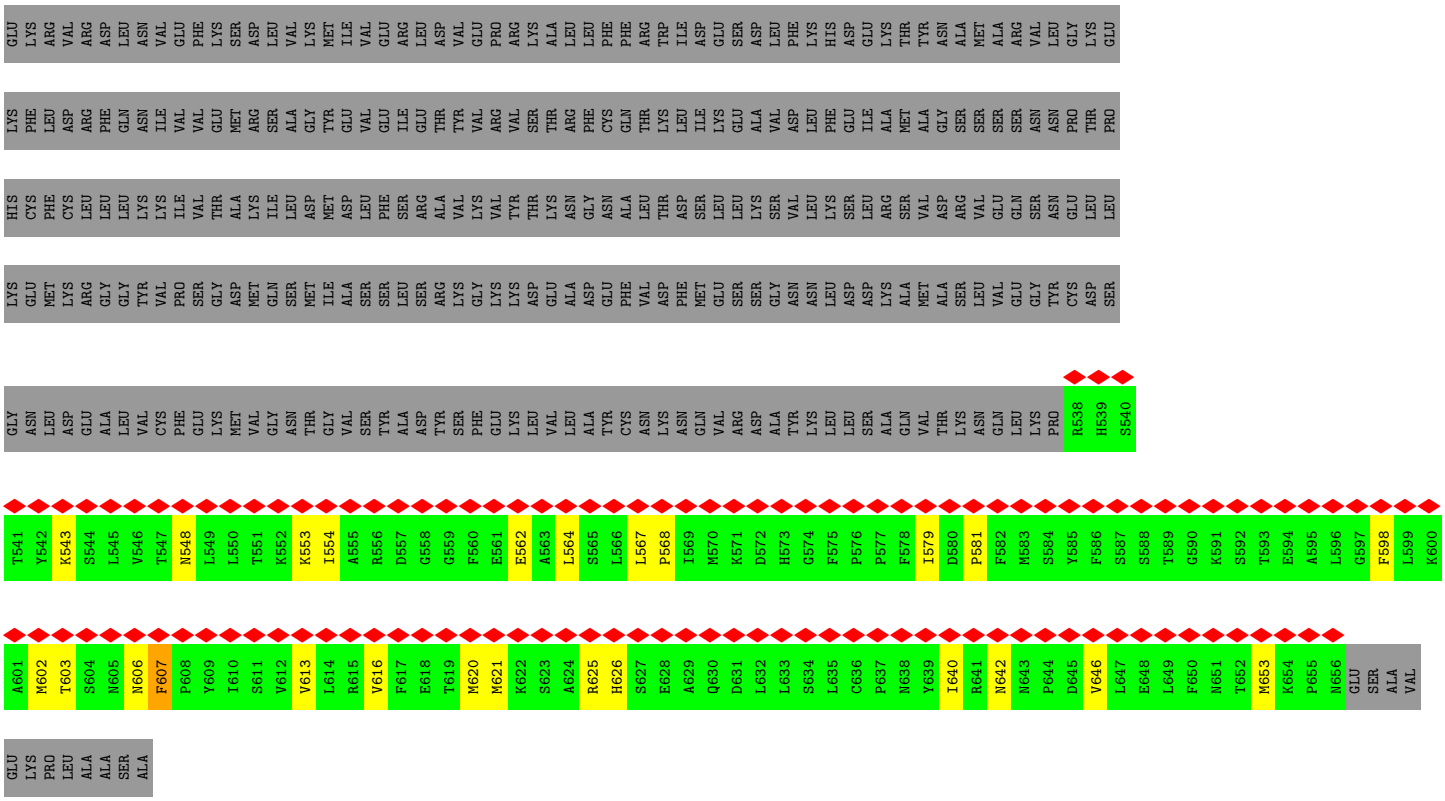


• Molecule 35: Small ribosomal subunit protein mS81 (rPPR8)

Chain g:



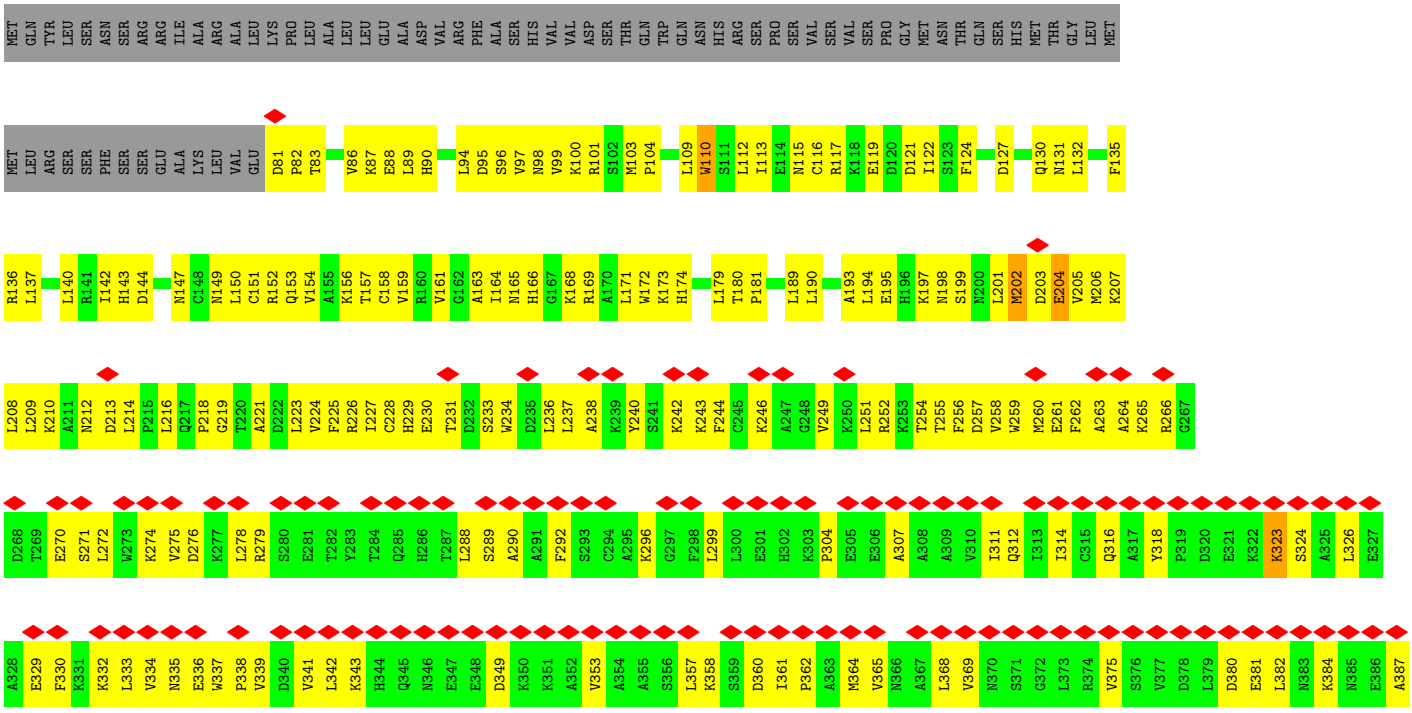




• Molecule 36: (rape) hypothetical protein

Chain h:



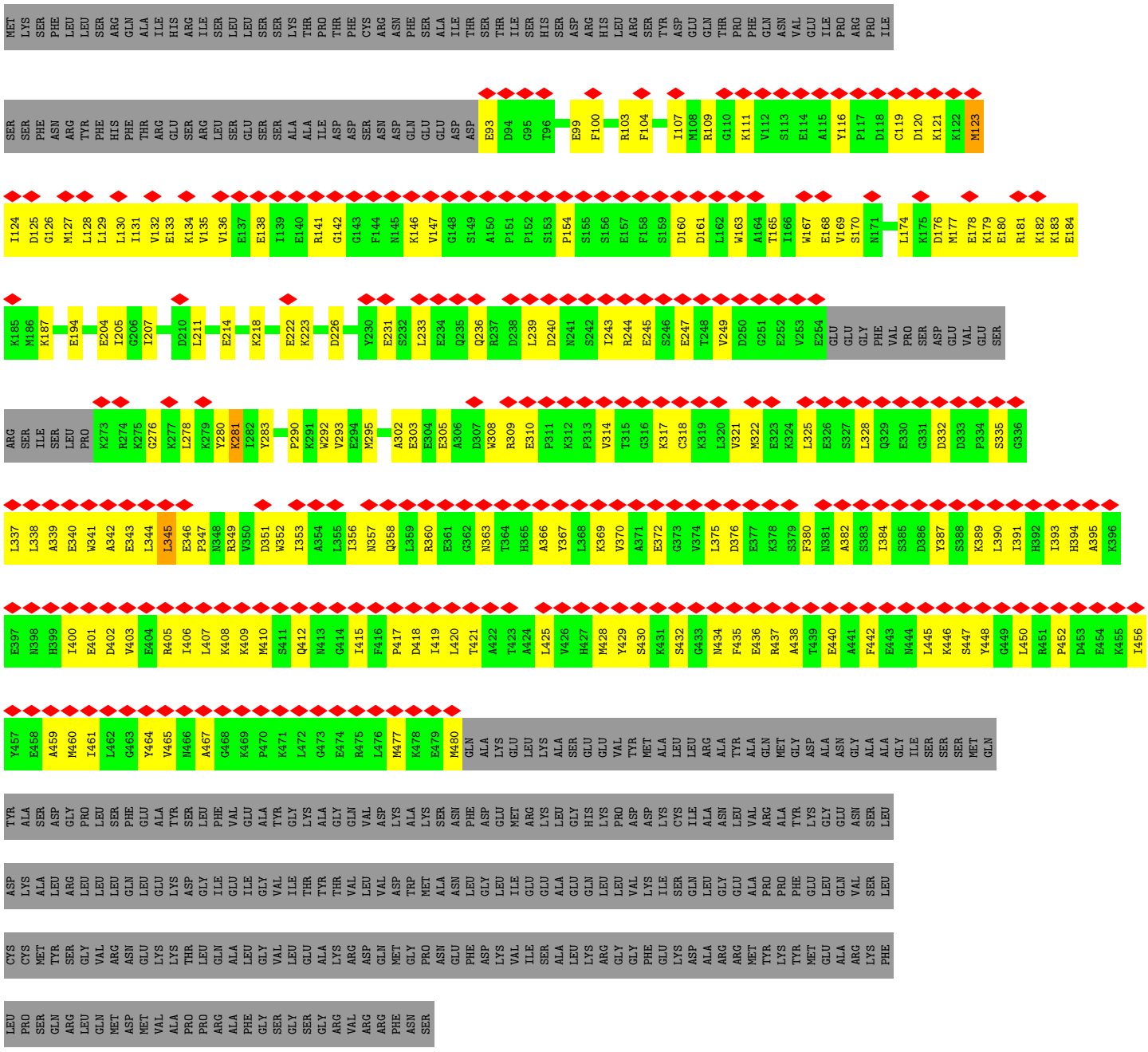




• Molecule 37: PROP1-like PPR domain-containing protein

Chain i:

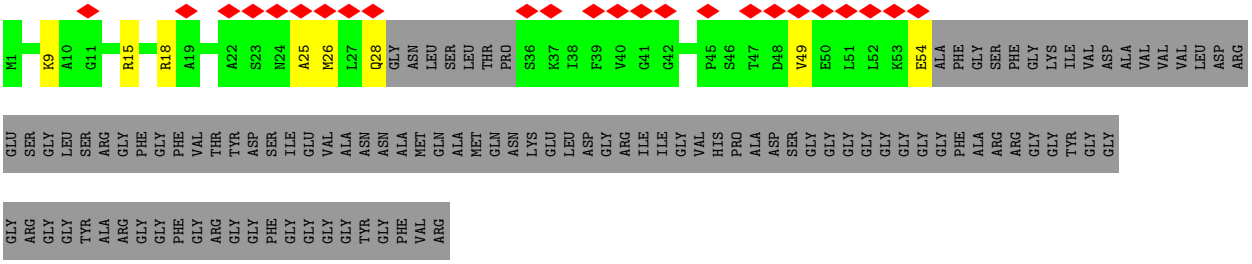




• Molecule 38: Small ribosomal subunit protein mS86

Chain k:

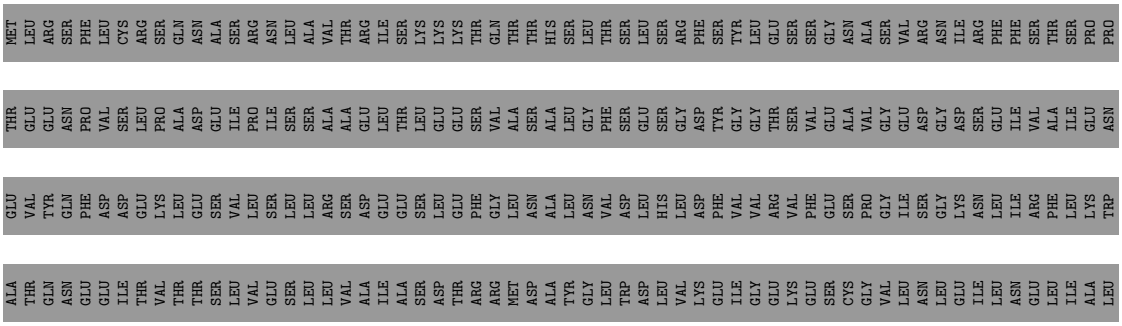


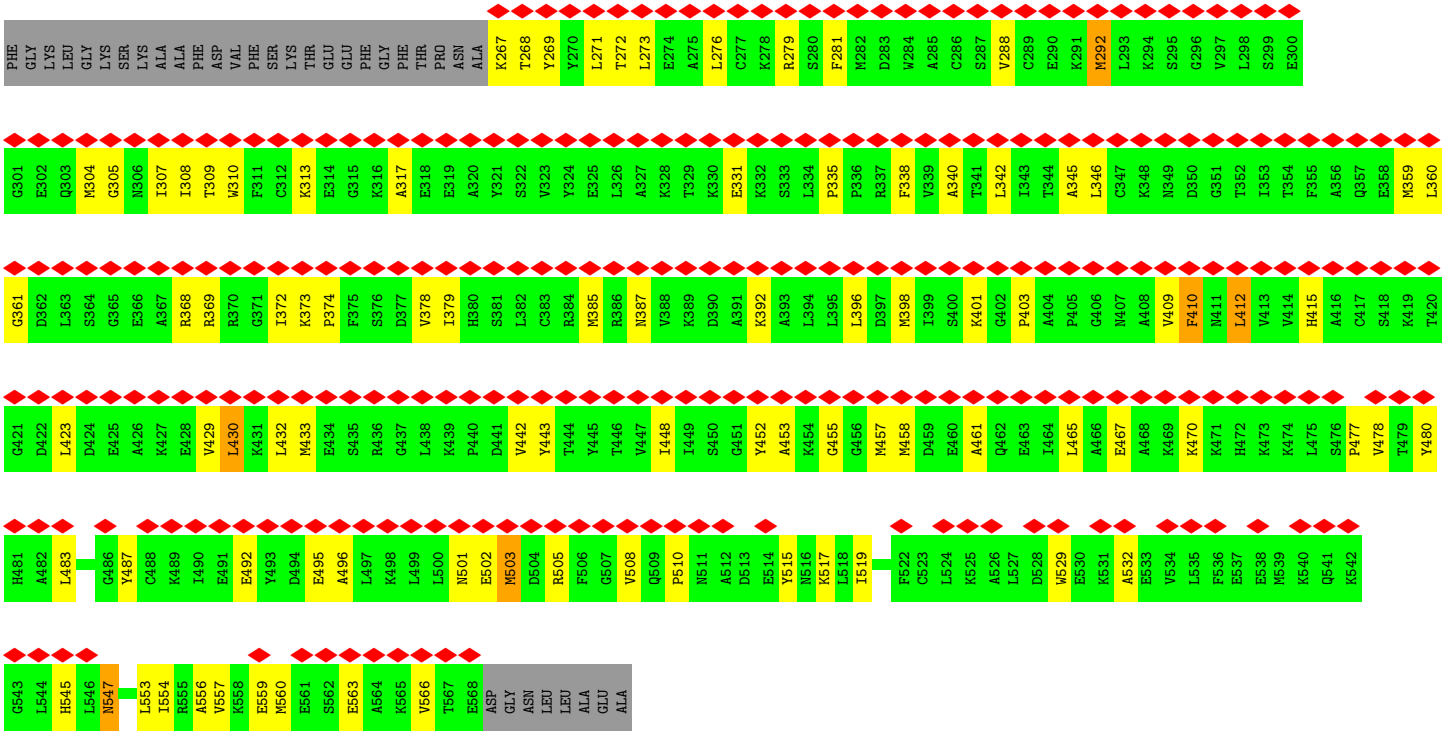


• Molecule 39: Small ribosomal subunit protein mS80 (rPPR6)

Chain l:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141355	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.786	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	676.2, 676.2, 676.2	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.966, 0.966, 0.966	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, 4OC, G7M, MA6, 2MG, ATP

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	0.67	2/38445 (0.0%)	0.90	57/59928 (0.1%)
2	8	0.69	1/891 (0.1%)	0.95	2/1191 (0.2%)
3	A	0.15	0/1647	0.29	0/2227
4	B	0.42	0/3969	0.60	1/5320 (0.0%)
5	C	0.13	0/2859	0.32	0/3828
6	D	0.23	0/3438	0.38	0/4599
7	E	0.12	0/838	0.29	0/1121
8	F	0.34	0/1225	0.51	0/1641
9	G	0.13	0/1054	0.26	0/1418
10	H	0.35	0/1696	0.46	0/2273
11	I	0.41	0/964	0.52	0/1293
12	J	0.35	0/1000	0.47	0/1340
13	K	0.20	0/1010	0.42	0/1345
14	L	0.38	0/883	0.66	5/1176 (0.4%)
15	M	0.41	0/856	0.43	0/1134
16	N	0.12	0/958	0.25	0/1280
17	O	0.14	0/890	0.32	0/1196
18	P	0.12	0/730	0.28	0/984
19	Q	0.11	0/733	0.27	0/978
20	R	0.30	0/1323	0.42	0/1772
21	S	0.18	0/614	0.37	0/809
22	T	0.45	0/416	0.44	0/547
23	U	0.12	0/1036	0.34	0/1395
24	V	0.10	0/1423	0.24	0/1895
25	W	0.34	0/3139	0.44	0/4250
26	X	0.36	0/1644	0.54	0/2216
27	Y	0.36	0/807	0.43	0/1077
28	Z	0.11	0/669	0.34	0/900
29	a	0.39	0/2523	0.55	0/3386
30	b	0.60	0/618	0.94	1/822 (0.1%)
31	c	0.35	0/233	0.58	0/296
32	d	0.26	0/628	0.47	1/840 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
33	e	0.25	0/2118	0.45	1/2828 (0.0%)
34	f	0.11	0/2981	0.34	0/4033
35	g	0.16	0/969	0.44	0/1309
36	h	0.11	0/2511	0.34	0/3391
37	i	0.10	0/3048	0.31	0/4093
38	k	0.12	0/316	0.34	0/423
39	l	0.21	0/2409	0.44	0/3233
All	All	0.48	3/93511 (0.0%)	0.69	68/133787 (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
2	8	0	3
8	F	0	2
31	c	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8	249	HIS	C-O	-8.69	1.12	1.24
1	2	1524	A	N9-C4	-6.50	1.33	1.37
1	2	1524	A	N3-C4	-5.75	1.31	1.34

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8	249	HIS	O-C-N	-14.51	104.36	123.23
1	2	1542	A	N7-C8-N9	11.76	119.68	113.80
30	b	20	TYR	CB-CA-C	-11.15	96.81	111.42
1	2	1542	A	C5-N7-C8	-10.12	98.84	103.90
1	2	1387	C	N1-C2-O2	9.58	124.65	118.90
1	2	1542	A	C8-N9-C4	-8.71	102.31	105.80
1	2	1387	C	C2-N1-C1'	8.26	127.88	118.80
14	L	135	ALA	N-CA-C	-8.12	101.39	112.03
1	2	1387	C	N3-C2-O2	-7.92	116.36	121.90
1	2	1388	A	O4'-C1'-N9	7.37	114.09	108.20
1	2	1524	A	C2-N3-C4	-6.80	107.20	110.60
1	2	1524	A	C5-N7-C8	-6.78	100.51	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1387	C	C6-N1-C2	-6.70	117.62	120.30
1	2	1542	A	C4-C5-N7	6.55	113.98	110.70
1	2	1029	C	N3-C2-O2	-6.52	117.34	121.90
1	2	494	A	O4'-C1'-N9	6.43	113.00	108.50
1	2	1542	A	C6-C5-N7	-6.35	127.85	132.30
1	2	1542	A	N9-C1'-C2'	6.30	118.93	112.00
1	2	1524	A	N7-C8-N9	6.30	116.95	113.80
1	2	1132	C	C2-N1-C1'	6.19	125.61	118.80
1	2	1058	C	C6-N1-C2	-6.19	117.82	120.30
1	2	1565	C	C6-N1-C2	-6.11	117.85	120.30
1	2	1593	G	O4'-C1'-N9	6.09	113.07	108.20
1	2	1421	C	N1-C2-O2	6.08	122.55	118.90
4	B	410	PRO	CB-CA-C	6.06	121.56	111.56
1	2	1541	G	O5'-C5'-C4'	5.99	114.19	109.40
1	2	1117	U	P-O3'-C3'	5.98	126.88	119.70
32	d	104	LYS	O-C-N	-5.96	117.67	121.85
1	2	1706	C	C2-N1-C1'	5.83	125.21	118.80
1	2	1421	C	C2-N1-C1'	5.77	125.15	118.80
1	2	969	G	O5'-C5'-C4'	5.75	114.00	109.40
1	2	1814	G	C3'-C2'-C1'	5.73	105.31	101.30
1	2	1524	A	O4'-C1'-N9	5.72	112.50	108.50
1	2	964	G	O5'-C5'-C4'	5.71	113.97	109.40
1	2	986	G	C4-N9-C1'	5.62	133.81	126.50
1	2	153	A	P-O3'-C3'	5.60	126.42	119.70
1	2	1135	A	O4'-C1'-N9	5.49	112.60	108.20
1	2	1620	U	O4'-C1'-N1	5.49	112.34	108.50
14	L	134	ASN	CA-CB-CG	5.49	118.09	112.60
2	8	249	HIS	CA-C-O	5.47	126.61	120.70
1	2	839	C	O4'-C1'-N1	5.44	112.55	108.20
1	2	1395	A	O5'-C5'-C4'	5.43	113.74	109.40
1	2	1524	A	N3-C4-N9	-5.40	123.08	127.40
1	2	986	G	N3-C4-N9	5.40	129.24	126.00
1	2	1392	A	C2-N3-C4	-5.39	107.90	110.60
1	2	951	A	N9-C1'-C2'	5.39	117.93	112.00
1	2	1029	C	N1-C2-O2	5.39	122.13	118.90
1	2	1387	C	C6-N1-C1'	-5.38	114.34	120.80
33	e	256	ASP	CA-CB-CG	5.36	117.96	112.60
1	2	1651	C	O4'-C1'-N1	5.32	112.46	108.20
1	2	986	G	C8-N9-C1'	-5.32	120.09	127.00
1	2	1055	C	N1-C2-O2	-5.31	115.71	118.90
1	2	1392	A	N1-C2-N3	5.24	131.92	129.30
1	2	762	A	O5'-C5'-C4'	5.24	113.59	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1012	U	O5'-C5'-C4'	5.24	113.59	109.40
1	2	162	C	C1'-O4'-C4'	-5.18	106.08	109.70
14	L	139	LYS	CA-C-O	-5.16	115.25	121.34
1	2	1387	C	C5-C6-N1	5.12	123.56	121.00
1	2	883	G	C3'-C2'-C1'	-5.12	97.40	101.50
14	L	133	THR	CA-C-N	-5.09	114.83	122.47
14	L	133	THR	C-N-CA	-5.09	114.83	122.47
1	2	788	A	C3'-C2'-C1'	-5.09	97.43	101.50
1	2	1542	A	C4-N9-C1'	5.08	135.45	126.30
1	2	1524	A	N3-C4-C5	5.07	130.35	126.80
1	2	459	U	O5'-C5'-C4'	5.07	113.45	109.40
1	2	1025	C	O5'-C5'-C4'	5.07	113.45	109.40
1	2	1524	A	C8-N9-C4	-5.06	103.78	105.80
1	2	1504	G	N3-C4-C5	-5.05	126.08	128.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	8	196	ARG	Sidechain
2	8	248	ARG	Sidechain
2	8	249	HIS	Mainchain
8	F	140	ARG	Sidechain
8	F	146	ARG	Sidechain
31	c	128	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	34484	0	17382	553	0
2	8	874	927	926	22	0
3	A	1611	0	1633	32	0
4	B	3877	0	4008	62	0
5	C	2806	0	2971	108	0
6	D	3389	0	3419	109	0
7	E	823	0	879	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	1254	0	1268	14	0
9	G	1037	0	1058	15	0
10	H	1671	0	1713	58	0
11	I	941	0	970	6	0
12	J	988	0	1022	33	0
13	K	993	0	1052	20	0
14	L	873	0	904	5	0
15	M	843	0	884	3	0
16	N	941	0	978	18	0
17	O	869	0	898	9	0
18	P	717	0	755	9	0
19	Q	724	0	744	17	0
20	R	1299	0	1307	19	0
21	S	611	0	687	22	0
22	T	408	0	444	2	0
23	U	1014	0	1061	57	0
24	V	1399	0	1427	38	0
25	W	3062	0	3030	14	0
26	X	1613	0	1559	21	0
27	Y	793	0	834	7	0
28	Z	649	0	662	28	0
29	a	2486	0	2376	33	0
30	b	610	0	626	32	0
31	c	232	0	278	1	0
32	d	616	0	674	21	0
33	e	2074	0	2074	50	0
34	f	2922	0	2870	113	0
35	g	946	0	948	17	0
36	h	2463	0	2488	221	0
37	i	2993	0	2962	230	0
38	k	313	0	258	9	0
39	l	2371	0	2420	72	0
40	W	31	0	12	0	0
All	All	88620	927	72461	1908	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 12.

All (1908) 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)
36:h:166:HIS:HA	36:h:169:ARG:HD2	1.25	1.14
36:h:234:TRP:HA	36:h:237:LEU:HD12	1.25	1.14
1:2:1750:C:H3'	1:2:1751:U:H5"	1.30	1.14
1:2:1091:A:OP2	3:A:121:LYS:HD2	1.50	1.11
36:h:193:ALA:HB2	36:h:201:LEU:HD22	1.32	1.11
37:i:124:ILE:HA	37:i:127:MET:HE1	1.12	1.11
34:f:369:ASP:HB3	34:f:370:PRO:HD3	1.36	1.07
1:2:202:A:H2'	1:2:203:A:H5"	1.33	1.06
3:A:200:GLN:HA	3:A:203:MET:HE2	1.35	1.05
1:2:1385:A:H4'	39:l:517:LYS:HE3	1.40	1.02
1:2:162:C:H3'	1:2:163:A:H5"	1.37	1.01
5:C:204:THR:HA	6:D:116:GLU:HG2	1.42	1.01
5:C:287:LEU:HD22	6:D:178:LEU:HD23	1.45	0.99
3:A:203:MET:HE3	3:A:205:ILE:HD12	1.44	0.99
37:i:127:MET:HA	37:i:130:LEU:HD12	1.43	0.98
19:Q:227:MET:HE2	21:S:52:MET:HG2	1.46	0.98
1:2:1726:U:H3	1:2:1744:C:N4	1.62	0.97
36:h:197:LYS:HE2	36:h:230:GLU:HB2	1.45	0.97
1:2:1763:U:H4'	1:2:1764:A:H5'	1.47	0.95
1:2:922:G:H1	1:2:1650:C:H42	1.14	0.94
5:C:21:THR:HG21	5:C:77:LEU:HD11	1.48	0.94
23:U:58:ARG:HD2	23:U:103:MET:HE3	1.48	0.94
1:2:1745:A:OP1	36:h:149:ASN:HB3	1.68	0.94
1:2:669:G:H2'	1:2:670:G:C8	2.02	0.94
3:A:200:GLN:HG2	3:A:205:ILE:HB	1.47	0.93
36:h:311:ILE:HD11	36:h:368:LEU:HD21	1.49	0.93
1:2:458:U:H2'	1:2:459:U:H5"	1.48	0.93
1:2:1726:U:H3	1:2:1744:C:H42	0.94	0.93
6:D:218:MET:HE3	33:e:167:LEU:HB3	1.52	0.92
1:2:1567:G:H21	1:2:1594:A:H2	1.17	0.91
37:i:363:ASN:HB3	37:i:366:ALA:HB3	1.53	0.91
1:2:200:C:H5	1:2:246:G:H1	1.19	0.89
5:C:257:LEU:HD12	6:D:194:MET:CE	2.01	0.89
23:U:61:ARG:C	23:U:62:LYS:HD2	1.97	0.89
1:2:1540:C:HO2'	1:2:1542:A:H8	0.93	0.89
1:2:1139:A:H61	1:2:1382:C:H42	1.21	0.88
5:C:180:ILE:HG22	5:C:191:TRP:CZ2	2.08	0.88
36:h:361:ILE:HG22	36:h:362:PRO:HD3	1.55	0.88
5:C:175:LEU:HD11	5:C:198:TRP:HB3	1.51	0.88
37:i:127:MET:O	37:i:131:ILE:HD12	1.74	0.88
1:2:202:A:C2'	1:2:203:A:H5"	2.04	0.88
1:2:65:G:H1	1:2:374:C:H5	1.21	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:163:A:H4'	1:2:164:A:H5'	1.54	0.87
30:b:26:LEU:HD23	38:k:49:VAL:CB	2.03	0.87
37:i:165:THR:HA	37:i:168:GLU:HG2	1.56	0.87
21:S:93:ILE:CD1	30:b:19:LEU:HD22	2.04	0.87
37:i:429:TYR:HB3	37:i:438:ALA:HB2	1.54	0.87
1:2:835:U:H2'	1:2:836:A:O4'	1.74	0.86
5:C:252:MET:HE2	33:e:150:SER:HB3	1.57	0.86
6:D:138:GLU:HB2	6:D:141:ARG:HB2	1.57	0.86
34:f:157:ILE:HA	34:f:162:ARG:HD2	1.56	0.86
1:2:164:A:H2'	1:2:165:A:C8	2.10	0.86
33:e:230:GLU:HG3	33:e:236:PRO:HA	1.57	0.85
36:h:279:ARG:HH22	36:h:290:ALA:HB1	1.40	0.85
23:U:101:ASP:O	23:U:105:VAL:HG12	1.74	0.85
1:2:26:U:H3	1:2:910:G:H1	1.22	0.85
1:2:670:G:H2'	1:2:671:A:H8	1.41	0.84
1:2:1801:A:H5'	13:K:44:LYS:HE2	1.58	0.84
10:H:225:ILE:HA	10:H:228:PRO:HG3	1.58	0.84
36:h:147:ASN:OD1	36:h:150:LEU:HD23	1.77	0.84
36:h:82:PRO:HB2	36:h:87:LYS:HD2	1.60	0.84
13:K:44:LYS:HD2	13:K:44:LYS:H	1.41	0.83
37:i:375:LEU:HD12	37:i:387:TYR:HE1	1.42	0.83
16:N:399:LEU:HD11	16:N:403:LYS:HD2	1.60	0.83
34:f:301:THR:O	34:f:305:VAL:HG23	1.78	0.83
5:C:289:LEU:HD21	33:e:151:ARG:HG2	1.59	0.83
5:C:257:LEU:HD12	6:D:194:MET:HE2	1.59	0.83
30:b:26:LEU:CD2	38:k:49:VAL:CB	2.56	0.83
33:e:147:ASN:HB3	33:e:151:ARG:HH12	1.43	0.82
1:2:612:U:H2'	1:2:613:C:C6	2.14	0.82
36:h:119:GLU:OE2	36:h:163:ALA:HB2	1.79	0.81
37:i:109:ARG:HH21	37:i:124:ILE:HG22	1.43	0.81
37:i:142:GLY:HA3	37:i:146:LYS:HD2	1.62	0.81
1:2:1664:4OC:HM23	1:2:1665:C:H5'	1.62	0.81
37:i:124:ILE:HA	37:i:127:MET:CE	2.03	0.81
37:i:132:VAL:O	37:i:136:VAL:HG12	1.79	0.81
1:2:3:C:O2'	1:2:4:A:H2'	1.79	0.81
5:C:325:THR:HG21	5:C:327:LYS:HZ1	1.46	0.81
34:f:139:PRO:HA	34:f:160:MET:HE3	1.61	0.80
1:2:491:G:H2'	1:2:492:G:C8	2.16	0.80
1:2:144:U:H2'	1:2:145:U:H6	1.46	0.80
1:2:1524:A:H2	1:2:1537:G:H21	1.26	0.80
10:H:207:GLU:HA	10:H:210:LYS:HD2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:242:LEU:HD12	37:i:205:ILE:HD11	1.64	0.80
36:h:342:LEU:HD21	36:h:387:ALA:HB1	1.62	0.80
1:2:1737:A:H3'	1:2:1738:G:H21	1.46	0.80
36:h:153:GLN:HA	36:h:156:LYS:HG2	1.63	0.79
17:O:91:MET:HE3	32:d:100:LEU:HD13	1.64	0.79
10:H:225:ILE:HG22	10:H:226:LYS:H	1.48	0.79
23:U:106:ALA:HA	23:U:109:GLU:OE2	1.82	0.79
1:2:1734:A:H2'	1:2:1735:C:H4'	1.64	0.79
36:h:234:TRP:CZ2	36:h:266:ARG:HG3	2.17	0.79
28:Z:62:ASN:O	28:Z:65:ILE:HD12	1.81	0.79
1:2:1746:A:H2'	1:2:1747:A:H8	1.48	0.78
38:k:25:ALA:HA	38:k:28:GLN:NE2	1.98	0.78
1:2:613:C:H2'	1:2:614:A:C8	2.18	0.78
1:2:1746:A:H2'	1:2:1747:A:C8	2.18	0.78
20:R:140:PRO:HB2	20:R:164:THR:HG21	1.65	0.78
37:i:290:PRO:HA	37:i:293:VAL:HG22	1.62	0.78
33:e:147:ASN:HB3	33:e:151:ARG:NH1	1.98	0.78
37:i:134:LYS:HD2	37:i:134:LYS:O	1.83	0.78
37:i:421:THR:O	37:i:425:LEU:HD13	1.83	0.78
21:S:93:ILE:HD12	30:b:19:LEU:HD22	1.63	0.78
37:i:391:ILE:HD13	37:i:425:LEU:HD11	1.66	0.78
16:N:325:MET:HE1	16:N:355:THR:HG22	1.67	0.77
39:l:373:LYS:HG3	39:l:374:PRO:HD3	1.64	0.77
5:C:260:LEU:CD2	6:D:181:LEU:HG	2.14	0.77
6:D:97:GLU:HA	6:D:100:ARG:HH21	1.49	0.77
34:f:367:LYS:HD2	34:f:367:LYS:O	1.83	0.77
10:H:241:ILE:HG12	10:H:246:LEU:HD13	1.66	0.77
5:C:204:THR:HA	6:D:116:GLU:CG	2.14	0.77
10:H:225:ILE:HA	10:H:228:PRO:CG	2.14	0.77
36:h:339:VAL:O	36:h:343:LYS:HG2	1.84	0.77
1:2:163:A:H1'	1:2:165:A:OP2	1.85	0.77
36:h:96:SER:HA	36:h:100:LYS:HE2	1.67	0.77
37:i:375:LEU:HD12	37:i:387:TYR:CE1	2.19	0.77
13:K:123:LYS:HE3	13:K:125:ILE:HG12	1.66	0.77
37:i:303:GLU:HB3	37:i:309:ARG:HH21	1.50	0.77
36:h:204:GLU:HA	36:h:207:LYS:HG2	1.66	0.76
1:2:659:A:H5"	19:Q:204:LYS:HD2	1.68	0.76
34:f:276:LEU:HB2	34:f:282:ILE:CD1	2.15	0.76
37:i:131:ILE:O	37:i:135:VAL:HG23	1.85	0.76
5:C:325:THR:HG21	5:C:327:LYS:NZ	2.01	0.76
10:H:230:ARG:HH11	10:H:230:ARG:HG3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:114:ARG:HB2	13:K:119:ALA:HB3	1.67	0.76
23:U:58:ARG:HD2	23:U:103:MET:CE	2.14	0.76
36:h:244:PHE:HD1	36:h:249:VAL:HG21	1.51	0.76
36:h:263:ALA:HB3	36:h:272:LEU:HD13	1.68	0.76
37:i:128:LEU:O	37:i:132:VAL:HG12	1.84	0.76
4:B:96:ARG:HH21	26:X:326:ALA:HB3	1.51	0.76
5:C:303:LEU:HB3	6:D:160:GLU:OE2	1.85	0.76
36:h:202:MET:C	36:h:206:MET:HE2	2.11	0.75
36:h:259:TRP:CZ3	36:h:275:VAL:HG12	2.21	0.75
1:2:492:G:O2'	1:2:494:A:H1'	1.86	0.75
1:2:356:G:H2'	1:2:357:A:C8	2.21	0.75
1:2:670:G:H2'	1:2:671:A:C8	2.21	0.75
5:C:260:LEU:HD21	6:D:181:LEU:HG	1.68	0.75
1:2:78:U:O2'	1:2:79:G:O5'	2.05	0.75
1:2:709:G:H2'	1:2:710:G:C8	2.22	0.75
1:2:1701:C:H2'	1:2:1702:G:C8	2.22	0.75
1:2:1703:G:H2'	1:2:1704:A:O4'	1.86	0.75
33:e:142:GLU:HA	33:e:145:LYS:HD2	1.69	0.75
1:2:573:G:O2'	1:2:817:G:H5'	1.86	0.75
36:h:229:HIS:HA	36:h:262:PHE:CZ	2.21	0.75
6:D:403:GLU:HG2	6:D:404:THR:HG23	1.69	0.74
36:h:137:LEU:HD21	36:h:143:HIS:CD2	2.21	0.74
37:i:452:PRO:HB3	37:i:456:ILE:HG21	1.68	0.74
1:2:710:G:H2'	1:2:711:A:C8	2.22	0.74
36:h:97:VAL:HG13	36:h:135:PHE:CD1	2.21	0.74
36:h:361:ILE:CG2	36:h:362:PRO:HD3	2.17	0.74
1:2:1797:G:H2'	1:2:1798:G:H8	1.50	0.74
5:C:182:LYS:CE	5:C:220:LEU:HB3	2.18	0.74
37:i:245:GLU:O	37:i:249:VAL:HG23	1.87	0.74
1:2:1769:C:H4'	1:2:1770:G:OP1	1.87	0.74
1:2:1833:U:H2'	1:2:1834:G:C8	2.23	0.74
5:C:210:LEU:HD12	6:D:87:VAL:HG22	1.69	0.74
5:C:183:LEU:HD12	5:C:220:LEU:HD23	1.68	0.73
1:2:1736:U:H4'	1:2:1737:A:C8	2.22	0.73
1:2:1137:G:H3'	1:2:1138:G:H21	1.52	0.73
33:e:168:LEU:O	33:e:172:LYS:HG2	1.88	0.73
1:2:323:C:C2'	1:2:324:G:H5'	2.19	0.73
5:C:285:SER:HB2	33:e:151:ARG:HH21	1.53	0.73
34:f:131:TYR:OH	34:f:407:PRO:HG3	1.87	0.73
36:h:103:MET:HE1	36:h:132:LEU:HD22	1.69	0.73
36:h:365:VAL:O	36:h:369:VAL:HG23	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:261:PHE:HB3	37:i:236:GLN:OE1	1.89	0.73
37:i:218:LYS:O	37:i:222:GLU:HG2	1.88	0.73
36:h:122:ILE:HD11	36:h:161:VAL:HG21	1.71	0.73
7:E:42:SER:HB2	7:E:65:MET:HE3	1.71	0.73
34:f:257:TYR:OH	37:i:293:VAL:HG12	1.89	0.73
34:f:369:ASP:HB3	34:f:370:PRO:CD	2.18	0.73
36:h:90:HIS:HE1	36:h:127:ASP:HB3	1.52	0.73
6:D:191:TYR:O	6:D:194:MET:HB2	1.88	0.72
37:i:176:ASP:O	37:i:180:GLU:HG2	1.89	0.72
1:2:660:G:H22	1:2:737:G:H1	1.37	0.72
36:h:203:ASP:O	36:h:207:LYS:HG2	1.88	0.72
1:2:368:G:O2'	1:2:369:G:H5'	1.90	0.72
1:2:1679:G:H5"	1:2:1680:A:OP1	1.90	0.72
1:2:997:G:H1	1:2:1029:C:H5	1.37	0.72
34:f:409:PHE:HD1	37:i:187:LYS:HZ1	1.38	0.72
9:G:17:GLU:HG3	9:G:68:VAL:CG1	2.19	0.72
1:2:81:U:H2'	1:2:82:C:H1'	1.72	0.72
1:2:1718:A:H2'	1:2:1719:G:H8	1.54	0.72
1:2:1750:C:C3'	1:2:1751:U:H5"	2.16	0.72
35:g:642:ASN:HB3	39:l:372:ILE:HG21	1.71	0.72
1:2:163:A:C4'	1:2:164:A:H5'	2.19	0.72
1:2:493:A:H4'	1:2:494:A:OP1	1.88	0.72
34:f:165:THR:O	34:f:168:THR:HG22	1.89	0.72
37:i:142:GLY:CA	37:i:146:LYS:HD2	2.20	0.72
1:2:458:U:C2'	1:2:459:U:H5"	2.20	0.71
5:C:252:MET:HE2	33:e:150:SER:CB	2.19	0.71
37:i:322:MET:HA	37:i:325:LEU:HG	1.69	0.71
1:2:1540:C:O2'	1:2:1542:A:H8	1.71	0.71
12:J:249:ARG:O	12:J:253:MET:HG2	1.90	0.71
36:h:103:MET:SD	36:h:104:PRO:HD2	2.30	0.71
36:h:193:ALA:CB	36:h:201:LEU:HD22	2.16	0.71
23:U:105:VAL:O	23:U:108:MET:HG2	1.90	0.71
1:2:323:C:H2'	1:2:324:G:H5'	1.73	0.71
24:V:178:PRO:HG2	24:V:179:LYS:HE2	1.73	0.71
21:S:97:LYS:HE2	38:k:54:GLU:HA	1.71	0.71
37:i:134:LYS:HD2	37:i:134:LYS:C	2.14	0.71
36:h:274:LYS:O	36:h:278:LEU:HG	1.90	0.71
37:i:417:PRO:HB3	37:i:421:THR:CG2	2.20	0.71
6:D:217:LEU:HD11	37:i:207:ILE:HD11	1.71	0.71
3:A:203:MET:HE3	3:A:205:ILE:CD1	2.19	0.71
36:h:197:LYS:HD2	36:h:230:GLU:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:457:C:H2'	1:2:458:U:O2	1.90	0.70
33:e:141:LYS:HB3	33:e:145:LYS:HE3	1.73	0.70
36:h:244:PHE:CD1	36:h:249:VAL:HG21	2.25	0.70
1:2:613:C:H2'	1:2:614:A:H8	1.55	0.70
1:2:1703:G:H3'	1:2:1704:A:H8	1.56	0.70
3:A:116:PHE:HD1	3:A:123:LEU:HD23	1.56	0.70
6:D:187:LEU:HB2	37:i:244:ARG:NH2	2.07	0.70
37:i:180:GLU:O	37:i:184:GLU:HG2	1.90	0.70
26:X:429:LYS:HA	26:X:429:LYS:HE3	1.72	0.70
4:B:144:ASN:HA	4:B:147:ARG:HB2	1.73	0.70
34:f:107:LEU:HD11	34:f:119:CYS:HA	1.72	0.70
18:P:58:ASP:OD2	18:P:72:ALA:HB2	1.91	0.70
1:2:144:U:H2'	1:2:145:U:C6	2.27	0.70
1:2:1739:U:H2'	1:2:1740:C:C6	2.27	0.70
37:i:339:ALA:O	37:i:343:GLU:HG2	1.91	0.70
37:i:429:TYR:CB	37:i:438:ALA:HB2	2.22	0.70
1:2:1686:U:H2'	1:2:1687:U:H6	1.57	0.69
1:2:50:A:H2'	1:2:51:U:C6	2.27	0.69
4:B:161:ARG:HH12	4:B:426:PHE:HB2	1.57	0.69
12:J:189:LEU:HD23	19:Q:246:GLU:HG2	1.74	0.69
36:h:194:LEU:HD11	36:h:226:ARG:HG2	1.73	0.69
36:h:335:ASN:OD1	36:h:381:GLU:HG2	1.93	0.69
3:A:74:PRO:HA	3:A:77:ASP:OD1	1.93	0.69
34:f:297:TRP:O	34:f:301:THR:HG23	1.92	0.69
1:2:1702:G:H2'	1:2:1703:G:C8	2.28	0.69
5:C:260:LEU:O	5:C:264:LYS:HB3	1.91	0.69
36:h:86:VAL:HG21	36:h:121:ASP:HB2	1.74	0.69
37:i:337:LEU:O	37:i:340:GLU:HG3	1.93	0.69
1:2:1801:A:O2'	1:2:1802:A:H5'	1.93	0.69
36:h:227:ILE:O	36:h:230:GLU:HG3	1.92	0.69
37:i:400:ILE:O	37:i:403:VAL:HG12	1.93	0.69
5:C:176:VAL:HA	5:C:180:ILE:CG2	2.22	0.69
1:2:151:A:O2'	1:2:153:A:H1'	1.93	0.69
1:2:292:A:O2'	1:2:293:A:H5'	1.93	0.69
1:2:1730:U:H2'	1:2:1731:A:C8	2.28	0.69
4:B:461:LYS:HE2	4:B:526:VAL:HG13	1.73	0.69
5:C:180:ILE:HG13	5:C:181:GLY:N	2.07	0.69
5:C:43:ARG:HB2	6:D:144:GLU:HG3	1.74	0.68
36:h:150:LEU:O	36:h:154:VAL:HG12	1.93	0.68
36:h:227:ILE:HD12	36:h:228:CYS:N	2.08	0.68
1:2:359:U:H3	1:2:368:G:H1	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:78:ARG:HB3	6:D:78:ARG:NH1	2.08	0.68
23:U:68:LEU:O	23:U:71:PRO:HD2	1.93	0.68
34:f:227:LEU:O	34:f:231:GLU:HG2	1.93	0.68
5:C:257:LEU:HD12	6:D:194:MET:HE1	1.73	0.68
1:2:1693:C:O2'	1:2:1694:G:H5'	1.93	0.68
5:C:305:MET:HG3	6:D:157:TRP:CH2	2.29	0.68
5:C:313:GLU:HG3	5:C:340:PRO:HB3	1.75	0.68
10:H:269:ASN:O	10:H:273:GLU:HG3	1.94	0.68
36:h:90:HIS:CE1	36:h:127:ASP:HB3	2.28	0.68
1:2:1683:U:H2'	1:2:1684:G:O4'	1.94	0.68
1:2:1767:G:H3'	1:2:1768:A:H5"	1.75	0.68
34:f:277:ASP:HB3	37:i:121:LYS:NZ	2.08	0.68
1:2:1686:U:H2'	1:2:1687:U:C6	2.28	0.68
1:2:1742:C:H2'	1:2:1743:A:C1'	2.24	0.68
23:U:62:LYS:HD2	23:U:62:LYS:N	2.08	0.68
36:h:193:ALA:HB2	36:h:201:LEU:CD2	2.19	0.68
1:2:922:G:H1	1:2:1650:C:N4	1.91	0.68
1:2:1752:U:H2'	1:2:1753:U:C6	2.29	0.68
6:D:236:ILE:HG22	33:e:171:VAL:HG11	1.74	0.68
28:Z:81:ILE:HD11	28:Z:84:ILE:CG2	2.24	0.68
2:8:200:LEU:HG	2:8:202:VAL:HG23	1.76	0.68
39:l:477:PRO:HG3	39:l:508:VAL:HG13	1.76	0.68
36:h:209:LEU:HD12	36:h:214:LEU:HB2	1.76	0.67
34:f:108:TYR:HE2	34:f:360:VAL:HG21	1.59	0.67
39:l:467:GLU:HA	39:l:470:LYS:HD3	1.74	0.67
1:2:48:C:H2'	1:2:49:U:C6	2.30	0.67
36:h:157:THR:O	36:h:161:VAL:HG22	1.94	0.67
1:2:129:A:O2'	1:2:130:A:H5'	1.95	0.67
1:2:654:G:H2'	1:2:655:A:C8	2.29	0.67
8:F:62:GLU:HA	8:F:132:LEU:HD11	1.76	0.67
24:V:180:GLU:O	24:V:184:LYS:HG2	1.94	0.67
37:i:179:LYS:HE2	37:i:183:LYS:HE3	1.77	0.67
23:U:68:LEU:C	23:U:71:PRO:HD2	2.19	0.67
36:h:330:PHE:HA	36:h:333:LEU:HD13	1.76	0.67
39:l:452:TYR:HB3	39:l:461:ALA:HB2	1.77	0.67
36:h:194:LEU:HG	36:h:230:GLU:OE2	1.94	0.67
36:h:260:MET:HE1	36:h:279:ARG:CZ	2.24	0.67
36:h:97:VAL:O	36:h:101:ARG:HD2	1.95	0.67
36:h:204:GLU:HA	36:h:207:LYS:CG	2.23	0.67
36:h:236:LEU:HD22	36:h:240:TYR:CE2	2.30	0.67
1:2:409:U:H2'	1:2:410:C:C6	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1710:G:O2'	1:2:1711:A:H5'	1.95	0.67
4:B:514:VAL:HB	4:B:517:GLN:HG3	1.77	0.67
10:H:225:ILE:HG23	10:H:228:PRO:HG3	1.77	0.67
18:P:82:SER:HB3	18:P:85:ALA:HB3	1.76	0.67
37:i:417:PRO:HB3	37:i:421:THR:HG21	1.75	0.67
1:2:647:C:O2'	1:2:648:U:H5'	1.94	0.66
5:C:182:LYS:HE3	5:C:220:LEU:HB3	1.77	0.66
16:N:399:LEU:CD1	16:N:403:LYS:HD2	2.24	0.66
20:R:86:ASN:HA	20:R:89:ILE:HD12	1.76	0.66
36:h:213:ASP:O	36:h:213:ASP:OD1	2.13	0.66
36:h:216:LEU:HD12	36:h:244:PHE:CE1	2.31	0.66
37:i:341:TRP:CH2	37:i:345:LEU:HG	2.30	0.66
2:8:227:ILE:HG22	2:8:227:ILE:O	1.93	0.66
36:h:259:TRP:CH2	36:h:275:VAL:HG12	2.29	0.66
32:d:66:ASP:OD2	32:d:68:SER:HB2	1.95	0.66
12:J:251:LYS:O	12:J:251:LYS:HD3	1.96	0.66
1:2:1744:C:H3'	1:2:1745:A:C5'	2.26	0.66
5:C:158:ASN:HD21	5:C:162:ARG:HH11	1.42	0.66
5:C:180:ILE:HG22	5:C:191:TRP:HZ2	1.61	0.66
25:W:372:THR:HG22	25:W:374:ARG:H	1.60	0.66
1:2:1618:G:H2'	1:2:1619:A:C8	2.31	0.66
1:2:1732:A:H2'	1:2:1733:C:O4'	1.96	0.66
23:U:76:ALA:HA	38:k:15:ARG:HH21	1.61	0.66
1:2:654:G:H2'	1:2:655:A:H8	1.60	0.66
34:f:171:ALA:HB2	34:f:206:LYS:HD2	1.76	0.66
1:2:718:A:H2	1:2:729:A:H61	1.43	0.66
37:i:407:LEU:O	37:i:410:MET:HG3	1.96	0.66
1:2:154:G:C6	36:h:172:TRP:CD1	2.83	0.65
1:2:673:U:H3	1:2:709:G:H22	1.41	0.65
5:C:46:ARG:CZ	6:D:148:SER:HB3	2.26	0.65
21:S:93:ILE:HD12	30:b:19:LEU:CD2	2.25	0.65
25:W:215:VAL:HG22	25:W:216:LYS:HG2	1.78	0.65
37:i:141:ARG:NH1	37:i:141:ARG:HA	2.11	0.65
37:i:356:ILE:HD12	37:i:357:ASN:N	2.11	0.65
2:8:217:LEU:HD11	2:8:238:ALA:HB2	1.79	0.65
37:i:165:THR:HA	37:i:168:GLU:CG	2.25	0.65
37:i:314:VAL:HG13	37:i:318:CYS:HB3	1.77	0.65
37:i:460:MET:HE2	37:i:460:MET:HA	1.78	0.65
33:e:191:ARG:HG2	33:e:191:ARG:HH11	1.61	0.65
34:f:90:LEU:HD12	34:f:141:ILE:HB	1.77	0.65
1:2:968:A:H4'	1:2:969:G:H5"	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:399:MET:HE3	29:a:102:ILE:HB	1.77	0.65
23:U:52:GLU:O	23:U:56:VAL:HG23	1.95	0.65
34:f:185:ALA:HA	34:f:188:TYR:CE2	2.32	0.65
39:l:317:ALA:HB1	39:l:346:LEU:HD22	1.79	0.65
1:2:1687:U:H2'	1:2:1688:U:C6	2.32	0.65
5:C:261:PHE:CD2	37:i:233:LEU:HD22	2.31	0.65
23:U:85:TYR:HE1	23:U:106:ALA:HB3	1.61	0.65
5:C:53:LYS:O	5:C:56:LYS:HG2	1.97	0.65
23:U:115:LYS:HZ2	23:U:116:GLU:HG3	1.61	0.65
37:i:366:ALA:HA	37:i:369:LYS:HG2	1.78	0.65
1:2:816:U:H4'	1:2:817:G:OP2	1.97	0.65
36:h:202:MET:SD	36:h:227:ILE:HD13	2.37	0.65
37:i:363:ASN:HD22	37:i:366:ALA:HB2	1.60	0.65
1:2:1318:A:H3'	1:2:1319:A:H8	1.61	0.65
1:2:1744:C:H2'	1:2:1746:A:N7	2.12	0.65
24:V:128:ARG:HE	24:V:132:GLN:HE21	1.44	0.65
36:h:234:TRP:CH2	36:h:266:ARG:HG3	2.31	0.65
1:2:134:A:O2'	1:2:135:A:H5'	1.96	0.64
25:W:372:THR:HB	25:W:375:SER:HB3	1.79	0.64
1:2:837:U:O2'	23:U:61:ARG:HG2	1.97	0.64
36:h:296:LYS:HE3	36:h:333:LEU:HG	1.79	0.64
3:A:144:SER:O	3:A:148:GLU:HG3	1.96	0.64
7:E:7:MET:HE1	7:E:66:GLN:HB2	1.79	0.64
23:U:115:LYS:HD2	23:U:115:LYS:C	2.22	0.64
34:f:280:GLU:O	34:f:284:GLU:HG2	1.97	0.64
36:h:279:ARG:HH22	36:h:290:ALA:CB	2.10	0.64
1:2:1697:G:H2'	1:2:1698:C:C6	2.33	0.64
1:2:1729:G:O2'	1:2:1730:U:H5'	1.97	0.64
34:f:276:LEU:HB2	34:f:282:ILE:HD12	1.78	0.64
5:C:255:ASN:ND2	33:e:146:ASP:HB3	2.12	0.64
6:D:452:THR:HG22	6:D:452:THR:O	1.96	0.64
34:f:157:ILE:HA	34:f:162:ARG:CD	2.26	0.64
1:2:1703:G:H3'	1:2:1704:A:C8	2.32	0.64
34:f:58:ARG:HH12	34:f:66:SER:HB3	1.62	0.64
1:2:1574:C:H5'	20:R:136:VAL:HG22	1.80	0.64
4:B:239:MET:HB2	26:X:448:MET:HE2	1.80	0.64
37:i:111:LYS:HD2	37:i:111:LYS:C	2.23	0.64
1:2:212:G:O2'	1:2:213:C:H5'	1.98	0.64
10:H:263:PRO:HB2	10:H:266:GLU:OE2	1.97	0.64
37:i:322:MET:HE3	37:i:358:GLN:CD	2.23	0.64
36:h:228:CYS:HA	36:h:231:THR:OG1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:26:LEU:HD21	38:k:49:VAL:CB	2.28	0.63
1:2:991:A:H2'	1:2:992:U:C6	2.33	0.63
12:J:250:VAL:O	12:J:253:MET:HG3	1.98	0.63
1:2:450:U:H4'	1:2:451:A:O5'	1.99	0.63
1:2:1744:C:H3'	1:2:1745:A:H5"	1.80	0.63
12:J:190:GLU:HB2	19:Q:247:TYR:CZ	2.33	0.63
16:N:298:PRO:HD2	16:N:301:LEU:HD12	1.81	0.63
34:f:113:GLU:HG3	34:f:113:GLU:O	1.97	0.63
36:h:171:LEU:HD11	36:h:189:LEU:HD12	1.81	0.63
12:J:189:LEU:HD23	19:Q:246:GLU:CG	2.28	0.63
25:W:118:PRO:O	25:W:121:ARG:HG3	1.98	0.63
1:2:1481:C:H2'	1:2:1482:U:C6	2.34	0.63
1:2:1769:C:H2'	1:2:1770:G:C8	2.33	0.63
36:h:169:ARG:HH11	36:h:169:ARG:HG3	1.63	0.63
36:h:299:LEU:HB3	36:h:337:TRP:HH2	1.62	0.63
37:i:240:ASP:HA	37:i:243:ILE:HG22	1.81	0.63
1:2:147:U:H2'	1:2:148:U:C6	2.33	0.63
5:C:256:LEU:HD12	5:C:286:SER:HB2	1.81	0.63
34:f:280:GLU:OE2	34:f:373:LEU:HG	1.99	0.63
23:U:47:LYS:NZ	23:U:47:LYS:HB3	2.13	0.63
39:l:517:LYS:O	39:l:517:LYS:HD3	1.98	0.63
1:2:609:U:H3	1:2:625:G:H22	1.47	0.63
1:2:1392:A:C2	39:l:545:HIS:HB3	2.34	0.63
13:K:39:THR:HG22	13:K:51:LYS:HD3	1.80	0.63
28:Z:68:HIS:HA	28:Z:79:TYR:O	1.99	0.63
36:h:316:GLN:OE1	36:h:316:GLN:HA	1.99	0.63
1:2:939:A:H2'	1:2:940:G:C8	2.34	0.62
1:2:1679:G:H2'	1:2:1791:G:N2	2.14	0.62
4:B:399:MET:HE1	29:a:101:ILE:HB	1.81	0.62
5:C:287:LEU:CD2	6:D:178:LEU:HD23	2.25	0.62
34:f:356:ARG:HA	34:f:360:VAL:HB	1.80	0.62
12:J:294:TYR:OH	21:S:30:LYS:HD2	2.00	0.62
37:i:335:SER:HA	37:i:338:LEU:CD2	2.29	0.62
37:i:99:GLU:O	37:i:103:ARG:HG3	2.00	0.62
23:U:88:ARG:NH1	37:i:420:LEU:HD22	2.15	0.62
32:d:60:LEU:HD21	32:d:83:ILE:HD11	1.82	0.62
33:e:149:HIS:HA	33:e:152:VAL:HG12	1.80	0.62
36:h:288:LEU:HB2	36:h:318:TYR:HE2	1.64	0.62
37:i:400:ILE:HD13	37:i:429:TYR:HE1	1.64	0.62
1:2:81:U:H2'	1:2:82:C:C1'	2.29	0.62
4:B:62:ILE:HD13	4:B:71:ILE:HG12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:318:LYS:HA	6:D:321:GLU:OE2	1.99	0.62
1:2:1135:A:HO2'	1:2:1136:A:H8	1.48	0.62
37:i:401:GLU:O	37:i:405:ARG:HD3	1.99	0.62
1:2:724:A:H2'	1:2:725:A:C8	2.35	0.62
1:2:1693:C:C2'	1:2:1694:G:H5'	2.29	0.62
36:h:296:LYS:HD2	36:h:337:TRP:CE2	2.35	0.62
36:h:323:LYS:HG2	36:h:324:SER:N	2.13	0.62
37:i:177:MET:HB3	37:i:181:ARG:NH2	2.14	0.62
36:h:358:LYS:O	36:h:362:PRO:HG2	2.00	0.62
37:i:366:ALA:O	37:i:370:VAL:HG23	2.00	0.62
1:2:151:A:HO2'	1:2:153:A:H1'	1.65	0.62
1:2:1763:U:C4'	1:2:1764:A:H5'	2.24	0.62
1:2:356:G:H2'	1:2:357:A:H8	1.63	0.62
4:B:282:GLN:HA	4:B:285:ILE:HD12	1.82	0.62
34:f:367:LYS:HD2	34:f:367:LYS:C	2.24	0.62
1:2:644:G:O2'	1:2:645:A:H5'	2.00	0.61
10:H:225:ILE:HA	10:H:228:PRO:CB	2.28	0.61
30:b:31:LYS:HG2	30:b:32:PRO:HD2	1.81	0.61
34:f:164:ALA:HB1	34:f:168:THR:HG21	1.81	0.61
1:2:162:C:C3'	1:2:163:A:H5"	2.22	0.61
1:2:1750:C:H3'	1:2:1751:U:C5'	2.17	0.61
6:D:76:ALA:O	6:D:79:VAL:HG12	2.00	0.61
10:H:240:GLY:C	37:i:295:MET:HE1	2.25	0.61
36:h:90:HIS:CD2	36:h:94:LEU:HD13	2.35	0.61
36:h:165:ASN:HA	36:h:168:LYS:NZ	2.14	0.61
1:2:365:G:C2'	1:2:366:G:H5'	2.30	0.61
1:2:1388:A:O2'	1:2:1389:A:H8	1.84	0.61
13:K:44:LYS:H	13:K:44:LYS:CD	2.11	0.61
24:V:61:ASP:O	24:V:65:MET:HG3	2.01	0.61
34:f:210:VAL:HG22	34:f:256:VAL:HG21	1.82	0.61
37:i:290:PRO:HA	37:i:293:VAL:CG2	2.30	0.61
1:2:648:U:H1'	1:2:649:U:O2	2.01	0.61
1:2:918:G:H5"	1:2:918:G:H8	1.66	0.61
1:2:1729:G:H2'	1:2:1730:U:H6	1.65	0.61
6:D:180:THR:HG21	6:D:193:TRP:CZ2	2.35	0.61
23:U:113:GLU:HA	23:U:116:GLU:OE1	1.99	0.61
36:h:81:ASP:HB2	36:h:82:PRO:HD3	1.83	0.61
10:H:204:GLU:HA	10:H:207:GLU:HG3	1.82	0.61
23:U:115:LYS:NZ	23:U:116:GLU:HG3	2.15	0.61
30:b:22:ASN:H	30:b:25:LYS:HD3	1.65	0.61
34:f:272:ARG:HD2	34:f:273:TYR:HE1	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:341:TRP:NE1	37:i:347:PRO:HG3	2.15	0.61
1:2:1791:G:H5"	1:2:1792:A:OP1	2.01	0.61
6:D:504:GLN:HG3	6:D:509:ARG:O	2.01	0.61
37:i:322:MET:HE3	37:i:358:GLN:NE2	2.16	0.61
1:2:68:A:H4'	1:2:69:G:O5'	2.00	0.61
1:2:649:U:O2	1:2:649:U:H2'	2.00	0.61
1:2:1772:A:H3'	1:2:1772:A:OP2	2.01	0.61
5:C:72:THR:HG21	5:C:85:THR:OG1	2.01	0.61
9:G:68:VAL:HG21	9:G:71:CYS:SG	2.40	0.61
5:C:117:LEU:HD13	5:C:123:ALA:HA	1.81	0.61
39:l:465:LEU:HD22	39:l:483:LEU:HD23	1.83	0.61
1:2:150:A:H3'	1:2:151:A:C8	2.35	0.60
1:2:1797:G:H2'	1:2:1798:G:C8	2.34	0.60
37:i:435:PHE:HD1	37:i:436:GLU:N	1.99	0.60
35:g:564:LEU:HD11	35:g:598:PHE:HA	1.83	0.60
36:h:229:HIS:HA	36:h:262:PHE:CE2	2.36	0.60
1:2:1392:A:H2	39:l:545:HIS:HB3	1.66	0.60
4:B:176:SER:HG	4:B:230:VAL:N	1.99	0.60
36:h:171:LEU:HA	36:h:181:PRO:HB3	1.82	0.60
1:2:1726:U:H4'	1:2:1727:G:OP1	2.00	0.60
28:Z:86:LEU:HD21	28:Z:90:GLY:HA2	1.81	0.60
29:a:86:ILE:HD13	29:a:101:ILE:HD12	1.84	0.60
34:f:232:GLU:OE2	34:f:236:LYS:HE3	2.02	0.60
1:2:142:U:H2'	1:2:143:U:C6	2.37	0.60
1:2:530:A:N7	4:B:529:ARG:NE	2.49	0.60
1:2:969:G:H22	1:2:1625:A:H5'	1.65	0.60
16:N:306:LYS:O	16:N:310:VAL:HG23	2.01	0.60
34:f:108:TYR:CE2	34:f:360:VAL:HG21	2.35	0.60
37:i:100:PHE:O	37:i:104:PHE:HB2	2.02	0.60
37:i:129:LEU:HA	37:i:132:VAL:CG1	2.31	0.60
1:2:545:A:H4'	1:2:546:G:O5'	2.01	0.60
6:D:306:GLU:OE1	6:D:306:GLU:HA	2.02	0.60
23:U:81:PRO:HA	23:U:84:VAL:HG12	1.83	0.60
37:i:408:LYS:N	37:i:408:LYS:HD2	2.17	0.60
1:2:386:U:H5	1:2:412:A:N1	1.99	0.60
3:A:200:GLN:HG2	3:A:205:ILE:CB	2.28	0.60
37:i:109:ARG:O	37:i:109:ARG:HD3	2.01	0.60
1:2:866:A:H5'	1:2:866:A:H8	1.67	0.60
34:f:389:THR:CG2	34:f:397:GLU:HG3	2.32	0.60
36:h:171:LEU:HD11	36:h:189:LEU:CD1	2.30	0.60
36:h:197:LYS:CE	36:h:230:GLU:HB2	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:347:PRO:HA	37:i:351:ASP:OD2	2.02	0.60
1:2:1167:U:H2'	1:2:1168:U:C6	2.37	0.60
33:e:173:GLU:HG2	33:e:176:ALA:HB2	1.84	0.60
1:2:714:G:N2	19:Q:192:ILE:HG22	2.17	0.59
5:C:176:VAL:HA	5:C:180:ILE:HG23	1.84	0.59
6:D:138:GLU:HB2	6:D:141:ARG:CB	2.31	0.59
23:U:88:ARG:HA	23:U:91:GLU:CD	2.27	0.59
33:e:354:VAL:HG21	33:e:362:ARG:NH1	2.17	0.59
36:h:236:LEU:HD22	36:h:240:TYR:HE2	1.66	0.59
1:2:1560:C:H4'	1:2:1561:A:H5"	1.84	0.59
5:C:204:THR:CA	6:D:116:GLU:HG2	2.25	0.59
25:W:347:LYS:H	25:W:347:LYS:HD2	1.68	0.59
35:g:621:MET:HG2	35:g:653:MET:HE2	1.84	0.59
37:i:204:GLU:HG3	37:i:204:GLU:O	2.02	0.59
37:i:335:SER:O	37:i:338:LEU:HG	2.02	0.59
1:2:242:G:O2'	1:2:243:U:H5'	2.01	0.59
2:8:200:LEU:HD13	2:8:244:VAL:HG22	1.84	0.59
5:C:46:ARG:NH2	6:D:148:SER:HB3	2.18	0.59
6:D:175:LYS:O	6:D:179:GLN:HG2	2.02	0.59
36:h:83:THR:O	36:h:86:VAL:HG22	2.02	0.59
36:h:271:SER:HA	36:h:274:LYS:HB2	1.84	0.59
5:C:256:LEU:HD22	5:C:257:LEU:HD22	1.85	0.59
6:D:343:GLU:O	6:D:347:LEU:HD12	2.02	0.59
34:f:192:LEU:HB3	34:f:193:PRO:HD2	1.84	0.59
1:2:1701:C:H2'	1:2:1702:G:H8	1.67	0.59
1:2:1792:A:H2'	1:2:1793:C:O4'	2.02	0.59
5:C:256:LEU:CD2	5:C:257:LEU:HD22	2.32	0.59
6:D:174:HIS:HB2	6:D:200:PHE:HE2	1.67	0.59
36:h:223:LEU:O	36:h:227:ILE:HG13	2.02	0.59
37:i:303:GLU:HB3	37:i:309:ARG:NH2	2.18	0.59
6:D:452:THR:O	6:D:452:THR:CG2	2.50	0.59
37:i:408:LYS:HA	37:i:408:LYS:HE2	1.82	0.59
1:2:1727:G:H1'	1:2:1728:U:H5'	1.84	0.59
5:C:178:LYS:NZ	5:C:224:MET:HE1	2.18	0.59
10:H:238:LYS:HD2	37:i:302:ALA:HB2	1.85	0.59
36:h:225:PHE:HA	36:h:228:CYS:SG	2.43	0.59
37:i:244:ARG:HA	37:i:247:GLU:OE1	2.01	0.59
1:2:842:A:O2'	1:2:843:U:H5'	2.03	0.59
10:H:222:THR:OG1	23:U:120:ALA:HB1	2.02	0.59
34:f:177:ILE:HD12	34:f:358:ARG:HG3	1.85	0.59
35:g:621:MET:HE1	35:g:626:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1450:G:H5'	10:H:415:LYS:HE2	1.85	0.58
1:2:1687:U:H2'	1:2:1688:U:H6	1.65	0.58
10:H:222:THR:HA	10:H:225:ILE:HD12	1.85	0.58
10:H:236:ILE:HG23	10:H:241:ILE:CG2	2.32	0.58
1:2:1730:U:H2'	1:2:1731:A:H8	1.68	0.58
6:D:227:LYS:HE3	33:e:286:GLU:HG2	1.85	0.58
37:i:170:SER:O	37:i:174:LEU:HD23	2.02	0.58
3:A:197:VAL:CG1	10:H:258:VAL:HG13	2.33	0.58
6:D:403:GLU:HG2	6:D:404:THR:CG2	2.31	0.58
24:V:56:PRO:HG3	24:V:65:MET:SD	2.43	0.58
28:Z:124:ILE:HG22	28:Z:127:LEU:H	1.68	0.58
34:f:127:TYR:OH	34:f:182:ASP:HB2	2.03	0.58
36:h:82:PRO:HB2	36:h:87:LYS:CD	2.32	0.58
39:l:272:THR:HG21	39:l:288:VAL:HG11	1.85	0.58
10:H:241:ILE:HA	37:i:295:MET:HE2	1.84	0.58
26:X:447:ARG:HA	26:X:450:GLU:HG3	1.85	0.58
34:f:402:THR:O	34:f:407:PRO:HD3	2.04	0.58
34:f:408:TYR:O	37:i:187:LYS:HD3	2.04	0.58
36:h:330:PHE:CD2	36:h:375:VAL:HG11	2.38	0.58
1:2:1729:G:H2'	1:2:1730:U:C6	2.39	0.58
6:D:258:GLY:HA3	6:D:356:TYR:CE2	2.37	0.58
10:H:225:ILE:HG22	10:H:226:LYS:N	2.18	0.58
37:i:109:ARG:HD3	37:i:109:ARG:C	2.28	0.58
37:i:477:MET:HA	37:i:480:MET:HG2	1.84	0.58
1:2:998:A:H4'	1:2:999:G:O5'	2.02	0.58
36:h:296:LYS:HD2	36:h:337:TRP:CD2	2.39	0.58
37:i:178:GLU:OE1	37:i:178:GLU:HA	2.03	0.58
37:i:335:SER:HA	37:i:338:LEU:HD21	1.84	0.58
1:2:629:G:H2'	1:2:630:C:H6	1.69	0.58
1:2:836:A:H5"	1:2:837:U:C4	2.39	0.58
1:2:1165:U:H2'	1:2:1166:U:C6	2.39	0.58
1:2:1752:U:H2'	1:2:1753:U:H6	1.68	0.58
3:A:197:VAL:HG12	10:H:258:VAL:HG13	1.85	0.58
1:2:1757:U:O2'	1:2:1758:G:H5'	2.04	0.58
2:8:213:PRO:HA	2:8:216:LEU:HD13	1.85	0.58
30:b:44:MET:HE1	30:b:51:ASP:HA	1.84	0.58
32:d:107:ALA:O	32:d:109:ALA:N	2.37	0.58
34:f:393:ASP:HB3	34:f:396:SER:OG	2.03	0.58
1:2:1490:A:OP2	14:L:139:LYS:HE3	2.04	0.58
6:D:308:LEU:HD22	6:D:344:ARG:NH1	2.19	0.58
6:D:339:ASP:HA	6:D:342:GLU:OE1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:105:LEU:HB3	34:f:106:PRO:HD3	1.86	0.58
37:i:154:PRO:HG3	37:i:160:ASP:OD2	2.04	0.58
39:l:379:ILE:HG13	39:l:412:LEU:HD11	1.85	0.58
1:2:541:G:O2'	1:2:542:G:H5'	2.04	0.57
1:2:1670:A:H2'	1:2:1671:C:C6	2.39	0.57
5:C:57:ILE:O	6:D:364:VAL:HG23	2.04	0.57
36:h:86:VAL:HG21	36:h:121:ASP:CB	2.33	0.57
37:i:328:LEU:HD23	37:i:369:LYS:HD2	1.86	0.57
37:i:345:LEU:O	37:i:345:LEU:HD13	2.04	0.57
1:2:1430:A:H2'	1:2:1432:A:N7	2.19	0.57
30:b:51:ASP:HB3	30:b:58:LYS:NZ	2.19	0.57
1:2:318:U:H5'	1:2:319:C:C5	2.39	0.57
1:2:467:G:H2'	1:2:468:U:C6	2.39	0.57
1:2:1600:G:H2'	1:2:1601:A:C8	2.40	0.57
13:K:123:LYS:HE3	13:K:125:ILE:CG1	2.34	0.57
33:e:304:LEU:O	33:e:308:GLU:HG2	2.03	0.57
34:f:272:ARG:HD2	34:f:273:TYR:CE1	2.38	0.57
36:h:221:ALA:HA	36:h:224:VAL:HG12	1.86	0.57
37:i:419:ILE:HD11	37:i:448:TYR:HE2	1.68	0.57
3:A:121:LYS:O	3:A:122:LYS:HB2	2.04	0.57
4:B:306:ALA:HA	4:B:309:ARG:HG2	1.87	0.57
35:g:613:VAL:HG11	35:g:640:ILE:HD13	1.86	0.57
12:J:283:SER:CB	12:J:288:ASP:HB3	2.34	0.57
36:h:258:VAL:O	36:h:261:GLU:HG2	2.05	0.57
36:h:304:PRO:O	36:h:364:MET:HE1	2.04	0.57
39:l:342:LEU:O	39:l:346:LEU:HD23	2.05	0.57
1:2:553:U:H2'	1:2:554:C:C6	2.40	0.57
8:F:146:ARG:HH21	30:b:31:LYS:HB3	1.69	0.57
36:h:121:ASP:HA	36:h:124:PHE:CD1	2.40	0.57
36:h:270:GLU:H	36:h:270:GLU:CD	2.13	0.57
36:h:307:ALA:HB3	36:h:364:MET:CE	2.35	0.57
37:i:278:LEU:HD12	37:i:278:LEU:O	2.03	0.57
37:i:356:ILE:HB	37:i:367:TYR:HE1	1.69	0.57
39:l:385:MET:SD	39:l:387:ASN:HB2	2.45	0.57
1:2:298:A:H5"	1:2:300:G:O4'	2.04	0.57
11:I:139:ASN:HB2	11:I:142:LYS:HE3	1.87	0.57
36:h:229:HIS:CD2	36:h:258:VAL:HG13	2.40	0.57
1:2:1622:A:C8	15:M:121:THR:HG22	2.39	0.57
1:2:1767:G:C3'	1:2:1768:A:H5"	2.34	0.57
1:2:1768:A:H2'	1:2:1769:C:H5'	1.86	0.57
37:i:305:GLU:O	37:i:305:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:148:U:H2'	1:2:149:U:C6	2.40	0.57
24:V:129:LYS:HB3	24:V:129:LYS:HZ2	1.70	0.57
36:h:153:GLN:OE1	36:h:156:LYS:HD3	2.03	0.57
37:i:418:ASP:H	37:i:421:THR:HB	1.69	0.57
1:2:1731:A:H5'	36:h:218:PRO:HD2	1.86	0.56
5:C:161:ILE:O	5:C:165:GLU:HG3	2.05	0.56
12:J:283:SER:HB2	12:J:288:ASP:HB3	1.87	0.56
34:f:369:ASP:O	34:f:371:PRO:HD3	2.05	0.56
1:2:236:A:OP1	1:2:236:A:H4'	2.05	0.56
1:2:1169:U:H2'	1:2:1170:U:H6	1.70	0.56
2:8:200:LEU:HD12	2:8:201:ALA:H	1.69	0.56
6:D:229:LYS:O	6:D:233:GLN:HG3	2.05	0.56
25:W:281:ARG:HD2	25:W:349:VAL:HG21	1.87	0.56
1:2:369:G:H2'	1:2:370:G:C8	2.40	0.56
1:2:845:U:H2'	1:2:846:G:C8	2.41	0.56
1:2:1679:G:N2	1:2:1791:G:H2'	2.20	0.56
10:H:250:ILE:O	10:H:251:ALA:HB3	2.06	0.56
33:e:382:LYS:HB3	33:e:382:LYS:NZ	2.19	0.56
36:h:227:ILE:O	36:h:231:THR:HG23	2.05	0.56
36:h:357:LEU:O	36:h:361:ILE:HG22	2.06	0.56
37:i:389:LYS:O	37:i:393:ILE:HG22	2.05	0.56
39:l:308:ILE:HG21	39:l:338:PHE:HB3	1.87	0.56
39:l:415:HIS:HE2	39:l:443:TYR:HE2	1.53	0.56
1:2:163:A:H4'	1:2:164:A:C5'	2.33	0.56
24:V:194:THR:HG22	24:V:195:LEU:H	1.69	0.56
30:b:22:ASN:O	30:b:25:LYS:HB2	2.05	0.56
34:f:36:ASP:O	34:f:39:VAL:HG12	2.06	0.56
1:2:150:A:H3'	1:2:151:A:C5	2.41	0.56
1:2:1706:C:H2'	1:2:1707:A:O5'	2.05	0.56
34:f:215:CYS:SG	34:f:264:LEU:HD11	2.45	0.56
1:2:1670:A:H2'	1:2:1671:C:H6	1.70	0.56
1:2:1802:A:O2'	1:2:1803:G:H5"	2.06	0.56
3:A:83:THR:HG23	3:A:193:THR:OG1	2.05	0.56
5:C:183:LEU:O	5:C:184:LEU:HD12	2.06	0.56
6:D:181:LEU:HD13	6:D:193:TRP:CB	2.36	0.56
17:O:21:MET:HE1	17:O:36:VAL:HG22	1.86	0.56
24:V:110:ASN:O	24:V:113:ARG:HG2	2.06	0.56
36:h:151:CYS:SG	36:h:179:LEU:HA	2.45	0.56
36:h:380:ASP:O	36:h:384:LYS:HG3	2.06	0.56
37:i:124:ILE:CA	37:i:127:MET:HE1	2.08	0.56
37:i:328:LEU:HD23	37:i:369:LYS:CD	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:436:GLU:HG2	37:i:437:ARG:N	2.19	0.56
1:2:1793:C:O2'	1:2:1794:U:H5'	2.06	0.56
2:8:249:HIS:O	2:8:250:ALA:C	2.43	0.56
6:D:186:THR:HG23	37:i:244:ARG:HH12	1.70	0.56
6:D:309:ASN:O	6:D:313:LYS:HG2	2.06	0.56
12:J:260:VAL:HG11	12:J:275:ILE:HD13	1.87	0.56
23:U:88:ARG:HA	23:U:91:GLU:OE2	2.06	0.56
28:Z:67:TYR:O	28:Z:80:GLU:HA	2.05	0.56
37:i:407:LEU:HD12	37:i:410:MET:HE2	1.87	0.56
1:2:573:G:H4'	1:2:574:G:OP1	2.03	0.56
1:2:1706:C:C2'	1:2:1707:A:O5'	2.53	0.56
3:A:93:ASN:HB3	3:A:96:ARG:HB3	1.88	0.56
37:i:460:MET:HE2	37:i:460:MET:CA	2.36	0.56
5:C:139:VAL:HG11	5:C:144:LEU:HD22	1.86	0.56
23:U:90:LEU:C	23:U:90:LEU:HD13	2.31	0.56
34:f:284:GLU:HA	34:f:284:GLU:OE2	2.06	0.56
36:h:116:CYS:O	36:h:117:ARG:HD2	2.06	0.56
1:2:1166:U:H2'	1:2:1167:U:C6	2.40	0.56
6:D:95:ARG:O	6:D:99:GLN:HB2	2.06	0.56
34:f:96:LYS:O	34:f:96:LYS:HD3	2.06	0.56
39:l:331:GLU:HG2	39:l:331:GLU:O	2.05	0.56
27:Y:20:GLU:H	27:Y:20:GLU:CD	2.14	0.55
33:e:354:VAL:O	33:e:355:SER:HB3	2.05	0.55
34:f:210:VAL:CG2	34:f:256:VAL:HG21	2.36	0.55
34:f:302:LEU:O	34:f:306:LYS:HG2	2.06	0.55
1:2:84:A:O4'	1:2:157:G:N2	2.39	0.55
1:2:211:G:O2'	1:2:212:G:H5'	2.05	0.55
36:h:337:TRP:HB3	36:h:338:PRO:HD3	1.88	0.55
1:2:1705:C:H4'	1:2:1706:C:OP2	2.05	0.55
21:S:94:LEU:O	21:S:98:VAL:HG12	2.05	0.55
36:h:83:THR:HG23	36:h:86:VAL:HG13	1.88	0.55
36:h:136:ARG:O	36:h:140:LEU:HB2	2.06	0.55
37:i:419:ILE:HD11	37:i:448:TYR:CE2	2.41	0.55
1:2:1711:A:H2'	1:2:1712:U:O4'	2.07	0.55
26:X:348:MET:HE1	26:X:352:ILE:CG2	2.37	0.55
36:h:292:PHE:CE1	36:h:333:LEU:HD11	2.42	0.55
3:A:130:MET:HA	3:A:130:MET:HE2	1.88	0.55
29:a:405:GLN:HA	29:a:408:ILE:HG12	1.87	0.55
34:f:401:PRO:HG2	34:f:405:ARG:HG3	1.87	0.55
37:i:239:LEU:HD13	37:i:239:LEU:C	2.31	0.55
1:2:64:U:H2'	1:2:65:G:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:612:U:H2'	1:2:613:C:H6	1.67	0.55
1:2:1316:A:H2'	1:2:1317:A:C8	2.41	0.55
1:2:1549:A:H2'	1:2:1550:A:C8	2.42	0.55
1:2:1736:U:OP1	1:2:1737:A:H1'	2.06	0.55
30:b:56:LYS:HE2	30:b:56:LYS:HA	1.89	0.55
34:f:214:ALA:HB1	34:f:264:LEU:HD22	1.89	0.55
36:h:121:ASP:O	36:h:124:PHE:HB2	2.07	0.55
1:2:376:G:O2'	1:2:377:U:H5'	2.07	0.55
1:2:1688:U:O2'	1:2:1689:C:H5'	2.06	0.55
2:8:227:ILE:O	2:8:227:ILE:CG2	2.55	0.55
5:C:158:ASN:HD21	5:C:162:ARG:NH1	2.05	0.55
6:D:117:ASP:OD1	6:D:120:GLY:HA2	2.06	0.55
29:a:230:ASP:O	29:a:233:GLU:HG2	2.07	0.55
1:2:1388:A:H4'	29:a:393:ARG:NE	2.22	0.55
1:2:1805:C:H2'	1:2:1806:G:O4'	2.07	0.55
4:B:63:LEU:HD13	29:a:167:MET:HE1	1.88	0.55
24:V:97:ARG:HB3	24:V:97:ARG:HH11	1.71	0.55
1:2:1378:A:H2'	1:2:1379:C:O2	2.06	0.55
1:2:1689:C:H2'	1:2:1690:G:H8	1.72	0.55
10:H:238:LYS:HD2	37:i:302:ALA:CB	2.37	0.55
16:N:331:LYS:HB2	16:N:331:LYS:NZ	2.22	0.54
33:e:283:ASP:HB3	33:e:286:GLU:HB2	1.89	0.54
5:C:93:ARG:HD2	5:C:98:PRO:HG2	1.89	0.54
5:C:224:MET:HE2	33:e:251:PHE:CE1	2.42	0.54
10:H:225:ILE:H	10:H:228:PRO:HA	1.72	0.54
23:U:57:ARG:O	23:U:60:ALA:HB3	2.07	0.54
33:e:182:LYS:HB2	33:e:185:GLU:HG3	1.88	0.54
37:i:430:SER:OG	37:i:459:ALA:HB1	2.07	0.54
39:l:346:LEU:HG	39:l:359:MET:HE1	1.90	0.54
1:2:77:U:O2'	1:2:78:U:H5'	2.06	0.54
1:2:1567:G:N2	1:2:1594:A:H2	1.98	0.54
5:C:97:ILE:HD11	5:C:354:SER:HB3	1.89	0.54
5:C:182:LYS:HD2	5:C:224:MET:SD	2.48	0.54
37:i:435:PHE:CD2	37:i:467:ALA:HA	2.42	0.54
10:H:241:ILE:HD12	10:H:245:MET:HE2	1.90	0.54
23:U:52:GLU:OE2	23:U:52:GLU:N	2.35	0.54
12:J:292:ILE:O	21:S:31:VAL:HG11	2.07	0.54
36:h:234:TRP:CH2	36:h:266:ARG:CG	2.91	0.54
37:i:133:GLU:HA	37:i:136:VAL:CG1	2.38	0.54
1:2:247:A:O2'	1:2:248:U:H5'	2.07	0.54
5:C:178:LYS:HZ1	5:C:224:MET:HE1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:171:LEU:O	36:h:181:PRO:HB3	2.08	0.54
37:i:321:VAL:HG11	37:i:340:GLU:OE1	2.07	0.54
1:2:568:G:H1'	1:2:816:U:C4	2.42	0.54
5:C:256:LEU:HD12	5:C:286:SER:CB	2.38	0.54
27:Y:10:VAL:HG22	29:a:385:ILE:HD11	1.89	0.54
28:Z:68:HIS:ND1	28:Z:128:SER:HA	2.23	0.54
34:f:198:GLU:HG3	34:f:320:ILE:HG21	1.89	0.54
39:l:368:ARG:HH21	39:l:401:LYS:HB2	1.71	0.54
1:2:491:G:H4'	1:2:492:G:OP1	2.07	0.54
4:B:309:ARG:HA	4:B:312:HIS:HB2	1.88	0.54
6:D:97:GLU:HA	6:D:100:ARG:NH2	2.20	0.54
3:A:116:PHE:CD1	3:A:123:LEU:HD23	2.41	0.54
7:E:7:MET:CE	7:E:66:GLN:HB2	2.37	0.54
23:U:83:ARG:HH22	38:k:9:LYS:HA	1.73	0.54
30:b:52:ASP:O	30:b:53:LYS:HG2	2.08	0.54
36:h:380:ASP:HB3	36:h:384:LYS:HE3	1.89	0.54
39:l:410:PHE:CE1	39:l:429:VAL:HG13	2.43	0.54
1:2:1169:U:H2'	1:2:1170:U:C6	2.43	0.54
1:2:1320:A:H2'	1:2:1321:A:H4'	1.89	0.54
8:F:143:ALA:C	8:F:145:PHE:H	2.16	0.54
14:L:46:LYS:HE3	14:L:64:LEU:HD12	1.90	0.54
34:f:277:ASP:HB3	37:i:121:LYS:HZ1	1.73	0.54
36:h:83:THR:O	36:h:87:LYS:HG3	2.08	0.54
36:h:227:ILE:HD12	36:h:228:CYS:H	1.71	0.54
39:l:379:ILE:HG23	39:l:412:LEU:HD21	1.90	0.54
6:D:315:LEU:HG	6:D:340:LEU:HD13	1.90	0.53
1:2:48:C:H2'	1:2:49:U:H6	1.73	0.53
1:2:178:U:O2'	1:2:179:G:H5'	2.09	0.53
1:2:1429:G:H5"	30:b:76:TRP:CZ2	2.43	0.53
6:D:150:SER:OG	6:D:152:LEU:HD23	2.08	0.53
6:D:181:LEU:HD13	6:D:193:TRP:HB2	1.88	0.53
17:O:52:MET:HG3	17:O:53:GLY:N	2.23	0.53
21:S:100:GLY:O	21:S:101:LEU:HD23	2.09	0.53
28:Z:71:LYS:HD2	28:Z:74:TRP:CZ2	2.43	0.53
37:i:314:VAL:HG13	37:i:318:CYS:CB	2.38	0.53
1:2:949:U:O2	1:2:953:U:H5	1.91	0.53
1:2:1711:A:O2'	1:2:1712:U:H5'	2.08	0.53
33:e:383:ILE:O	33:e:384:LEU:HG	2.08	0.53
6:D:85:ALA:O	6:D:89:LYS:HD3	2.08	0.53
9:G:97:GLN:HA	9:G:97:GLN:NE2	2.23	0.53
12:J:196:ILE:HD12	12:J:209:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:107:ALA:C	32:d:109:ALA:N	2.66	0.53
37:i:369:LYS:HA	37:i:372:GLU:OE1	2.08	0.53
1:2:629:G:H2'	1:2:630:C:C6	2.43	0.53
1:2:1037:C:H5'	27:Y:78:LEU:HD21	1.91	0.53
1:2:1054:U:H2'	1:2:1055:C:C6	2.43	0.53
37:i:342:ALA:HA	37:i:347:PRO:CD	2.37	0.53
6:D:318:LYS:HA	6:D:321:GLU:HG2	1.91	0.53
4:B:464:ARG:HG3	4:B:465:ARG:HG2	1.89	0.53
1:2:1757:U:H2'	1:2:1758:G:C8	2.43	0.53
4:B:481:ARG:HG3	29:a:154:GLU:HB3	1.91	0.53
21:S:27:ILE:HD12	21:S:47:MET:SD	2.49	0.53
30:b:47:ASN:O	30:b:48:ASN:C	2.51	0.53
33:e:149:HIS:HA	33:e:152:VAL:CG1	2.39	0.53
37:i:407:LEU:HG	37:i:410:MET:HE3	1.90	0.53
1:2:50:A:H2'	1:2:51:U:H6	1.74	0.53
1:2:143:U:O2'	1:2:144:U:H5'	2.08	0.53
1:2:386:U:O2	1:2:386:U:H2'	2.08	0.53
5:C:293:SER:HA	5:C:296:CYS:SG	2.48	0.53
25:W:462:TYR:HA	25:W:472:MET:HE2	1.91	0.53
32:d:45:PHE:CE2	32:d:49:ILE:HD11	2.44	0.53
34:f:66:SER:OG	34:f:69:MET:HG3	2.09	0.53
34:f:276:LEU:HB2	34:f:282:ILE:HD11	1.91	0.53
36:h:97:VAL:HG13	36:h:135:PHE:HD1	1.74	0.53
36:h:311:ILE:HD11	36:h:368:LEU:CD2	2.31	0.53
6:D:242:LEU:HD12	37:i:205:ILE:CD1	2.37	0.53
6:D:314:LYS:O	6:D:318:LYS:HD2	2.08	0.53
12:J:198:ILE:HB	12:J:262:VAL:HG12	1.91	0.53
36:h:228:CYS:SG	36:h:237:LEU:HD23	2.49	0.53
37:i:93:GLU:O	37:i:93:GLU:HG2	2.09	0.53
37:i:352:TRP:HB3	37:i:380:PHE:CE1	2.44	0.53
1:2:43:G:H2'	1:2:44:C:C6	2.45	0.52
1:2:158:A:H5'	1:2:159:G:OP2	2.09	0.52
1:2:466:A:O2'	1:2:467:G:H5'	2.09	0.52
1:2:1071:G:H2'	1:2:1072:A:C8	2.44	0.52
10:H:219:LYS:HD2	23:U:127:LEU:HD11	1.91	0.52
36:h:332:LYS:HD2	36:h:336:GLU:HB2	1.91	0.52
1:2:866:A:H5'	1:2:866:A:C8	2.44	0.52
6:D:334:GLU:O	6:D:338:ARG:HG3	2.09	0.52
10:H:218:GLU:N	10:H:218:GLU:OE2	2.43	0.52
10:H:245:MET:HB2	37:i:292:TRP:CH2	2.45	0.52
12:J:260:VAL:HG11	12:J:275:ILE:CD1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:280:GLU:HA	34:f:283:ILE:CG2	2.39	0.52
36:h:203:ASP:HA	36:h:206:MET:CE	2.39	0.52
1:2:275:U:O2'	1:2:276:U:H5'	2.08	0.52
1:2:1826:G:H3'	1:2:1827:MA6:H8	1.91	0.52
29:a:217:LEU:HA	29:a:220:LYS:HE3	1.91	0.52
35:g:640:ILE:HG23	35:g:646:VAL:HG21	1.91	0.52
36:h:265:LYS:O	36:h:341:VAL:HA	2.10	0.52
36:h:329:GLU:O	36:h:332:LYS:HB2	2.09	0.52
37:i:461:ILE:O	37:i:465:VAL:HG23	2.09	0.52
1:2:530:A:N7	4:B:529:ARG:CZ	2.73	0.52
1:2:956:G:N2	11:I:171:VAL:HG11	2.25	0.52
1:2:1029:C:H2'	1:2:1030:U:H5"	1.91	0.52
1:2:1144:A:H2'	1:2:1145:A:H8	1.74	0.52
6:D:189:GLU:HA	6:D:192:LYS:HD2	1.92	0.52
36:h:224:VAL:HG11	36:h:244:PHE:HE2	1.74	0.52
37:i:127:MET:O	37:i:130:LEU:HB2	2.10	0.52
4:B:478:ILE:HD12	4:B:482:VAL:HG21	1.92	0.52
24:V:128:ARG:O	24:V:132:GLN:HG2	2.08	0.52
24:V:159:GLU:OE2	24:V:162:LYS:HE2	2.08	0.52
31:c:133:LYS:O	31:c:137:LYS:HE3	2.08	0.52
37:i:429:TYR:HA	37:i:432:SER:OG	2.10	0.52
17:O:98:ARG:O	17:O:100:THR:HG23	2.10	0.52
23:U:112:ALA:HA	23:U:115:LYS:HE3	1.90	0.52
33:e:233:LEU:HD11	33:e:235:ARG:NH1	2.24	0.52
34:f:171:ALA:HB2	34:f:206:LYS:CD	2.38	0.52
36:h:88:GLU:HA	36:h:88:GLU:OE2	2.09	0.52
36:h:89:LEU:HB3	36:h:112:LEU:HG	1.91	0.52
37:i:430:SER:CB	37:i:459:ALA:HB1	2.39	0.52
37:i:442:PHE:CE2	37:i:446:LYS:HE3	2.44	0.52
4:B:313:PHE:HD2	4:B:316:LEU:HB2	1.73	0.52
5:C:183:LEU:HD12	5:C:220:LEU:CD2	2.36	0.52
16:N:313:TYR:CE1	24:V:168:LEU:HD21	2.44	0.52
24:V:156:LYS:NZ	24:V:156:LYS:HB3	2.24	0.52
32:d:84:PRO:O	32:d:88:ARG:HG3	2.08	0.52
36:h:158:CYS:SG	36:h:166:HIS:HB2	2.49	0.52
36:h:204:GLU:CA	36:h:207:LYS:HG2	2.38	0.52
36:h:311:ILE:HA	36:h:314:ILE:HG22	1.90	0.52
1:2:4:A:OP1	24:V:35:ARG:HD3	2.10	0.52
1:2:163:A:H4'	1:2:164:A:OP1	2.09	0.52
1:2:718:A:H2'	1:2:718:A:N3	2.24	0.52
1:2:1704:A:H2	1:2:1706:C:H41	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:54:ALA:HA	3:A:192:ILE:CD1	2.40	0.52
12:J:202:ARG:O	12:J:234:MET:HG3	2.09	0.52
36:h:166:HIS:HA	36:h:169:ARG:CD	2.17	0.52
36:h:339:VAL:O	36:h:342:LEU:HD23	2.09	0.52
16:N:325:MET:CE	16:N:355:THR:HG22	2.39	0.52
35:g:543:LYS:NZ	35:g:581:PRO:HG3	2.25	0.52
36:h:219:GLY:O	36:h:223:LEU:HD13	2.10	0.52
36:h:271:SER:O	36:h:275:VAL:HG13	2.09	0.52
37:i:184:GLU:OE1	37:i:184:GLU:HA	2.10	0.52
8:F:146:ARG:NH2	30:b:31:LYS:HB3	2.25	0.52
10:H:238:LYS:CD	37:i:302:ALA:HB2	2.40	0.52
28:Z:68:HIS:HB3	28:Z:78:SER:HB2	1.92	0.52
34:f:82:GLU:HA	34:f:82:GLU:OE1	2.10	0.52
36:h:121:ASP:HA	36:h:124:PHE:HD1	1.73	0.52
36:h:165:ASN:HA	36:h:168:LYS:HZ1	1.74	0.52
36:h:203:ASP:HA	36:h:206:MET:HE3	1.92	0.52
5:C:183:LEU:C	5:C:184:LEU:HD12	2.35	0.51
6:D:108:ILE:O	6:D:112:ASP:HB2	2.10	0.51
6:D:148:SER:O	6:D:149:ASP:HB2	2.10	0.51
1:2:488:C:OP1	17:O:109:ARG:HD3	2.09	0.51
1:2:1804:U:H5”	2:8:174:LYS:O	2.09	0.51
5:C:303:LEU:O	5:C:303:LEU:HD23	2.10	0.51
10:H:219:LYS:O	23:U:124:LEU:HD21	2.10	0.51
1:2:364:C:H4’	1:2:365:G:C4	2.45	0.51
6:D:78:ARG:HB3	6:D:78:ARG:HH11	1.75	0.51
6:D:227:LYS:HD2	33:e:289:TYR:CD2	2.46	0.51
10:H:227:GLY:HA3	10:H:230:ARG:CZ	2.40	0.51
34:f:310:PRO:HB3	34:f:373:LEU:HA	1.93	0.51
34:f:325:PHE:CD1	37:i:103:ARG:HG2	2.46	0.51
36:h:233:SER:OG	36:h:236:LEU:HG	2.10	0.51
37:i:352:TRP:HB3	37:i:380:PHE:HE1	1.75	0.51
1:2:365:G:H2’	1:2:366:G:H5’	1.92	0.51
5:C:158:ASN:O	5:C:161:ILE:HG22	2.10	0.51
5:C:176:VAL:O	5:C:180:ILE:HG12	2.10	0.51
6:D:171:PHE:O	6:D:175:LYS:HG3	2.11	0.51
36:h:202:MET:CE	36:h:236:LEU:HD13	2.41	0.51
37:i:179:LYS:HE2	37:i:183:LYS:CE	2.39	0.51
37:i:394:HIS:CE1	37:i:402:ASP:HB3	2.46	0.51
1:2:153:A:C2	28:Z:59:PHE:HZ	2.28	0.51
1:2:636:A:OP1	24:V:117:LYS:HE3	2.11	0.51
1:2:1766:U:H2’	1:2:1767:G:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:227:GLU:O	5:C:231:ARG:HG3	2.11	0.51
37:i:328:LEU:HG	37:i:332:ASP:HB2	1.93	0.51
1:2:759:G:H2'	1:2:760:C:C6	2.46	0.51
1:2:1745:A:OP1	36:h:150:LEU:HD22	2.09	0.51
5:C:259:SER:O	5:C:263:SER:HB2	2.10	0.51
23:U:85:TYR:HE1	23:U:106:ALA:CB	2.22	0.51
23:U:98:SER:OG	23:U:101:ASP:HB2	2.10	0.51
34:f:273:TYR:CD2	34:f:286:MET:HG2	2.45	0.51
5:C:61:LYS:HB3	5:C:65:SER:OG	2.10	0.51
5:C:162:ARG:NH1	5:C:162:ARG:HG2	2.25	0.51
10:H:427:TRP:HZ3	10:H:429:LYS:HD3	1.76	0.51
37:i:342:ALA:HA	37:i:347:PRO:HD3	1.93	0.51
5:C:175:LEU:O	5:C:180:ILE:HG23	2.11	0.51
12:J:297:ASP:OD2	21:S:47:MET:HE2	2.11	0.51
33:e:191:ARG:HG2	33:e:191:ARG:NH1	2.25	0.51
36:h:89:LEU:HB2	36:h:112:LEU:CD2	2.40	0.51
39:l:430:LEU:HA	39:l:433:MET:SD	2.51	0.51
1:2:1742:C:H2'	1:2:1743:A:H1'	1.91	0.51
2:8:200:LEU:CG	2:8:202:VAL:HG23	2.40	0.51
37:i:369:LYS:O	37:i:372:GLU:HG2	2.11	0.51
37:i:407:LEU:HG	37:i:410:MET:CE	2.41	0.51
37:i:464:TYR:O	37:i:467:ALA:HB3	2.11	0.51
1:2:341:C:H2'	1:2:342:U:C6	2.46	0.51
1:2:499:C:H2'	1:2:500:C:C6	2.46	0.51
7:E:16:LYS:CE	24:V:186:THR:HG23	2.40	0.51
34:f:279:VAL:O	34:f:283:ILE:HG22	2.11	0.51
39:l:272:THR:O	39:l:276:LEU:HB2	2.11	0.51
1:2:1625:A:N3	1:2:1625:A:H2'	2.25	0.50
1:2:1742:C:H3'	1:2:1743:A:C8	2.46	0.50
8:F:43:GLU:O	8:F:44:ARG:HG2	2.10	0.50
9:G:17:GLU:OE1	9:G:66:GLY:HA2	2.12	0.50
13:K:76:GLU:O	13:K:77:HIS:HB2	2.10	0.50
23:U:88:ARG:O	23:U:91:GLU:HG2	2.10	0.50
23:U:89:VAL:O	23:U:93:THR:HG23	2.11	0.50
33:e:334:ILE:O	33:e:354:VAL:O	2.28	0.50
1:2:162:C:O2	1:2:162:C:O2'	2.25	0.50
1:2:490:A:H2'	1:2:491:G:C8	2.46	0.50
1:2:1715:C:O2'	1:2:1716:C:H5'	2.12	0.50
4:B:297:THR:HG21	4:B:312:HIS:NE2	2.26	0.50
20:R:206:LYS:HZ1	20:R:208:HIS:CE1	2.29	0.50
34:f:284:GLU:O	34:f:287:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:839:C:O2'	1:2:840:U:O5'	2.28	0.50
36:h:292:PHE:CE1	36:h:329:GLU:HB3	2.46	0.50
2:8:231:LEU:HD21	2:8:255:PRO:HD3	1.93	0.50
10:H:241:ILE:CA	37:i:295:MET:HE2	2.41	0.50
35:g:625:ARG:CZ	35:g:625:ARG:HB2	2.41	0.50
36:h:83:THR:HG23	36:h:86:VAL:HG22	1.94	0.50
36:h:206:MET:O	36:h:209:LEU:HB3	2.12	0.50
39:l:304:MET:HE1	39:l:308:ILE:HD13	1.92	0.50
23:U:47:LYS:HB3	23:U:47:LYS:HZ1	1.75	0.50
37:i:165:THR:O	37:i:168:GLU:HG3	2.11	0.50
1:2:1012:U:H5'	1:2:1013:A:OP2	2.12	0.50
5:C:162:ARG:HH11	5:C:162:ARG:HG2	1.77	0.50
6:D:340:LEU:O	6:D:343:GLU:HG2	2.11	0.50
37:i:452:PRO:CB	37:i:456:ILE:HG21	2.39	0.50
1:2:763:A:H2'	1:2:764:A:C8	2.47	0.50
5:C:217:LEU:HD23	5:C:220:LEU:HD12	1.94	0.50
5:C:305:MET:HG3	6:D:157:TRP:CZ3	2.47	0.50
36:h:156:LYS:HA	36:h:159:VAL:HG12	1.94	0.50
1:2:868:C:H4'	9:G:18:ARG:HH12	1.76	0.50
5:C:238:GLU:HG2	5:C:239:LYS:N	2.27	0.50
5:C:317:HIS:HB3	33:e:255:HIS:O	2.11	0.50
6:D:347:LEU:HD12	6:D:347:LEU:H	1.76	0.50
28:Z:81:ILE:HD11	28:Z:84:ILE:HG22	1.93	0.50
34:f:286:MET:HE1	34:f:301:THR:OG1	2.12	0.50
34:f:404:GLN:H	34:f:404:GLN:CD	2.20	0.50
36:h:136:ARG:HA	36:h:140:LEU:HD12	1.92	0.50
36:h:238:ALA:O	36:h:242:LYS:HD2	2.12	0.50
1:2:1594:A:H2'	1:2:1595:A:O4'	2.12	0.50
1:2:1742:C:H3'	1:2:1743:A:H8	1.77	0.50
6:D:174:HIS:O	6:D:178:LEU:HD13	2.12	0.50
26:X:346:LYS:HB3	26:X:347:LYS:NZ	2.27	0.50
34:f:157:ILE:O	34:f:162:ARG:HD3	2.11	0.50
37:i:400:ILE:CD1	37:i:429:TYR:HE1	2.25	0.50
1:2:57:U:O4	1:2:384:U:H5	1.94	0.49
1:2:1839:G:H2'	1:2:1840:A:C8	2.46	0.49
19:Q:248:GLU:HG2	19:Q:250:ILE:H	1.77	0.49
34:f:267:ILE:HG12	37:i:276:GLY:O	2.11	0.49
37:i:322:MET:HA	37:i:325:LEU:CG	2.40	0.49
37:i:429:TYR:CD1	37:i:434:ASN:HB2	2.47	0.49
1:2:145:U:H2'	1:2:146:U:C6	2.47	0.49
1:2:292:A:C2'	1:2:293:A:H5'	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1388:A:H4'	29:a:393:ARG:HE	1.77	0.49
1:2:1688:U:H2'	1:2:1689:C:H6	1.77	0.49
1:2:390:A:H2'	1:2:391:C:O4'	2.12	0.49
1:2:669:G:H2'	1:2:670:G:H8	1.72	0.49
6:D:186:THR:CG2	37:i:244:ARG:HH12	2.25	0.49
32:d:37:ALA:N	32:d:107:ALA:HB2	2.27	0.49
34:f:161:PHE:C	34:f:162:ARG:HG3	2.36	0.49
36:h:169:ARG:HG3	36:h:169:ARG:NH1	2.26	0.49
1:2:1134:U:C2'	1:2:1135:A:H5'	2.42	0.49
6:D:403:GLU:CG	6:D:404:THR:HG23	2.41	0.49
21:S:85:ASP:OD1	21:S:85:ASP:C	2.56	0.49
36:h:82:PRO:HG3	36:h:124:PHE:CZ	2.46	0.49
36:h:338:PRO:O	36:h:342:LEU:HD22	2.12	0.49
1:2:522:G:H2'	1:2:523:C:C6	2.47	0.49
2:8:188:LEU:CD2	2:8:227:ILE:HG23	2.42	0.49
5:C:176:VAL:HA	5:C:180:ILE:HG21	1.95	0.49
10:H:427:TRP:CZ3	10:H:429:LYS:HD3	2.47	0.49
36:h:136:ARG:CG	36:h:140:LEU:HD12	2.42	0.49
36:h:209:LEU:HD12	36:h:214:LEU:CB	2.41	0.49
1:2:848:G:OP2	1:2:864:U:H5	1.96	0.49
10:H:219:LYS:HD2	23:U:127:LEU:CD1	2.43	0.49
23:U:102:ALA:HA	23:U:105:VAL:CG1	2.43	0.49
30:b:51:ASP:HB3	30:b:58:LYS:HZ3	1.77	0.49
36:h:204:GLU:O	36:h:208:LEU:HB2	2.11	0.49
1:2:638:A:N3	9:G:104:THR:HG22	2.27	0.49
1:2:1430:A:P	30:b:76:TRP:HH2	2.34	0.49
1:2:1754:U:C2'	1:2:1755:G:H5'	2.42	0.49
34:f:355:ILE:O	34:f:359:LEU:HB2	2.13	0.49
34:f:389:THR:HG23	34:f:397:GLU:HG3	1.94	0.49
39:l:559:GLU:O	39:l:563:GLU:HG2	2.13	0.49
1:2:1524:A:H8	29:a:338:LYS:NZ	2.10	0.49
1:2:1720:C:C2	1:2:1721:A:C8	3.00	0.49
1:2:1728:U:O2'	1:2:1729:G:H8	1.96	0.49
2:8:172:THR:HG23	2:8:174:LYS:H	1.77	0.49
37:i:134:LYS:NZ	37:i:138:GLU:HB2	2.27	0.49
37:i:243:ILE:HG12	37:i:247:GLU:CD	2.38	0.49
1:2:177:G:H2'	1:2:178:U:C6	2.48	0.49
1:2:553:U:H2'	1:2:554:C:H6	1.77	0.49
1:2:1014:A:H2'	1:2:1015:C:C6	2.48	0.49
1:2:1412:C:H2'	1:2:1413:A:C8	2.47	0.49
1:2:1734:A:H1'	1:2:1737:A:C2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:376:VAL:HG13	4:B:379:LEU:HD23	1.95	0.49
5:C:93:ARG:CD	5:C:98:PRO:HG2	2.42	0.49
12:J:205:THR:HG21	12:J:239:ALA:HA	1.94	0.49
26:X:346:LYS:HB3	26:X:347:LYS:HZ2	1.78	0.49
36:h:342:LEU:HD11	36:h:387:ALA:O	2.13	0.49
37:i:194:GLU:OE1	37:i:223:LYS:HD3	2.13	0.49
39:l:515:TYR:O	39:l:519:ILE:HG13	2.13	0.49
1:2:691:A:H2'	1:2:692:A:C8	2.48	0.49
1:2:989:A:H2'	1:2:990:U:C6	2.48	0.49
4:B:453:ALA:O	4:B:524:VAL:HG11	2.13	0.49
5:C:117:LEU:HD13	5:C:123:ALA:CA	2.42	0.49
9:G:49:PHE:HA	9:G:61:THR:O	2.13	0.49
14:L:45:LEU:HD11	14:L:77:LEU:HD11	1.94	0.49
34:f:58:ARG:NH1	34:f:66:SER:HB3	2.27	0.49
34:f:258:PRO:HD3	37:i:280:TYR:CZ	2.48	0.49
37:i:420:LEU:HD12	37:i:421:THR:N	2.28	0.49
4:B:302:CYS:SG	4:B:305:GLU:HB2	2.52	0.48
4:B:371:LEU:HA	4:B:375:LYS:HE3	1.93	0.48
13:K:59:ASN:O	13:K:60:ARG:HB2	2.12	0.48
36:h:254:THR:HA	36:h:257:ASP:OD2	2.13	0.48
37:i:366:ALA:HA	37:i:369:LYS:CG	2.43	0.48
1:2:145:U:C2	1:2:146:U:C5	3.01	0.48
1:2:440:A:H3'	1:2:441:U:H4'	1.94	0.48
1:2:1767:G:H2'	1:2:1768:A:C4'	2.42	0.48
32:d:67:LEU:O	32:d:71:LEU:HG	2.13	0.48
35:g:543:LYS:HZ3	35:g:581:PRO:HG3	1.78	0.48
37:i:394:HIS:ND1	37:i:402:ASP:HB3	2.28	0.48
1:2:317:U:H4'	1:2:318:U:OP1	2.12	0.48
1:2:732:U:H2'	1:2:733:C:H6	1.77	0.48
4:B:171:LYS:HG2	26:X:447:ARG:NH2	2.29	0.48
10:H:330:VAL:HG22	10:H:365:CYS:SG	2.53	0.48
34:f:38:ASP:HA	34:f:41:ASP:OD2	2.13	0.48
39:l:502:GLU:HA	39:l:505:ARG:HD2	1.96	0.48
4:B:96:ARG:NH2	26:X:326:ALA:HB3	2.24	0.48
4:B:490:SER:O	4:B:533:LEU:HG	2.14	0.48
34:f:96:LYS:O	34:f:96:LYS:CD	2.61	0.48
36:h:198:ASN:ND2	36:h:201:LEU:HB2	2.28	0.48
1:2:81:U:O5'	1:2:81:U:H6	1.97	0.48
1:2:611:G:H2'	1:2:612:U:C6	2.48	0.48
1:2:1773:U:C2'	1:2:1774:A:OP1	2.61	0.48
5:C:180:ILE:HG22	5:C:191:TRP:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:104:LYS:HG2	32:d:105:PRO:HD2	1.96	0.48
36:h:307:ALA:HB3	36:h:364:MET:HE2	1.94	0.48
30:b:84:GLN:HE21	30:b:84:GLN:HB3	1.49	0.48
34:f:187:TYR:O	34:f:191:ARG:HD2	2.14	0.48
34:f:202:LEU:HD22	34:f:313:LEU:HD23	1.96	0.48
34:f:257:TYR:CD1	34:f:258:PRO:HD2	2.48	0.48
39:l:453:ALA:HA	39:l:458:MET:HE1	1.95	0.48
6:D:308:LEU:HD22	6:D:344:ARG:CZ	2.44	0.48
8:F:38:ARG:HB3	8:F:39:PRO:HD3	1.94	0.48
21:S:60:GLN:HG3	21:S:62:HIS:O	2.13	0.48
1:2:37:A:O2'	1:2:38:G:H5'	2.14	0.48
1:2:150:A:H3'	1:2:151:A:C4	2.49	0.48
1:2:226:A:O2'	1:2:227:A:H5'	2.13	0.48
1:2:342:U:H2'	1:2:343:G:O4'	2.13	0.48
1:2:836:A:H3'	1:2:837:U:C6	2.49	0.48
1:2:1429:G:H5"	30:b:76:TRP:CH2	2.48	0.48
1:2:1744:C:H3'	1:2:1745:A:C4'	2.44	0.48
4:B:14:LYS:O	4:B:15:ASN:HB3	2.13	0.48
7:E:16:LYS:NZ	24:V:189:LEU:HD11	2.29	0.48
19:Q:189:GLU:HG2	21:S:50:SER:HB3	1.95	0.48
36:h:95:ASP:O	36:h:99:VAL:HB	2.13	0.48
1:2:161:A:H2'	1:2:161:A:N3	2.29	0.48
1:2:1700:U:H2'	1:2:1701:C:C6	2.49	0.48
8:F:144:HIS:C	8:F:146:ARG:H	2.22	0.48
10:H:219:LYS:C	23:U:124:LEU:HD21	2.38	0.48
13:K:42:PRO:HD3	13:K:48:ALA:O	2.14	0.48
21:S:96:LYS:HA	38:k:26:MET:HE1	1.96	0.48
36:h:225:PHE:HA	36:h:228:CYS:HG	1.79	0.48
39:l:309:THR:HG22	39:l:313:LYS:HE3	1.95	0.48
1:2:1567:G:OP2	22:T:49:GLY:HA2	2.14	0.48
1:2:1721:A:H5'	1:2:1722:C:OP2	2.14	0.48
3:A:50:LEU:HD23	3:A:50:LEU:C	2.39	0.48
5:C:168:ARG:O	5:C:172:LYS:HB2	2.14	0.48
7:E:89:LEU:C	7:E:90:ARG:HG2	2.39	0.48
22:T:52:ASP:OD2	22:T:55:THR:HG23	2.14	0.48
24:V:194:THR:HG22	24:V:195:LEU:N	2.28	0.48
36:h:154:VAL:HG11	36:h:179:LEU:HD22	1.95	0.48
36:h:201:LEU:O	36:h:204:GLU:HG2	2.14	0.48
37:i:435:PHE:CD1	37:i:436:GLU:N	2.79	0.48
1:2:18:A:OP2	6:D:481:ARG:HD2	2.14	0.47
1:2:732:U:H2'	1:2:733:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:793:C:OP1	12:J:312:ARG:HD2	2.14	0.47
1:2:1721:A:H2'	1:2:1721:A:N3	2.28	0.47
7:E:89:LEU:O	7:E:90:ARG:HG2	2.14	0.47
16:N:298:PRO:CD	16:N:301:LEU:HD12	2.44	0.47
37:i:448:TYR:CD2	37:i:450:LEU:HD11	2.49	0.47
1:2:289:A:H2'	1:2:290:C:C6	2.49	0.47
1:2:1691:C:O2	1:2:1691:C:H2'	2.15	0.47
3:A:9:GLN:HE22	10:H:234:ASP:HA	1.79	0.47
7:E:16:LYS:HZ1	24:V:189:LEU:HD11	1.78	0.47
16:N:306:LYS:HD3	24:V:177:GLU:OE1	2.13	0.47
20:R:89:ILE:O	20:R:93:ASN:HB2	2.14	0.47
32:d:104:LYS:HB2	32:d:104:LYS:HE2	1.68	0.47
33:e:164:MET:O	33:e:168:LEU:HG	2.13	0.47
37:i:131:ILE:HD12	37:i:131:ILE:H	1.79	0.47
39:l:279:ARG:HD3	39:l:281:PHE:CE2	2.49	0.47
1:2:1123:A:H8	1:2:1123:A:OP2	1.97	0.47
5:C:178:LYS:O	5:C:182:LYS:HB3	2.14	0.47
5:C:221:ARG:HD3	33:e:250:GLU:OE2	2.14	0.47
6:D:186:THR:HG23	37:i:244:ARG:NH1	2.29	0.47
10:H:241:ILE:HA	37:i:295:MET:CE	2.44	0.47
36:h:221:ALA:HB2	36:h:244:PHE:CZ	2.49	0.47
37:i:129:LEU:HA	37:i:132:VAL:HG12	1.96	0.47
39:l:465:LEU:HD21	39:l:480:TYR:HE1	1.79	0.47
1:2:136:A:H2'	1:2:137:A:H8	1.79	0.47
1:2:1726:U:N3	1:2:1744:C:N4	2.34	0.47
5:C:256:LEU:HD11	5:C:287:LEU:HD23	1.96	0.47
10:H:226:LYS:HB3	23:U:113:GLU:OE1	2.15	0.47
36:h:136:ARG:HG2	36:h:140:LEU:HD12	1.97	0.47
36:h:204:GLU:O	36:h:208:LEU:HD13	2.14	0.47
1:2:1700:U:H2'	1:2:1701:C:H6	1.79	0.47
6:D:150:SER:O	6:D:151:GLU:HB2	2.14	0.47
10:H:220:GLU:HG3	23:U:124:LEU:HD11	1.96	0.47
23:U:116:GLU:HA	23:U:119:LYS:HD3	1.97	0.47
36:h:173:LYS:HG3	36:h:212:ASN:HA	1.95	0.47
1:2:192:G:O2'	1:2:193:A:H5'	2.14	0.47
1:2:499:C:H2'	1:2:500:C:H6	1.79	0.47
1:2:1825:2MG:HM21	1:2:1828:MA6:N7	2.29	0.47
6:D:129:LYS:O	6:D:133:LEU:HD13	2.14	0.47
23:U:81:PRO:HA	23:U:84:VAL:CG1	2.44	0.47
23:U:112:ALA:O	23:U:115:LYS:HE3	2.15	0.47
26:X:436:GLU:O	26:X:440:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:185:ARG:HA	29:a:185:ARG:HD3	1.64	0.47
30:b:47:ASN:O	30:b:49:ILE:N	2.48	0.47
36:h:349:ASP:O	36:h:353:VAL:HG23	2.14	0.47
1:2:158:A:H2'	1:2:158:A:N3	2.30	0.47
1:2:280:U:H2'	1:2:282:A:OP2	2.14	0.47
1:2:411:C:H2'	1:2:412:A:H8	1.80	0.47
1:2:468:U:H3'	1:2:469:G:H5"	1.97	0.47
1:2:1129:G:H2'	1:2:1130:C:C6	2.50	0.47
6:D:204:HIS:C	6:D:205:PHE:HD1	2.23	0.47
13:K:110:ARG:HD2	13:K:110:ARG:HA	1.74	0.47
15:M:140:PHE:HB3	15:M:142:MET:HE3	1.96	0.47
23:U:67:LYS:HG3	23:U:69:VAL:HG23	1.96	0.47
23:U:88:ARG:NH1	37:i:420:LEU:CD2	2.78	0.47
26:X:401:PRO:HG3	29:a:361:ARG:HG2	1.96	0.47
28:Z:55:GLU:HG3	28:Z:91:ARG:HG3	1.96	0.47
30:b:21:ILE:HD11	30:b:79:ILE:HG12	1.95	0.47
32:d:64:LEU:CD1	32:d:70:LEU:HD13	2.45	0.47
35:g:606:ASN:O	35:g:607:PHE:CD1	2.68	0.47
36:h:171:LEU:C	36:h:181:PRO:HB3	2.39	0.47
36:h:234:TRP:HA	36:h:237:LEU:CD1	2.19	0.47
37:i:353:ILE:HA	37:i:356:ILE:CG1	2.45	0.47
39:l:335:PRO:HD2	39:l:338:PHE:HD2	1.80	0.47
39:l:487:TYR:HB2	39:l:496:ALA:HB2	1.97	0.47
1:2:164:A:H2'	1:2:165:A:H8	1.68	0.47
1:2:1841:U:O4	21:S:75:LYS:HE3	2.15	0.47
4:B:204:THR:HG23	4:B:207:PHE:H	1.80	0.47
7:E:12:PRO:HD3	7:E:61:GLN:O	2.14	0.47
12:J:251:LYS:HE3	12:J:282:TYR:CZ	2.50	0.47
13:K:89:ASP:O	13:K:91:PRO:HD3	2.14	0.47
17:O:105:PRO:O	33:e:319:LYS:O	2.33	0.47
23:U:112:ALA:CA	23:U:115:LYS:HE3	2.44	0.47
37:i:107:ILE:HG21	37:i:169:VAL:HG13	1.95	0.47
37:i:281:LYS:HB2	37:i:281:LYS:HE3	1.56	0.47
37:i:452:PRO:HB3	37:i:456:ILE:CG2	2.42	0.47
1:2:275:U:H2'	1:2:276:U:C6	2.50	0.47
4:B:242:PHE:CD1	26:X:449:LYS:HD3	2.50	0.47
5:C:204:THR:HG22	6:D:116:GLU:HG2	1.97	0.47
6:D:439:TYR:CE2	6:D:488:LYS:HD3	2.50	0.47
37:i:126:GLY:O	37:i:129:LEU:HG	2.15	0.47
37:i:407:LEU:CD1	37:i:410:MET:HE2	2.44	0.47
37:i:408:LYS:O	37:i:412:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1736:U:H5'	1:2:1737:A:O4'	2.15	0.47
5:C:210:LEU:HD12	6:D:87:VAL:CG2	2.40	0.47
10:H:419:ALA:HB3	10:H:423:LYS:HD3	1.97	0.47
28:Z:68:HIS:CE1	28:Z:128:SER:HA	2.50	0.47
36:h:202:MET:HE1	36:h:236:LEU:HD13	1.97	0.47
39:l:379:ILE:HG21	39:l:409:VAL:HG13	1.96	0.47
1:2:763:A:H2'	1:2:764:A:H8	1.80	0.46
1:2:913:U:H2'	1:2:914:U:C6	2.50	0.46
1:2:1385:A:H3'	1:2:1386:A:C8	2.49	0.46
5:C:257:LEU:CD1	6:D:194:MET:HE1	2.42	0.46
12:J:251:LYS:HD3	12:J:251:LYS:C	2.39	0.46
34:f:351:PHE:O	34:f:355:ILE:HG13	2.15	0.46
36:h:330:PHE:CG	36:h:375:VAL:HG11	2.49	0.46
37:i:99:GLU:CD	37:i:177:MET:HE3	2.40	0.46
37:i:222:GLU:HA	37:i:222:GLU:OE2	2.15	0.46
37:i:363:ASN:ND2	37:i:366:ALA:HB2	2.27	0.46
37:i:460:MET:HE2	37:i:460:MET:N	2.31	0.46
1:2:66:C:O2	1:2:66:C:H2'	2.14	0.46
1:2:581:A:H2'	1:2:582:G:O4'	2.15	0.46
1:2:753:U:H2'	1:2:754:G:O4'	2.15	0.46
1:2:926:G:H2'	1:2:928:A:N7	2.30	0.46
15:M:109:TYR:HB2	20:R:147:MET:HE2	1.96	0.46
23:U:115:LYS:HD2	23:U:116:GLU:N	2.30	0.46
33:e:304:LEU:HD12	33:e:304:LEU:HA	1.72	0.46
34:f:210:VAL:HG22	34:f:256:VAL:CG2	2.43	0.46
1:2:1110:C:H1'	1:2:1442:A:C4	2.49	0.46
5:C:254:ARG:O	5:C:258:LYS:HB2	2.14	0.46
7:E:5:ASP:OD1	7:E:68:THR:HG23	2.15	0.46
23:U:105:VAL:HA	23:U:108:MET:SD	2.56	0.46
33:e:149:HIS:CA	33:e:152:VAL:HG12	2.45	0.46
36:h:153:GLN:CA	36:h:156:LYS:HG2	2.42	0.46
36:h:342:LEU:HD21	36:h:387:ALA:CB	2.42	0.46
1:2:1091:A:OP2	3:A:121:LYS:CD	2.43	0.46
1:2:1683:U:H3	1:2:1788:U:H3	1.63	0.46
1:2:1701:C:H4'	1:2:1702:G:OP1	2.16	0.46
1:2:1754:U:O2'	1:2:1755:G:H5'	2.16	0.46
5:C:236:GLY:O	5:C:240:VAL:HG23	2.15	0.46
6:D:208:ALA:HB1	6:D:210:GLU:OE2	2.15	0.46
24:V:162:LYS:HZ3	24:V:162:LYS:HB2	1.80	0.46
29:a:390:VAL:HG11	39:l:553:LEU:HA	1.97	0.46
33:e:367:VAL:O	33:e:370:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:103:ARG:O	37:i:107:ILE:HG22	2.15	0.46
37:i:141:ARG:HA	37:i:141:ARG:CZ	2.45	0.46
39:l:529:TRP:CD1	39:l:557:VAL:HG23	2.51	0.46
1:2:3:C:H1'	1:2:4:A:C8	2.50	0.46
1:2:683:A:C2	1:2:700:A:C5	3.04	0.46
1:2:1384:A:H2'	1:2:1385:A:H8	1.81	0.46
6:D:138:GLU:CD	6:D:141:ARG:HD2	2.41	0.46
29:a:412:LYS:HA	29:a:412:LYS:HD2	1.73	0.46
39:l:501:ASN:ND2	39:l:505:ARG:HH22	2.14	0.46
1:2:1733:C:H42	1:2:1737:A:N6	2.13	0.46
4:B:524:VAL:HG12	4:B:535:VAL:HB	1.98	0.46
34:f:144:MET:CE	34:f:212:MET:HE1	2.46	0.46
36:h:289:SER:HA	36:h:292:PHE:HB3	1.98	0.46
1:2:549:U:H2'	1:2:550:U:H6	1.81	0.46
5:C:175:LEU:HD22	5:C:199:PHE:HE1	1.81	0.46
16:N:379:VAL:HG12	16:N:383:LYS:HZ2	1.80	0.46
20:R:28:TYR:HA	20:R:106:VAL:HG11	1.97	0.46
23:U:27:LEU:O	23:U:31:GLU:HG3	2.16	0.46
25:W:286:ARG:HD2	25:W:286:ARG:HA	1.61	0.46
34:f:102:ALA:HB1	34:f:122:PHE:CZ	2.51	0.46
1:2:172:A:H5'	1:2:173:A:H5"	1.97	0.46
1:2:902:A:C2'	1:2:903:C:H5'	2.46	0.46
4:B:171:LYS:HG2	26:X:447:ARG:CZ	2.46	0.46
13:K:56:ARG:HE	13:K:56:ARG:HB2	1.56	0.46
20:R:141:PHE:O	20:R:164:THR:HG22	2.15	0.46
26:X:491:ARG:NH2	27:Y:30:LEU:O	2.48	0.46
34:f:202:LEU:HD22	34:f:313:LEU:CD2	2.46	0.46
37:i:322:MET:HA	37:i:325:LEU:CD1	2.45	0.46
37:i:442:PHE:HE1	37:i:452:PRO:HG2	1.81	0.46
1:2:158:A:H3'	1:2:159:G:H8	1.81	0.46
1:2:746:C:H2'	1:2:747:C:C6	2.51	0.46
1:2:1701:C:O2'	1:2:1702:G:P	2.73	0.46
10:H:318:ARG:HH21	10:H:366:THR:HG21	1.81	0.46
12:J:189:LEU:HD12	19:Q:248:GLU:HA	1.97	0.46
12:J:293:VAL:O	21:S:31:VAL:HG12	2.16	0.46
27:Y:14:VAL:HG11	29:a:327:HIS:HB3	1.98	0.46
35:g:602:MET:SD	35:g:603:THR:HB	2.56	0.46
36:h:116:CYS:C	36:h:117:ARG:HD2	2.41	0.46
36:h:252:ARG:O	36:h:255:THR:HG22	2.15	0.46
39:l:267:LYS:NZ	39:l:271:LEU:HD11	2.30	0.46
6:D:88:GLU:OE1	6:D:88:GLU:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:443:LYS:HD3	6:D:445:TYR:CE1	2.51	0.46
10:H:225:ILE:HA	10:H:228:PRO:CA	2.46	0.46
10:H:357:THR:HB	10:H:361:TRP:HE1	1.81	0.46
16:N:331:LYS:HB2	16:N:331:LYS:HZ3	1.81	0.46
36:h:152:ARG:HD2	36:h:153:GLN:NE2	2.30	0.46
37:i:460:MET:HA	37:i:460:MET:CE	2.43	0.46
1:2:162:C:H3'	1:2:163:A:C5'	2.28	0.45
1:2:1836:C:O2'	1:2:1837:U:H5'	2.16	0.45
5:C:303:LEU:HD23	5:C:303:LEU:C	2.42	0.45
9:G:104:THR:O	9:G:122:GLY:HA3	2.15	0.45
12:J:249:ARG:HG3	12:J:249:ARG:NH1	2.31	0.45
25:W:394:MET:HE3	25:W:394:MET:HB3	1.83	0.45
36:h:202:MET:O	36:h:206:MET:HE2	2.17	0.45
1:2:857:A:H2'	1:2:858:A:C8	2.52	0.45
1:2:1119:G:H5'	1:2:1543:A:O2'	2.17	0.45
1:2:1802:A:C4'	1:2:1803:G:OP1	2.64	0.45
6:D:115:GLU:O	6:D:115:GLU:HG3	2.17	0.45
10:H:238:LYS:HE3	10:H:238:LYS:HB2	1.63	0.45
29:a:99:PRO:HA	29:a:102:ILE:HG22	1.99	0.45
33:e:245:LEU:HD23	33:e:252:PHE:CE2	2.51	0.45
37:i:310:GLU:OE2	37:i:310:GLU:N	2.39	0.45
39:l:510:PRO:HB2	39:l:515:TYR:HE1	1.82	0.45
1:2:65:G:H2'	1:2:66:C:C6	2.51	0.45
1:2:1791:G:O3'	1:2:1792:A:H8	1.99	0.45
36:h:361:ILE:CG2	36:h:362:PRO:CD	2.92	0.45
4:B:62:ILE:CD1	4:B:71:ILE:HG12	2.45	0.45
10:H:241:ILE:CA	37:i:295:MET:CE	2.94	0.45
26:X:343:LYS:HE3	26:X:343:LYS:HB3	1.84	0.45
34:f:174:GLU:O	34:f:177:ILE:HG22	2.16	0.45
34:f:290:VAL:O	34:f:294:GLY:HA2	2.15	0.45
34:f:300:LYS:NZ	34:f:300:LYS:HB2	2.32	0.45
39:l:268:THR:O	39:l:272:THR:HG22	2.16	0.45
39:l:503:MET:HB2	39:l:510:PRO:HG3	1.98	0.45
1:2:341:C:O2'	1:2:342:U:H5'	2.16	0.45
1:2:692:A:H2'	1:2:693:U:H6	1.81	0.45
1:2:740:U:H2'	1:2:741:C:H6	1.81	0.45
1:2:1576:C:H2'	1:2:1577:U:C6	2.52	0.45
1:2:1686:U:O2'	1:2:1687:U:H5'	2.16	0.45
2:8:228:GLY:HA2	2:8:263:MET:HB3	1.99	0.45
3:A:95:ASN:OD1	3:A:122:LYS:HG2	2.16	0.45
12:J:249:ARG:HG3	12:J:249:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:553:LYS:HD3	35:g:553:LYS:HA	1.71	0.45
37:i:104:PHE:CE1	37:i:169:VAL:HG12	2.52	0.45
37:i:290:PRO:CA	37:i:293:VAL:HG22	2.40	0.45
37:i:322:MET:CA	37:i:325:LEU:HG	2.44	0.45
1:2:78:U:O4	1:2:162:C:N3	2.50	0.45
1:2:1680:A:H2'	1:2:1681:A:O4'	2.17	0.45
1:2:1717:C:H2'	1:2:1718:A:H5'	1.98	0.45
7:E:10:PHE:HB2	7:E:63:GLN:HB2	1.99	0.45
7:E:48:LEU:HD12	7:E:59:HIS:O	2.17	0.45
28:Z:63:TRP:CD1	36:h:137:LEU:HD12	2.52	0.45
29:a:211:LYS:HD3	29:a:211:LYS:HA	1.79	0.45
34:f:286:MET:HE2	34:f:302:LEU:HG	1.99	0.45
37:i:147:VAL:HG12	37:i:147:VAL:O	2.17	0.45
39:l:556:ALA:O	39:l:560:MET:HB2	2.17	0.45
1:2:64:U:H2'	1:2:65:G:H8	1.82	0.45
1:2:218:U:H4'	1:2:219:C:OP2	2.16	0.45
1:2:914:U:O2'	6:D:373:VAL:O	2.34	0.45
1:2:1170:U:H2'	1:2:1171:U:H6	1.82	0.45
1:2:1499:A:H2'	1:2:1500:C:C6	2.52	0.45
1:2:1728:U:C2	1:2:1729:G:C8	3.05	0.45
4:B:333:PHE:CE2	4:B:336:PHE:HE2	2.34	0.45
5:C:252:MET:CE	33:e:150:SER:HA	2.47	0.45
10:H:215:GLU:O	10:H:219:LYS:HB2	2.17	0.45
24:V:135:PHE:CE2	24:V:139:LEU:HD11	2.52	0.45
37:i:133:GLU:HA	37:i:136:VAL:HG12	1.98	0.45
37:i:207:ILE:HG23	37:i:211:LEU:HD23	1.99	0.45
37:i:448:TYR:HD2	37:i:450:LEU:CG	2.30	0.45
39:l:269:TYR:HB3	39:l:292:MET:HE2	1.99	0.45
1:2:135:A:H2'	1:2:136:A:O4'	2.15	0.45
1:2:200:C:O2	1:2:200:C:O4'	2.35	0.45
1:2:216:A:H2'	1:2:217:A:C8	2.52	0.45
1:2:286:C:O2'	1:2:287:U:H5'	2.17	0.45
1:2:411:C:H2'	1:2:412:A:C8	2.52	0.45
1:2:1717:C:C2'	1:2:1718:A:H5'	2.46	0.45
18:P:15:LYS:HA	18:P:44:ASP:O	2.17	0.45
18:P:64:SER:OG	18:P:67:LYS:HB2	2.16	0.45
34:f:165:THR:HA	34:f:222:CYS:O	2.17	0.45
34:f:338:ILE:HG23	34:f:384:TYR:HD2	1.82	0.45
36:h:271:SER:O	36:h:275:VAL:HG22	2.17	0.45
39:l:269:TYR:O	39:l:273:LEU:HG	2.17	0.45
39:l:529:TRP:HE1	39:l:557:VAL:HB	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:681:G:O2'	1:2:682:G:H5'	2.17	0.45
1:2:701:U:C5	1:2:702:C:C5	3.05	0.45
1:2:918:G:H5"	1:2:918:G:C8	2.50	0.45
1:2:1312:A:H2	35:g:579:ILE:HD12	1.82	0.45
1:2:1724:U:O2	1:2:1724:U:H2'	2.15	0.45
4:B:262:ALA:H	29:a:196:THR:HG21	1.81	0.45
5:C:183:LEU:HB3	6:D:71:ILE:HD12	1.99	0.45
10:H:230:ARG:HG3	10:H:230:ARG:NH1	2.24	0.45
36:h:223:LEU:HD12	36:h:223:LEU:N	2.32	0.45
1:2:244:U:O2	1:2:244:U:O4'	2.35	0.45
1:2:703:U:H2'	1:2:704:A:C8	2.51	0.45
1:2:1798:G:H2'	1:2:1799:U:C6	2.52	0.45
2:8:245:VAL:HG22	2:8:247:VAL:HG13	1.98	0.45
29:a:405:GLN:OE1	29:a:405:GLN:C	2.60	0.45
30:b:50:LYS:HE2	30:b:50:LYS:HA	1.99	0.45
36:h:190:LEU:HG	36:h:205:VAL:HG11	1.98	0.45
1:2:494:A:H5"	1:2:495:G:OP2	2.17	0.44
1:2:1379:C:H5	1:2:1381:C:C2	2.35	0.44
28:Z:86:LEU:CD2	28:Z:90:GLY:HA2	2.48	0.44
34:f:277:ASP:HB3	37:i:121:LYS:HZ3	1.82	0.44
37:i:445:LEU:HD22	37:i:452:PRO:HG3	1.99	0.44
1:2:129:A:H2'	1:2:130:A:H8	1.81	0.44
1:2:1144:A:H2'	1:2:1145:A:C8	2.52	0.44
1:2:1748:G:H2'	1:2:1749:A:C8	2.52	0.44
2:8:184:SER:HA	2:8:227:ILE:HD11	1.99	0.44
3:A:123:LEU:C	3:A:123:LEU:HD12	2.42	0.44
4:B:333:PHE:CE2	4:B:336:PHE:CE2	3.06	0.44
16:N:320:SER:OG	16:N:323:GLU:HG3	2.18	0.44
27:Y:77:LYS:HB2	27:Y:77:LYS:HE3	1.70	0.44
28:Z:87:TYR:HB2	28:Z:92:HIS:O	2.17	0.44
34:f:253:SER:HB3	37:i:283:TYR:OH	2.17	0.44
35:g:621:MET:HG2	35:g:653:MET:CE	2.45	0.44
36:h:122:ILE:HG21	36:h:158:CYS:SG	2.57	0.44
36:h:326:LEU:C	36:h:326:LEU:HD12	2.42	0.44
1:2:83:U:H1'	1:2:158:A:C6	2.52	0.44
1:2:129:A:H2'	1:2:130:A:C8	2.53	0.44
1:2:174:C:H2'	1:2:175:G:O4'	2.17	0.44
1:2:242:G:H2'	1:2:243:U:H6	1.82	0.44
1:2:1137:G:C8	1:2:1138:G:C2	3.05	0.44
1:2:1167:U:H2'	1:2:1168:U:H6	1.83	0.44
1:2:1710:G:H2'	1:2:1711:A:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:285:ILE:HA	4:B:288:ARG:HG3	2.00	0.44
5:C:252:MET:HE2	33:e:150:SER:CA	2.47	0.44
6:D:166:MET:O	6:D:170:LYS:HG3	2.17	0.44
6:D:322:LEU:HG	6:D:322:LEU:O	2.18	0.44
13:K:46:ASN:HD22	13:K:89:ASP:CG	2.26	0.44
32:d:69:LYS:HD2	32:d:69:LYS:HA	1.85	0.44
36:h:210:LYS:HD3	36:h:243:LYS:NZ	2.31	0.44
36:h:228:CYS:HA	36:h:231:THR:HG1	1.81	0.44
37:i:317:LYS:HE2	37:i:344:LEU:HD11	1.98	0.44
37:i:360:ARG:HG3	37:i:367:TYR:CE2	2.53	0.44
37:i:395:ALA:HA	37:i:428:MET:SD	2.57	0.44
39:l:517:LYS:HD3	39:l:517:LYS:C	2.42	0.44
1:2:1718:A:H2'	1:2:1719:G:C8	2.42	0.44
1:2:1726:U:H2'	1:2:1727:G:C8	2.53	0.44
4:B:447:GLN:HB3	29:a:155:ASP:HA	2.00	0.44
6:D:109:ASP:C	6:D:111:GLU:H	2.25	0.44
6:D:464:MET:HE2	6:D:464:MET:HB3	1.82	0.44
28:Z:91:ARG:HG2	28:Z:91:ARG:HH11	1.82	0.44
1:2:43:G:H2'	1:2:44:C:H6	1.82	0.44
1:2:150:A:H5'	1:2:151:A:OP2	2.17	0.44
1:2:1413:A:H2'	1:2:1414:C:C6	2.52	0.44
4:B:309:ARG:HA	4:B:309:ARG:HD3	1.74	0.44
12:J:199:LYS:HB3	12:J:199:LYS:HE3	1.49	0.44
28:Z:101:LYS:O	28:Z:102:ASP:OD1	2.34	0.44
39:l:410:PHE:HE1	39:l:429:VAL:HG13	1.82	0.44
1:2:83:U:H1'	1:2:158:A:C5	2.52	0.44
1:2:225:G:H1'	1:2:226:A:N7	2.33	0.44
1:2:1488:A:H2'	1:2:1489:C:C6	2.53	0.44
8:F:132:LEU:HD12	8:F:132:LEU:O	2.18	0.44
20:R:154:LEU:HD11	20:R:169:TYR:CG	2.52	0.44
24:V:141:LYS:HE2	24:V:141:LYS:CA	2.47	0.44
29:a:380:LYS:HE3	29:a:380:LYS:HB3	1.68	0.44
30:b:38:VAL:HG22	30:b:42:ASN:HD21	1.82	0.44
30:b:54:CYS:SG	30:b:54:CYS:O	2.76	0.44
32:d:110:ILE:HG23	32:d:111:LYS:N	2.33	0.44
36:h:258:VAL:HA	36:h:261:GLU:HG2	1.99	0.44
37:i:303:GLU:CB	37:i:309:ARG:HH21	2.25	0.44
39:l:547:ASN:C	39:l:547:ASN:HD22	2.23	0.44
1:2:161:A:C2	1:2:162:C:H1'	2.53	0.44
1:2:254:U:H2'	1:2:255:G:H8	1.83	0.44
1:2:364:C:H4'	1:2:365:G:C2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1135:A:O2'	1:2:1136:A:H8	1.98	0.44
1:2:1737:A:H3'	1:2:1738:G:N2	2.25	0.44
4:B:263:PRO:HB3	29:a:200:GLU:OE1	2.17	0.44
12:J:246:ILE:O	12:J:250:VAL:HG23	2.17	0.44
19:Q:189:GLU:CG	21:S:50:SER:HB3	2.47	0.44
20:R:206:LYS:NZ	20:R:208:HIS:CE1	2.85	0.44
26:X:401:PRO:HD2	29:a:365:LEU:HD22	2.00	0.44
28:Z:65:ILE:HD11	36:h:143:HIS:CG	2.52	0.44
34:f:318:GLN:O	34:f:322:GLU:HB2	2.17	0.44
37:i:134:LYS:HZ2	37:i:163:TRP:HH2	1.66	0.44
1:2:389:G:O2'	1:2:390:A:H5'	2.16	0.44
1:2:1740:C:OP2	1:2:1740:C:H6	1.99	0.44
24:V:141:LYS:HD3	24:V:141:LYS:HA	1.90	0.44
34:f:280:GLU:HA	34:f:283:ILE:HG22	1.99	0.44
37:i:141:ARG:HA	37:i:141:ARG:HH11	1.81	0.44
39:l:519:ILE:CG2	39:l:554:ILE:HD11	2.48	0.44
1:2:241:U:H2'	1:2:242:G:H8	1.83	0.44
1:2:711:A:H2'	1:2:712:A:C8	2.52	0.44
1:2:733:C:H2'	1:2:734:U:H6	1.83	0.44
1:2:995:A:H2'	1:2:996:C:C6	2.52	0.44
1:2:1732:A:H3'	1:2:1733:C:H6	1.83	0.44
4:B:408:GLY:O	4:B:409:ILE:HB	2.18	0.44
7:E:47:GLU:OE1	7:E:61:GLN:HG3	2.18	0.44
12:J:310:ARG:HD2	12:J:311:LYS:O	2.17	0.44
17:O:60:LYS:HG2	24:V:84:TYR:CD1	2.53	0.44
20:R:206:LYS:HE2	20:R:206:LYS:HB2	1.48	0.44
34:f:388:ALA:HB3	34:f:397:GLU:OE1	2.17	0.44
37:i:214:GLU:O	37:i:218:LYS:HG2	2.18	0.44
37:i:349:ARG:O	37:i:349:ARG:HD3	2.18	0.44
39:l:340:ALA:HB1	39:l:374:PRO:HG3	2.00	0.44
39:l:519:ILE:HG23	39:l:532:ALA:HB1	2.00	0.44
1:2:156:U:O2'	1:2:157:G:H8	2.01	0.43
1:2:1696:A:H2'	1:2:1697:G:O4'	2.18	0.43
6:D:517:LEU:HD21	33:e:271:LYS:HD3	1.99	0.43
20:R:24:GLY:HA2	20:R:27:ARG:HE	1.82	0.43
36:h:171:LEU:HD12	36:h:208:LEU:HD23	1.99	0.43
37:i:109:ARG:C	37:i:109:ARG:CD	2.91	0.43
1:2:400:C:H2'	1:2:401:A:O4'	2.18	0.43
1:2:672:A:H2'	1:2:673:U:H6	1.81	0.43
1:2:674:U:H2'	1:2:675:U:C6	2.53	0.43
1:2:1710:G:H2'	1:2:1711:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1802:A:H1'	1:2:1803:G:P	2.58	0.43
3:A:200:GLN:HG3	3:A:205:ILE:HD12	2.00	0.43
4:B:494:LYS:HD3	4:B:494:LYS:HA	1.82	0.43
6:D:223:VAL:O	6:D:223:VAL:CG1	2.67	0.43
23:U:59:PHE:HA	23:U:62:LYS:HG2	2.00	0.43
23:U:92:LEU:HB3	23:U:97:ILE:HG21	1.99	0.43
34:f:42:GLN:HG2	34:f:58:ARG:HB2	1.99	0.43
35:g:548:ASN:O	35:g:554:ILE:HD12	2.18	0.43
36:h:94:LEU:O	36:h:98:ASN:HB2	2.18	0.43
1:2:24:A:H2'	1:2:25:U:H5'	2.01	0.43
1:2:775:C:O2'	1:2:776:G:H5'	2.18	0.43
1:2:1679:G:C6	1:2:1791:G:C6	3.06	0.43
3:A:16:SER:HB2	3:A:178:ALA:HB1	2.00	0.43
3:A:61:ALA:HB2	3:A:196:PHE:CE1	2.53	0.43
4:B:383:PHE:HD1	4:B:389:ILE:HG12	1.83	0.43
12:J:245:ASN:OD1	12:J:245:ASN:C	2.61	0.43
20:R:32:LYS:HE2	20:R:76:PHE:HB3	2.00	0.43
34:f:175:VAL:HG23	34:f:312:SER:HB3	2.00	0.43
36:h:234:TRP:CG	36:h:237:LEU:HD12	2.53	0.43
37:i:243:ILE:HG12	37:i:247:GLU:OE2	2.19	0.43
37:i:417:PRO:HB3	37:i:421:THR:HG22	1.97	0.43
39:l:423:LEU:HD21	39:l:448:ILE:O	2.18	0.43
1:2:79:G:H22	1:2:161:A:H2	1.66	0.43
1:2:500:C:H2'	1:2:501:C:O4'	2.18	0.43
1:2:587:U:H5"	9:G:30:SER:HB3	2.01	0.43
1:2:1722:C:O2	1:2:1722:C:H2'	2.18	0.43
4:B:171:LYS:HE3	26:X:447:ARG:NH2	2.33	0.43
7:E:33:LYS:HA	7:E:33:LYS:HD3	1.63	0.43
8:F:98:LYS:O	8:F:101:ILE:HG22	2.19	0.43
8:F:143:ALA:O	8:F:144:HIS:ND1	2.51	0.43
27:Y:29:MET:HE2	27:Y:29:MET:HB2	1.83	0.43
32:d:107:ALA:C	32:d:109:ALA:H	2.25	0.43
36:h:312:GLN:O	36:h:316:GLN:HG2	2.19	0.43
1:2:1673:C:H2'	1:2:1674:C:C6	2.52	0.43
1:2:1687:U:O2'	1:2:1688:U:H5'	2.18	0.43
2:8:231:LEU:HB2	2:8:250:ALA:HB2	2.00	0.43
4:B:290:ALA:O	4:B:294:GLU:HG2	2.19	0.43
5:C:239:LYS:HD2	6:D:211:TYR:CE2	2.54	0.43
9:G:87:GLU:OE1	9:G:87:GLU:HA	2.19	0.43
24:V:183:LYS:O	24:V:187:GLU:HG3	2.17	0.43
25:W:189:ARG:HB3	25:W:189:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:110:LEU:HA	29:a:110:LEU:HD23	1.73	0.43
34:f:185:ALA:O	34:f:189:LEU:HB2	2.17	0.43
37:i:123:MET:O	37:i:127:MET:SD	2.77	0.43
37:i:360:ARG:HA	37:i:367:TYR:HB2	2.00	0.43
37:i:380:PHE:CD2	37:i:382:ALA:HB2	2.54	0.43
1:2:991:A:H2'	1:2:992:U:H6	1.79	0.43
1:2:1090:U:OP2	3:A:120:HIS:CD2	2.71	0.43
5:C:161:ILE:HD12	5:C:161:ILE:HA	1.81	0.43
10:H:242:THR:O	10:H:246:LEU:HB2	2.18	0.43
29:a:130:PHE:CE1	29:a:132:ASP:HB3	2.53	0.43
36:h:142:ILE:HG23	36:h:142:ILE:O	2.17	0.43
36:h:339:VAL:HA	36:h:342:LEU:CD2	2.49	0.43
1:2:1383:G:C6	1:2:1384:A:C5	3.06	0.43
1:2:1727:G:O2'	1:2:1728:U:H5'	2.18	0.43
2:8:188:LEU:HD23	2:8:227:ILE:HG12	2.01	0.43
4:B:314:ILE:H	4:B:314:ILE:HD12	1.84	0.43
4:B:465:ARG:HB2	4:B:469:SER:OG	2.17	0.43
18:P:13:MET:HB2	18:P:16:SER:HB2	2.00	0.43
28:Z:62:ASN:OD1	36:h:144:ASP:HA	2.19	0.43
28:Z:122:LYS:HE2	28:Z:124:ILE:CD1	2.48	0.43
34:f:327:THR:OG1	34:f:330:GLN:HG3	2.18	0.43
36:h:195:GLU:OE2	36:h:195:GLU:C	2.62	0.43
37:i:104:PHE:CE2	37:i:135:VAL:HG21	2.54	0.43
1:2:310:U:O2'	1:2:311:G:H5'	2.18	0.43
1:2:325:A:C2	1:2:326:U:C6	3.07	0.43
4:B:303:LEU:HD23	4:B:303:LEU:HA	1.92	0.43
12:J:191:THR:HG22	19:Q:246:GLU:OE1	2.18	0.43
13:K:8:ILE:HD11	18:P:32:ARG:HB2	2.00	0.43
21:S:93:ILE:HD13	30:b:19:LEU:HD22	1.94	0.43
29:a:150:ASP:OD1	29:a:152:GLU:HG2	2.19	0.43
34:f:389:THR:HG22	34:f:397:GLU:HG3	2.00	0.43
37:i:390:LEU:HB3	37:i:406:ILE:HD13	2.00	0.43
1:2:129:A:C5	1:2:150:A:C2	3.07	0.43
1:2:131:A:H2'	1:2:132:A:H8	1.83	0.43
1:2:1680:A:C5	1:2:1681:A:H1'	2.53	0.43
1:2:1692:C:C2	1:2:1693:C:C5	3.06	0.43
1:2:1705:C:C4'	1:2:1706:C:OP2	2.67	0.43
4:B:145:GLU:H	4:B:145:GLU:CD	2.26	0.43
6:D:338:ARG:O	6:D:342:GLU:HG2	2.18	0.43
13:K:39:THR:HA	13:K:50:ARG:O	2.19	0.43
18:P:82:SER:HB3	18:P:85:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:53:ASP:N	23:U:54:PRO:HD2	2.34	0.43
24:V:127:GLU:OE1	24:V:127:GLU:O	2.37	0.43
34:f:160:MET:HG2	34:f:161:PHE:CE2	2.54	0.43
34:f:314:LYS:HD2	34:f:376:VAL:HB	2.01	0.43
36:h:122:ILE:HD11	36:h:161:VAL:CG2	2.46	0.43
39:l:317:ALA:HB2	39:l:345:ALA:HB1	2.00	0.43
1:2:130:A:O2'	1:2:131:A:H5'	2.18	0.43
1:2:1519:A:H5'	1:2:1521:G:H1'	2.00	0.43
4:B:287:SER:N	4:B:321:ARG:HH12	2.17	0.43
4:B:383:PHE:CD1	4:B:389:ILE:HG12	2.54	0.43
5:C:55:ARG:HA	5:C:55:ARG:HD2	1.74	0.43
6:D:258:GLY:O	6:D:355:LEU:HD22	2.19	0.43
19:Q:227:MET:CE	21:S:52:MET:HG2	2.32	0.43
33:e:312:LEU:HA	33:e:315:LYS:HB2	2.01	0.43
37:i:116:TYR:HB3	37:i:119:CYS:SG	2.59	0.43
37:i:127:MET:O	37:i:130:LEU:N	2.51	0.43
1:2:72:G:H4'	1:2:73:A:H5"	2.00	0.42
1:2:74:A:O2'	1:2:75:C:H5'	2.18	0.42
1:2:82:C:O2	1:2:158:A:N1	2.52	0.42
1:2:432:G:N7	5:C:37:ILE:HD12	2.34	0.42
1:2:458:U:H5	1:2:493:A:N7	2.17	0.42
1:2:460:U:O2	1:2:460:U:H2'	2.19	0.42
1:2:498:G:H2'	1:2:499:C:C6	2.54	0.42
1:2:893:A:H2'	1:2:894:A:C8	2.54	0.42
5:C:254:ARG:NH2	37:i:226:ASP:HA	2.34	0.42
9:G:105:THR:HB	9:G:120:VAL:HG22	2.00	0.42
10:H:224:VAL:C	10:H:225:ILE:HG13	2.43	0.42
10:H:224:VAL:O	10:H:225:ILE:CB	2.66	0.42
11:I:177:GLU:HG2	11:I:179:PHE:CE1	2.54	0.42
23:U:59:PHE:CD1	23:U:85:TYR:CD2	3.06	0.42
1:2:479:G:OP1	32:d:75:THR:HB	2.19	0.42
1:2:786:A:H2'	1:2:787:G:C8	2.54	0.42
1:2:1412:C:H2'	1:2:1413:A:H8	1.83	0.42
1:2:1757:U:H2'	1:2:1758:G:H8	1.81	0.42
1:2:1793:C:C2'	1:2:1794:U:H5'	2.50	0.42
1:2:1822:A:H2'	1:2:1823:G:C8	2.53	0.42
3:A:157:VAL:HG22	3:A:174:TYR:HB2	2.01	0.42
5:C:182:LYS:HE3	5:C:220:LEU:HD22	2.00	0.42
18:P:13:MET:CB	18:P:16:SER:HB2	2.48	0.42
19:Q:181:ARG:NH2	19:Q:234:PHE:HE2	2.16	0.42
32:d:42:ILE:N	32:d:43:PRO:HD2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:82:PRO:HB2	36:h:87:LYS:CG	2.49	0.42
36:h:199:SER:HB2	36:h:231:THR:HB	2.01	0.42
1:2:1848:C:O2	1:2:1848:C:H2'	2.18	0.42
4:B:334:PRO:O	11:I:202:PHE:CZ	2.73	0.42
6:D:180:THR:HG21	6:D:193:TRP:CE2	2.54	0.42
8:F:91:TRP:HH2	8:F:132:LEU:HD23	1.85	0.42
13:K:31:LEU:HD11	13:K:102:LYS:HD2	2.00	0.42
28:Z:87:TYR:CE2	28:Z:93:GLY:HA2	2.55	0.42
1:2:428:U:O2'	1:2:429:G:H5'	2.19	0.42
1:2:549:U:H2'	1:2:550:U:C6	2.55	0.42
1:2:1034:A:O2'	1:2:1035:U:H5'	2.19	0.42
1:2:1792:A:C2'	1:2:1793:C:H5'	2.49	0.42
2:8:178:LYS:O	2:8:181:LYS:HB3	2.19	0.42
3:A:73:ASN:HB3	3:A:76:PHE:CD2	2.54	0.42
4:B:478:ILE:HD13	4:B:478:ILE:HA	1.87	0.42
5:C:285:SER:HA	5:C:288:SER:OG	2.20	0.42
10:H:321:ILE:HG22	10:H:363:ILE:HG12	2.01	0.42
20:R:132:MET:HE3	20:R:134:ARG:HB2	2.00	0.42
34:f:160:MET:HE2	34:f:160:MET:HB2	1.91	0.42
36:h:316:GLN:OE1	36:h:316:GLN:CA	2.67	0.42
37:i:120:ASP:O	37:i:124:ILE:HG13	2.20	0.42
37:i:127:MET:C	37:i:131:ILE:HD12	2.43	0.42
37:i:179:LYS:CE	37:i:183:LYS:HE3	2.47	0.42
37:i:407:LEU:O	37:i:410:MET:HE3	2.18	0.42
37:i:442:PHE:CE1	37:i:452:PRO:HG2	2.53	0.42
39:l:455:GLY:O	39:l:457:MET:HE2	2.19	0.42
39:l:501:ASN:ND2	39:l:505:ARG:HH12	2.18	0.42
1:2:611:G:O2'	1:2:612:U:H5'	2.18	0.42
6:D:445:TYR:CE1	6:D:478:ILE:HD12	2.54	0.42
9:G:12:THR:HG22	9:G:24:VAL:HG21	2.02	0.42
13:K:79:GLN:O	13:K:103:ASP:HB2	2.19	0.42
24:V:128:ARG:NE	24:V:132:GLN:HG3	2.35	0.42
36:h:109:LEU:HD12	36:h:109:LEU:O	2.19	0.42
36:h:113:ILE:HD11	36:h:153:GLN:C	2.44	0.42
37:i:387:TYR:CE2	37:i:410:MET:HA	2.53	0.42
39:l:279:ARG:HD3	39:l:281:PHE:HE2	1.83	0.42
1:2:486:C:H2'	1:2:487:U:C6	2.54	0.42
1:2:1000:A:H2'	1:2:1001:A:O4'	2.20	0.42
1:2:1138:G:C5	1:2:1139:A:C8	3.07	0.42
1:2:1681:A:C6	1:2:1791:G:C2	3.08	0.42
4:B:487:ILE:HG12	4:B:537:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:21:THR:HG21	5:C:77:LEU:CD1	2.34	0.42
24:V:160:LYS:HE3	24:V:160:LYS:HB3	1.79	0.42
28:Z:53:LEU:HB3	28:Z:116:VAL:HG13	2.01	0.42
33:e:319:LYS:C	33:e:321:HIS:H	2.28	0.42
34:f:67:ALA:HB3	34:f:68:PRO:HD3	2.02	0.42
36:h:221:ALA:HB2	36:h:244:PHE:CE1	2.55	0.42
37:i:376:ASP:OD1	37:i:376:ASP:N	2.45	0.42
3:A:166:LEU:O	3:A:170:GLU:HG2	2.20	0.42
21:S:96:LYS:HG3	38:k:26:MET:CE	2.49	0.42
24:V:172:SER:HA	24:V:175:TRP:CD2	2.55	0.42
26:X:323:GLU:HG2	26:X:324:GLU:N	2.34	0.42
39:l:305:GLY:O	39:l:308:ILE:HG22	2.19	0.42
39:l:308:ILE:CG2	39:l:338:PHE:HB3	2.48	0.42
39:l:492:GLU:CD	39:l:495:GLU:H	2.28	0.42
1:2:154:G:H1’	36:h:174:HIS:HB2	2.01	0.42
1:2:1782:G:H2’	1:2:1783:G:O5’	2.20	0.42
6:D:362:VAL:HG12	6:D:386:MET:HE3	2.01	0.42
8:F:143:ALA:O	8:F:145:PHE:N	2.47	0.42
9:G:106:PRO:HD2	9:G:120:VAL:CG2	2.49	0.42
24:V:126:GLU:HA	24:V:126:GLU:OE2	2.19	0.42
25:W:416:LEU:HB2	25:W:419:VAL:HG11	2.02	0.42
26:X:505:ASP:HA	26:X:508:TYR:CE2	2.55	0.42
36:h:296:LYS:HA	36:h:337:TRP:CZ2	2.55	0.42
37:i:436:GLU:O	37:i:440:GLU:HG3	2.19	0.42
1:2:1380:U:H5’	20:R:70:ARG:HH22	1.85	0.42
1:2:1785:G:H2’	1:2:1786:U:C6	2.54	0.42
5:C:325:THR:N	5:C:326:PRO:HA	2.33	0.42
25:W:192:ASP:OD1	25:W:192:ASP:O	2.38	0.42
28:Z:58:GLN:HA	28:Z:63:TRP:CZ3	2.55	0.42
32:d:46:LEU:HD11	32:d:60:LEU:HD12	2.01	0.42
35:g:616:VAL:O	35:g:620:MET:HG2	2.20	0.42
1:2:1685:G:N3	1:2:1685:G:H2’	2.34	0.42
2:8:262:LEU:HD12	2:8:264:LYS:H	1.85	0.42
6:D:517:LEU:CD2	33:e:271:LYS:HD3	2.50	0.42
9:G:9:ALA:HB1	9:G:26:LEU:HD13	2.01	0.42
16:N:298:PRO:CG	16:N:301:LEU:HD12	2.49	0.42
24:V:178:PRO:HG2	24:V:179:LYS:CE	2.47	0.42
36:h:171:LEU:CA	36:h:181:PRO:HB3	2.47	0.42
36:h:229:HIS:HD2	36:h:258:VAL:HG13	1.79	0.42
36:h:338:PRO:O	36:h:341:VAL:HG22	2.20	0.42
37:i:161:ASP:N	37:i:161:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:366:ALA:HA	37:i:369:LYS:HD2	2.02	0.42
1:2:1144:A:H61	1:2:1379:C:N4	2.18	0.41
1:2:1376:A:H2'	1:2:1377:A:C8	2.55	0.41
1:2:1673:C:H2'	1:2:1674:C:H6	1.85	0.41
1:2:1773:U:H2'	1:2:1774:A:OP1	2.20	0.41
5:C:248:GLU:HG3	5:C:251:ARG:HH21	1.85	0.41
8:F:144:HIS:C	8:F:146:ARG:N	2.78	0.41
13:K:44:LYS:HD2	13:K:44:LYS:N	2.22	0.41
23:U:67:LYS:CG	23:U:69:VAL:HG23	2.50	0.41
34:f:286:MET:CE	34:f:302:LEU:HG	2.50	0.41
36:h:258:VAL:O	36:h:262:PHE:HB2	2.20	0.41
36:h:275:VAL:HG23	36:h:276:ASP:N	2.35	0.41
36:h:279:ARG:HH12	36:h:290:ALA:HB2	1.85	0.41
37:i:375:LEU:CD1	37:i:387:TYR:HE1	2.24	0.41
39:l:547:ASN:HD22	39:l:547:ASN:N	2.18	0.41
1:2:153:A:H3'	1:2:153:A:N3	2.35	0.41
1:2:924:C:H2'	1:2:925:U:O4'	2.20	0.41
1:2:1688:U:H2'	1:2:1689:C:C6	2.56	0.41
1:2:1845:A:N6	30:b:20:TYR:O	2.52	0.41
10:H:246:LEU:HD12	10:H:246:LEU:HA	1.91	0.41
10:H:427:TRP:CZ3	10:H:429:LYS:HA	2.55	0.41
12:J:248:ARG:HG2	12:J:281:GLY:O	2.20	0.41
21:S:64:ILE:HD12	21:S:64:ILE:N	2.35	0.41
23:U:88:ARG:HD3	23:U:91:GLU:OE1	2.20	0.41
24:V:62:ALA:HB1	32:d:102:LEU:HD23	2.02	0.41
28:Z:84:ILE:HD11	36:h:137:LEU:HD13	2.02	0.41
34:f:57:ASP:O	34:f:59:PRO:HD3	2.19	0.41
36:h:115:ASN:O	36:h:115:ASN:ND2	2.39	0.41
36:h:299:LEU:HG	36:h:360:ASP:OD2	2.20	0.41
37:i:205:ILE:HD13	37:i:205:ILE:HA	1.84	0.41
37:i:345:LEU:O	37:i:346:GLU:HB2	2.19	0.41
37:i:375:LEU:HD23	37:i:375:LEU:H	1.86	0.41
1:2:7:G:O2'	1:2:8:U:H5'	2.20	0.41
1:2:363:A:H8	1:2:363:A:OP1	2.02	0.41
1:2:1080:G:P	30:b:14:ARG:HH21	2.43	0.41
1:2:1093:A:H4'	1:2:1094:A:O5'	2.20	0.41
1:2:1686:U:H2'	1:2:1687:U:O4'	2.21	0.41
11:I:170:HIS:ND1	11:I:171:VAL:HG22	2.36	0.41
16:N:298:PRO:HG2	16:N:301:LEU:HG	2.01	0.41
19:Q:234:PHE:CZ	24:V:195:LEU:HD13	2.54	0.41
26:X:472:ARG:HG2	26:X:472:ARG:HH11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:179:LYS:HE2	37:i:183:LYS:NZ	2.34	0.41
1:2:79:G:H1	1:2:161:A:H2	1.64	0.41
1:2:368:G:C2'	1:2:369:G:H5'	2.50	0.41
1:2:674:U:H2'	1:2:675:U:H6	1.85	0.41
1:2:767:A:H2'	1:2:768:U:C6	2.55	0.41
1:2:1733:C:H42	1:2:1737:A:H61	1.67	0.41
2:8:188:LEU:HD23	2:8:227:ILE:HG23	2.02	0.41
5:C:174:ILE:HA	5:C:178:LYS:HG2	2.02	0.41
5:C:313:GLU:OE2	33:e:253:VAL:HB	2.21	0.41
9:G:29:ILE:HA	9:G:33:MET:CE	2.50	0.41
14:L:67:LEU:HD22	14:L:84:ASP:HB3	2.02	0.41
20:R:63:MET:HB3	20:R:72:ARG:HD3	2.02	0.41
30:b:60:LEU:HA	30:b:63:VAL:HG12	2.02	0.41
34:f:78:GLU:O	34:f:82:GLU:HG2	2.20	0.41
36:h:130:GLN:HG3	36:h:131:ASN:N	2.35	0.41
36:h:151:CYS:HA	36:h:154:VAL:CG1	2.51	0.41
36:h:361:ILE:HG21	36:h:382:LEU:HD21	2.02	0.41
37:i:127:MET:SD	37:i:127:MET:N	2.94	0.41
1:2:145:U:H2'	1:2:146:U:H6	1.86	0.41
1:2:628:U:H5"	1:2:629:G:C8	2.55	0.41
1:2:1383:G:H1'	39:l:478:VAL:HG13	2.02	0.41
1:2:1507:A:H2'	1:2:1508:A:C8	2.55	0.41
1:2:1819:C:H2'	1:2:1820:G:C8	2.55	0.41
2:8:246:ILE:N	2:8:246:ILE:HD12	2.36	0.41
4:B:152:LYS:HD3	4:B:152:LYS:HA	1.88	0.41
12:J:261:LYS:HE2	12:J:296:GLU:OE1	2.20	0.41
16:N:314:PHE:CE2	24:V:165:LYS:HE3	2.55	0.41
23:U:78:ILE:O	23:U:78:ILE:HG13	2.20	0.41
25:W:472:MET:HE3	25:W:472:MET:HB2	1.84	0.41
28:Z:119:ARG:HG2	28:Z:119:ARG:HH11	1.85	0.41
32:d:45:PHE:O	32:d:49:ILE:HG13	2.19	0.41
32:d:104:LYS:CG	32:d:105:PRO:HD2	2.49	0.41
36:h:82:PRO:HB2	36:h:87:LYS:HG2	2.01	0.41
37:i:125:ASP:O	37:i:129:LEU:HD23	2.21	0.41
37:i:309:ARG:HA	37:i:309:ARG:HD3	1.80	0.41
39:l:369:ARG:O	39:l:403:PRO:HB3	2.21	0.41
1:2:25:U:HO2'	1:2:26:U:H5	1.62	0.41
1:2:184:A:H1'	1:2:186:G:N7	2.36	0.41
1:2:365:G:H3'	1:2:365:G:N3	2.35	0.41
1:2:367:G:C2	1:2:368:G:C8	3.09	0.41
1:2:686:G:H2'	1:2:687:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1339:U:C2	1:2:1340:U:C5	3.09	0.41
1:2:1692:C:H2'	1:2:1693:C:H6	1.85	0.41
1:2:1719:G:C2	1:2:1720:C:C5	3.08	0.41
8:F:108:GLU:H	8:F:108:GLU:CD	2.25	0.41
20:R:132:MET:CE	20:R:134:ARG:HB2	2.51	0.41
34:f:230:VAL:HG22	34:f:252:TYR:HB3	2.02	0.41
37:i:290:PRO:C	37:i:293:VAL:HG22	2.46	0.41
39:l:442:VAL:H	39:l:442:VAL:HG22	1.64	0.41
1:2:144:U:C2	1:2:145:U:C5	3.09	0.41
1:2:1704:A:H2	1:2:1706:C:N4	2.19	0.41
1:2:1766:U:H2'	1:2:1767:G:H8	1.84	0.41
3:A:138:ASP:OD2	3:A:141:ARG:HA	2.20	0.41
4:B:199:ASP:HA	4:B:202:LYS:HE3	2.02	0.41
4:B:463:LYS:HA	4:B:463:LYS:HD3	1.83	0.41
5:C:160:ILE:HG13	5:C:161:ILE:N	2.35	0.41
6:D:498:GLU:HG2	6:D:503:VAL:CG2	2.50	0.41
14:L:77:LEU:HD22	14:L:81:GLU:HB3	2.03	0.41
19:Q:234:PHE:CE2	24:V:195:LEU:HD13	2.55	0.41
28:Z:60:LEU:HD23	28:Z:60:LEU:HA	1.91	0.41
29:a:394:LEU:HD23	29:a:394:LEU:HA	1.87	0.41
34:f:83:ASN:HB3	34:f:86:ILE:HD12	2.02	0.41
36:h:149:ASN:O	36:h:152:ARG:HB3	2.21	0.41
36:h:224:VAL:CG1	36:h:225:PHE:N	2.83	0.41
37:i:182:LYS:HA	37:i:182:LYS:HD2	1.71	0.41
37:i:317:LYS:CE	37:i:344:LEU:HD11	2.50	0.41
39:l:398:MET:SD	39:l:403:PRO:HD2	2.60	0.41
1:2:151:A:C2	1:2:156:U:C5	3.09	0.41
1:2:362:C:O2'	1:2:363:A:H2'	2.20	0.41
1:2:740:U:H2'	1:2:741:C:C6	2.55	0.41
1:2:1713:C:H2'	1:2:1714:A:C8	2.56	0.41
3:A:50:LEU:HD23	3:A:50:LEU:O	2.21	0.41
5:C:250:LYS:HD2	5:C:250:LYS:HA	1.71	0.41
16:N:314:PHE:CZ	24:V:168:LEU:HD23	2.56	0.41
18:P:77:LYS:HE3	18:P:77:LYS:HB3	1.66	0.41
20:R:207:LYS:H	20:R:207:LYS:HG2	1.78	0.41
23:U:45:LEU:HD12	23:U:45:LEU:HA	1.83	0.41
29:a:153:LEU:HD23	29:a:153:LEU:HA	1.85	0.41
34:f:185:ALA:HA	34:f:188:TYR:CZ	2.55	0.41
36:h:122:ILE:HD13	36:h:158:CYS:SG	2.60	0.41
36:h:251:LEU:HB2	36:h:256:PHE:CE2	2.55	0.41
37:i:384:ILE:HG22	37:i:415:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:8:U:O2	1:2:8:U:H2'	2.20	0.41
1:2:337:G:C2'	1:2:338:G:H5'	2.51	0.41
1:2:344:A:H2'	1:2:345:G:O4'	2.21	0.41
1:2:428:U:H2'	1:2:429:G:C8	2.56	0.41
1:2:639:C:C2	1:2:640:C:C5	3.09	0.41
1:2:1076:G:H5'	1:2:1094:A:OP2	2.21	0.41
1:2:1344:U:H2'	1:2:1345:U:C6	2.56	0.41
1:2:1541:G:H5"	1:2:1542:A:C8	2.56	0.41
3:A:186:TYR:CG	10:H:264:LEU:HD13	2.56	0.41
4:B:145:GLU:HG2	4:B:146:ILE:N	2.36	0.41
6:D:172:GLN:O	6:D:175:LYS:HB2	2.21	0.41
10:H:241:ILE:N	37:i:295:MET:CE	2.83	0.41
19:Q:226:THR:O	19:Q:226:THR:CG2	2.68	0.41
19:Q:248:GLU:OE2	19:Q:250:ILE:HB	2.20	0.41
26:X:326:ALA:HA	26:X:329:GLU:HB2	2.02	0.41
28:Z:118:LYS:O	28:Z:121:TRP:HD1	2.03	0.41
33:e:149:HIS:O	33:e:152:VAL:HG12	2.20	0.41
33:e:273:MET:HA	33:e:273:MET:HE3	2.02	0.41
33:e:319:LYS:O	33:e:320:CYS:HB2	2.21	0.41
33:e:384:LEU:C	33:e:384:LEU:HD12	2.46	0.41
37:i:134:LYS:HZ3	37:i:138:GLU:HB2	1.86	0.41
37:i:303:GLU:OE2	37:i:308:TRP:HE3	2.04	0.41
39:l:307:ILE:HD13	39:l:310:TRP:CZ3	2.56	0.41
39:l:374:PRO:O	39:l:378:VAL:HG23	2.20	0.41
1:2:77:U:C2'	1:2:78:U:H5'	2.51	0.41
1:2:203:A:H2'	1:2:204:C:O4'	2.21	0.41
1:2:476:C:O2	1:2:476:C:O4'	2.37	0.41
1:2:733:C:H2'	1:2:734:U:C6	2.56	0.41
1:2:1013:A:C2	1:2:1482:U:H1'	2.56	0.41
1:2:1338:U:H2'	1:2:1339:U:O4'	2.21	0.41
1:2:1693:C:H2'	1:2:1694:G:O4'	2.21	0.41
1:2:1723:U:H2'	1:2:1724:U:C6	2.56	0.41
5:C:63:LEU:HD11	6:D:363:HIS:NE2	2.36	0.41
5:C:256:LEU:HD23	5:C:257:LEU:HD22	2.03	0.41
16:N:376:ILE:HD13	16:N:376:ILE:HA	1.85	0.41
17:O:101:ARG:HA	17:O:102:PRO:HD3	1.98	0.41
33:e:149:HIS:C	33:e:152:VAL:HG12	2.46	0.41
36:h:164:ILE:H	36:h:164:ILE:HG12	1.65	0.41
39:l:410:PHE:HZ	39:l:432:LEU:HD23	1.86	0.41
1:2:352:C:C2	1:2:353:C:C5	3.09	0.40
1:2:521:A:C2	13:K:88:LYS:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1736:U:O3'	1:2:1737:A:H8	2.05	0.40
6:D:181:LEU:HD13	6:D:193:TRP:HB3	2.01	0.40
10:H:327:LYS:HE2	10:H:327:LYS:HB3	1.80	0.40
29:a:153:LEU:O	29:a:154:GLU:HB2	2.21	0.40
30:b:48:ASN:OD1	30:b:50:LYS:HG2	2.21	0.40
34:f:157:ILE:N	34:f:158:PRO:CD	2.84	0.40
34:f:189:LEU:O	34:f:192:LEU:HD12	2.21	0.40
35:g:567:LEU:HB2	35:g:568:PRO:HD3	2.03	0.40
36:h:201:LEU:HD23	36:h:201:LEU:C	2.45	0.40
36:h:288:LEU:HB2	36:h:318:TYR:CE2	2.51	0.40
36:h:299:LEU:HB3	36:h:337:TRP:CH2	2.49	0.40
37:i:290:PRO:O	37:i:293:VAL:HG22	2.20	0.40
37:i:375:LEU:HG	37:i:409:LYS:HZ2	1.86	0.40
1:2:265:A:C2	1:2:301:A:C5	3.08	0.40
1:2:1430:A:P	30:b:76:TRP:CH2	3.13	0.40
1:2:1675:C:H2'	1:2:1676:U:O4'	2.21	0.40
4:B:191:ILE:HG12	29:a:192:ILE:HD13	2.03	0.40
5:C:182:LYS:C	5:C:184:LEU:H	2.29	0.40
6:D:78:ARG:HB3	6:D:78:ARG:CZ	2.51	0.40
12:J:195:ILE:HD12	12:J:211:ASP:O	2.20	0.40
36:h:206:MET:HA	36:h:209:LEU:HB3	2.03	0.40
36:h:272:LEU:O	36:h:275:VAL:HG22	2.22	0.40
37:i:134:LYS:NZ	37:i:163:TRP:HH2	2.20	0.40
39:l:392:LYS:HD2	39:l:396:LEU:HG	2.04	0.40
1:2:609:U:O2	1:2:609:U:H2'	2.21	0.40
1:2:701:U:O2	1:2:701:U:H2'	2.20	0.40
1:2:861:C:H2'	1:2:862:G:O4'	2.21	0.40
1:2:1318:A:H3'	1:2:1319:A:C8	2.50	0.40
1:2:1745:A:OP1	36:h:110:TRP:HH2	2.05	0.40
6:D:109:ASP:O	6:D:110:ASP:CG	2.64	0.40
17:O:83:LEU:HD23	17:O:83:LEU:HA	1.92	0.40
24:V:184:LYS:HB3	24:V:184:LYS:HE2	1.79	0.40
29:a:385:ILE:C	29:a:385:ILE:HD12	2.45	0.40
34:f:147:VAL:HG13	34:f:149:MET:HE3	2.03	0.40
34:f:164:ALA:O	34:f:221:PHE:HA	2.21	0.40
34:f:273:TYR:O	34:f:276:LEU:HG	2.21	0.40
1:2:65:G:H2'	1:2:66:C:H6	1.85	0.40
1:2:1066:G:O2'	1:2:1093:A:N1	2.51	0.40
1:2:1312:A:H2'	1:2:1313:A:O4'	2.22	0.40
4:B:307:LYS:HD3	4:B:307:LYS:HA	1.88	0.40
5:C:312:ILE:HD13	5:C:312:ILE:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:134:LYS:HD2	6:D:134:LYS:HA	1.94	0.40
6:D:364:VAL:HG22	6:D:386:MET:SD	2.61	0.40
12:J:283:SER:HB3	12:J:288:ASP:HB3	2.00	0.40
20:R:25:SER:HA	20:R:28:TYR:OH	2.21	0.40
34:f:170:LEU:HD22	34:f:212:MET:HE3	2.03	0.40
37:i:363:ASN:HB3	37:i:366:ALA:CB	2.36	0.40
39:l:563:GLU:HA	39:l:566:VAL:HG22	2.04	0.40
1:2:129:A:N6	1:2:150:A:C6	2.90	0.40
1:2:408:A:H3'	1:2:409:U:H6	1.87	0.40
1:2:561:A:H2'	1:2:565:G:C8	2.57	0.40
1:2:921:G:O2'	1:2:1842:U:OP1	2.36	0.40
1:2:1052:U:O2'	11:I:168:SER:HB2	2.21	0.40
1:2:1328:A:H2'	1:2:1329:A:C8	2.56	0.40
1:2:1713:C:C2	1:2:1714:A:C8	3.10	0.40
4:B:282:GLN:CD	4:B:282:GLN:H	2.30	0.40
6:D:170:LYS:HD3	6:D:204:HIS:ND1	2.37	0.40
25:W:204:LYS:HD3	25:W:205:PRO:HD2	2.04	0.40
36:h:264:ALA:O	36:h:341:VAL:HG12	2.21	0.40
37:i:352:TRP:O	37:i:356:ILE:HG13	2.22	0.40
39:l:360:LEU:HD12	39:l:361:GLY:N	2.36	0.40
39:l:470:LYS:HB2	39:l:470:LYS:HE2	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	8	107/520 (21%)	89 (83%)	14 (13%)	4 (4%)	2 1
3	A	202/212 (95%)	191 (95%)	11 (5%)	0	100 100
4	B	457/554 (82%)	427 (93%)	28 (6%)	2 (0%)	30 36
5	C	329/362 (91%)	323 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	D	409/501 (82%)	393 (96%)	16 (4%)	0	100	100
7	E	99/138 (72%)	97 (98%)	2 (2%)	0	100	100
8	F	146/157 (93%)	141 (97%)	4 (3%)	1 (1%)	18	21
9	G	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
10	H	208/383 (54%)	200 (96%)	7 (3%)	1 (0%)	24	29
11	I	111/228 (49%)	107 (96%)	4 (4%)	0	100	100
12	J	125/304 (41%)	119 (95%)	6 (5%)	0	100	100
13	K	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
14	L	108/154 (70%)	105 (97%)	3 (3%)	0	100	100
15	M	99/155 (64%)	98 (99%)	1 (1%)	0	100	100
16	N	114/414 (28%)	114 (100%)	0	0	100	100
17	O	108/136 (79%)	108 (100%)	0	0	100	100
18	P	89/110 (81%)	89 (100%)	0	0	100	100
19	Q	88/237 (37%)	88 (100%)	0	0	100	100
20	R	162/212 (76%)	153 (94%)	9 (6%)	0	100	100
21	S	73/100 (73%)	73 (100%)	0	0	100	100
22	T	48/94 (51%)	45 (94%)	3 (6%)	0	100	100
23	U	125/192 (65%)	122 (98%)	3 (2%)	0	100	100
24	V	162/193 (84%)	158 (98%)	3 (2%)	1 (1%)	21	25
25	W	376/483 (78%)	374 (100%)	2 (0%)	0	100	100
26	X	202/496 (41%)	200 (99%)	1 (0%)	1 (0%)	24	29
27	Y	96/102 (94%)	96 (100%)	0	0	100	100
28	Z	78/153 (51%)	74 (95%)	4 (5%)	0	100	100
29	a	311/424 (73%)	303 (97%)	8 (3%)	0	100	100
30	b	75/80 (94%)	65 (87%)	9 (12%)	1 (1%)	9	9
31	c	24/128 (19%)	23 (96%)	1 (4%)	0	100	100
32	d	76/110 (69%)	74 (97%)	1 (1%)	1 (1%)	9	9
33	e	244/383 (64%)	240 (98%)	4 (2%)	0	100	100
34	f	375/410 (92%)	362 (96%)	13 (4%)	0	100	100
35	g	117/668 (18%)	109 (93%)	8 (7%)	0	100	100
36	h	308/384 (80%)	299 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	i	366/725 (50%)	356 (97%)	10 (3%)	0	100	100
38	k	43/155 (28%)	37 (86%)	6 (14%)	0	100	100
39	l	300/576 (52%)	296 (99%)	4 (1%)	0	100	100
All	All	6608/10887 (61%)	6386 (97%)	210 (3%)	12 (0%)	44	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	8	251	LYS
10	H	225	ILE
30	b	48	ASN
2	8	228	GLY
32	d	108	ASP
4	B	409	ILE
2	8	266	ILE
8	F	143	ALA
2	8	257	LYS
24	V	44	LEU
26	X	428	ILE
4	B	410	PRO

5.3.2 Protein sidechains (i)

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	8	95/461 (21%)	87 (92%)	8 (8%)	10	12
3	A	177/182 (97%)	176 (99%)	1 (1%)	78	87
4	B	421/492 (86%)	413 (98%)	8 (2%)	50	66
5	C	312/343 (91%)	307 (98%)	5 (2%)	55	71
6	D	366/444 (82%)	361 (99%)	5 (1%)	59	74
7	E	90/126 (71%)	88 (98%)	2 (2%)	45	62
8	F	124/124 (100%)	117 (94%)	7 (6%)	19	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	G	112/113 (99%)	110 (98%)	2 (2%)	51	68
10	H	175/320 (55%)	170 (97%)	5 (3%)	37	52
11	I	104/197 (53%)	103 (99%)	1 (1%)	68	81
12	J	108/256 (42%)	105 (97%)	3 (3%)	38	53
13	K	106/107 (99%)	104 (98%)	2 (2%)	50	66
14	L	93/128 (73%)	88 (95%)	5 (5%)	20	27
15	M	90/137 (66%)	88 (98%)	2 (2%)	45	62
16	N	107/362 (30%)	107 (100%)	0	100	100
17	O	93/117 (80%)	92 (99%)	1 (1%)	65	79
18	P	78/95 (82%)	76 (97%)	2 (3%)	40	56
19	Q	75/203 (37%)	74 (99%)	1 (1%)	61	76
20	R	141/180 (78%)	140 (99%)	1 (1%)	76	86
21	S	68/90 (76%)	66 (97%)	2 (3%)	37	52
22	T	44/79 (56%)	43 (98%)	1 (2%)	44	60
23	U	109/170 (64%)	107 (98%)	2 (2%)	51	68
24	V	147/173 (85%)	143 (97%)	4 (3%)	39	55
25	W	328/410 (80%)	321 (98%)	7 (2%)	47	63
26	X	174/395 (44%)	170 (98%)	4 (2%)	44	60
27	Y	84/86 (98%)	82 (98%)	2 (2%)	43	59
28	Z	65/119 (55%)	61 (94%)	4 (6%)	16	21
29	a	252/375 (67%)	246 (98%)	6 (2%)	43	59
30	b	68/71 (96%)	65 (96%)	3 (4%)	25	35
31	c	25/116 (22%)	25 (100%)	0	100	100
32	d	65/93 (70%)	65 (100%)	0	100	100
33	e	226/339 (67%)	220 (97%)	6 (3%)	39	55
34	f	321/351 (92%)	317 (99%)	4 (1%)	63	77
35	g	108/597 (18%)	106 (98%)	2 (2%)	50	66
36	h	271/337 (80%)	264 (97%)	7 (3%)	40	56
37	i	325/629 (52%)	319 (98%)	6 (2%)	51	68
38	k	21/106 (20%)	20 (95%)	1 (5%)	23	32
39	l	256/492 (52%)	250 (98%)	6 (2%)	44	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5824/9415 (62%)	5696 (98%)	128 (2%)	45 62

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	8	171	PHE
2	8	172	THR
2	8	176	GLU
2	8	188	LEU
2	8	189	LYS
2	8	231	LEU
2	8	245	VAL
2	8	249	HIS
3	A	123	LEU
4	B	10	VAL
4	B	15	ASN
4	B	18	SER
4	B	69	THR
4	B	368	TRP
4	B	478	ILE
4	B	510	THR
4	B	527	SER
5	C	52	ILE
5	C	68	GLN
5	C	122	GLN
5	C	125	GLN
5	C	221	ARG
6	D	90	GLU
6	D	161	ARG
6	D	375	LYS
6	D	386	MET
6	D	395	ILE
7	E	28	LYS
7	E	45	LYS
8	F	28	VAL
8	F	63	VAL
8	F	107	LEU
8	F	116	LEU
8	F	124	SER
8	F	130	GLU
8	F	138	THR
9	G	59	ARG

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Mol	Chain	Res	Type
9	G	86	GLU
10	H	276	SER
10	H	298	ARG
10	H	300	VAL
10	H	356	LYS
10	H	366	THR
11	I	207	TYR
12	J	205	THR
12	J	259	VAL
12	J	304	ASN
13	K	25	ASP
13	K	88	LYS
14	L	82	LEU
14	L	87	GLU
14	L	93	GLN
14	L	111	GLU
14	L	112	VAL
15	M	106	LYS
15	M	157	VAL
17	O	111	VAL
18	P	28	LYS
18	P	39	LYS
19	Q	226	THR
20	R	62	VAL
21	S	40	LEU
21	S	83	SER
22	T	73	GLN
23	U	59	PHE
23	U	63	HIS
24	V	33	HIS
24	V	119	GLU
24	V	159	GLU
24	V	177	GLU
25	W	97	LEU
25	W	139	ILE
25	W	256	GLN
25	W	275	VAL
25	W	279	GLU
25	W	349	VAL
25	W	456	GLU
26	X	335	VAL
26	X	432	GLU

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Mol	Chain	Res	Type
26	X	438	ILE
26	X	440	GLU
27	Y	7	LYS
27	Y	73	GLU
28	Z	51	LYS
28	Z	81	ILE
28	Z	84	ILE
28	Z	91	ARG
29	a	87	GLU
29	a	91	ASN
29	a	101	ILE
29	a	128	GLN
29	a	149	THR
29	a	208	HIS
30	b	43	CYS
30	b	47	ASN
30	b	84	GLN
33	e	203	GLU
33	e	224	GLU
33	e	229	GLU
33	e	286	GLU
33	e	304	LEU
33	e	315	LYS
34	f	90	LEU
34	f	148	THR
34	f	175	VAL
34	f	176	GLN
35	g	562	GLU
35	g	607	PHE
36	h	110	TRP
36	h	180	THR
36	h	202	MET
36	h	204	GLU
36	h	246	LYS
36	h	323	LYS
36	h	334	VAL
37	i	123	MET
37	i	167	TRP
37	i	231	GLU
37	i	281	LYS
37	i	345	LEU
37	i	447	SER

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Mol	Chain	Res	Type
38	k	18	ARG
39	l	292	MET
39	l	410	PHE
39	l	412	LEU
39	l	430	LEU
39	l	503	MET
39	l	547	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	9	GLN
4	B	244	ASN
4	B	351	ASN
4	B	468	HIS
5	C	88	HIS
5	C	135	ASN
5	C	158	ASN
5	C	284	ASN
6	D	252	ASN
6	D	353	GLN
7	E	96	HIS
8	F	34	GLN
8	F	37	HIS
9	G	50	GLN
9	G	119	ASN
9	G	123	GLN
10	H	299	GLN
11	I	139	ASN
11	I	217	GLN
12	J	267	HIS
13	K	61	HIS
14	L	36	ASN
14	L	61	HIS
16	N	349	GLN
19	Q	198	GLN
20	R	208	HIS
21	S	48	GLN
21	S	63	HIS
24	V	96	GLN
25	W	248	HIS
25	W	288	ASN

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Mol	Chain	Res	Type
25	W	405	HIS
26	X	521	ASN
27	Y	35	GLN
28	Z	73	HIS
28	Z	92	HIS
30	b	57	GLN
30	b	84	GLN
35	g	638	ASN
36	h	143	HIS
36	h	229	HIS
36	h	345	GLN
37	i	381	ASN
39	l	472	HIS
39	l	501	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1602/1611 (99%)	289 (18%)	21 (1%)

All (289) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	12	A
1	2	17	G
1	2	26	U
1	2	30	G
1	2	37	A
1	2	40	A
1	2	47	G
1	2	55	C
1	2	56	U
1	2	59	A
1	2	76	G
1	2	78	U
1	2	79	G
1	2	80	U
1	2	83	U
1	2	150	A
1	2	151	A
1	2	152	G

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Mol	Chain	Res	Type
1	2	154	G
1	2	155	U
1	2	156	U
1	2	157	G
1	2	158	A
1	2	161	A
1	2	162	C
1	2	163	A
1	2	164	A
1	2	183	A
1	2	184	A
1	2	185	G
1	2	195	U
1	2	203	A
1	2	205	A
1	2	206	G
1	2	210	G
1	2	214	U
1	2	215	A
1	2	225	G
1	2	226	A
1	2	233	G
1	2	236	A
1	2	237	G
1	2	238	C
1	2	245	U
1	2	264	U
1	2	266	G
1	2	270	G
1	2	277	A
1	2	285	G
1	2	286	C
1	2	288	G
1	2	308	G
1	2	317	U
1	2	318	U
1	2	347	C
1	2	348	A
1	2	351	G
1	2	363	A
1	2	364	C
1	2	365	G

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Mol	Chain	Res	Type
1	2	366	G
1	2	371	C
1	2	373	G
1	2	378	G
1	2	386	U
1	2	391	C
1	2	403	G
1	2	409	U
1	2	416	A
1	2	420	U
1	2	425	G
1	2	430	A
1	2	431	A
1	2	432	G
1	2	440	A
1	2	441	U
1	2	443	C
1	2	444	C
1	2	450	U
1	2	451	A
1	2	468	U
1	2	469	G
1	2	470	C
1	2	471	G
1	2	479	G
1	2	492	G
1	2	494	A
1	2	495	G
1	2	509	C
1	2	516	C
1	2	522	G
1	2	528	G
1	2	529	U
1	2	530	A
1	2	531	A
1	2	545	A
1	2	557	A
1	2	560	G
1	2	562	C
1	2	566	G
1	2	571	A
1	2	573	G

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Mol	Chain	Res	Type
1	2	574	G
1	2	575	G
1	2	579	G
1	2	629	G
1	2	649	U
1	2	658	C
1	2	661	A
1	2	699	G
1	2	717	A
1	2	718	A
1	2	720	A
1	2	745	A
1	2	751	G
1	2	762	A
1	2	773	A
1	2	786	A
1	2	789	U
1	2	790	A
1	2	811	A
1	2	813	C
1	2	836	A
1	2	837	U
1	2	838	U
1	2	839	C
1	2	840	U
1	2	841	G
1	2	846	G
1	2	851	U
1	2	865	A
1	2	866	A
1	2	867	A
1	2	903	C
1	2	907	A
1	2	914	U
1	2	916	A
1	2	918	G
1	2	919	G
1	2	920	G
1	2	922	G
1	2	926	G
1	2	927	C
1	2	928	A

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Mol	Chain	Res	Type
1	2	953	U
1	2	954	U
1	2	962	A
1	2	964	G
1	2	968	A
1	2	969	G
1	2	970	A
1	2	986	G
1	2	994	A
1	2	999	G
1	2	1000	A
1	2	1002	A
1	2	1007	A
1	2	1013	A
1	2	1027	G
1	2	1029	C
1	2	1030	U
1	2	1031	U
1	2	1036	A
1	2	1037	C
1	2	1057	U
1	2	1082	U
1	2	1086	G
1	2	1093	A
1	2	1112	U
1	2	1116	G
1	2	1117	U
1	2	1118	U
1	2	1123	A
1	2	1125	A
1	2	1127	A
1	2	1132	C
1	2	1134	U
1	2	1135	A
1	2	1136	A
1	2	1137	G
1	2	1140	G
1	2	1141	A
1	2	1143	A
1	2	1170	U
1	2	1172	U
1	2	1310	A

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Mol	Chain	Res	Type
1	2	1311	A
1	2	1316	A
1	2	1320	A
1	2	1321	A
1	2	1339	U
1	2	1380	U
1	2	1385	A
1	2	1386	A
1	2	1387	C
1	2	1388	A
1	2	1389	A
1	2	1392	A
1	2	1393	A
1	2	1395	A
1	2	1407	G
1	2	1420	A
1	2	1422	U
1	2	1423	G
1	2	1431	U
1	2	1432	A
1	2	1447	G
1	2	1450	G
1	2	1459	A
1	2	1460	A
1	2	1475	U
1	2	1476	A
1	2	1490	A
1	2	1491	C
1	2	1501	A
1	2	1515	U
1	2	1516	G
1	2	1523	A
1	2	1541	G
1	2	1543	A
1	2	1561	A
1	2	1564	U
1	2	1582	C
1	2	1600	G
1	2	1615	G
1	2	1625	A
1	2	1626	U
1	2	1647	G

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Mol	Chain	Res	Type
1	2	1652	C
1	2	1653	U
1	2	1659	C
1	2	1661	C
1	2	1662	C
1	2	1669	C
1	2	1680	A
1	2	1686	U
1	2	1694	G
1	2	1701	C
1	2	1702	G
1	2	1703	G
1	2	1704	A
1	2	1706	C
1	2	1707	A
1	2	1714	A
1	2	1721	A
1	2	1722	C
1	2	1724	U
1	2	1725	C
1	2	1727	G
1	2	1728	U
1	2	1731	A
1	2	1732	A
1	2	1735	C
1	2	1736	U
1	2	1738	G
1	2	1740	C
1	2	1743	A
1	2	1744	C
1	2	1745	A
1	2	1746	A
1	2	1747	A
1	2	1751	U
1	2	1753	U
1	2	1760	U
1	2	1762	U
1	2	1763	U
1	2	1764	A
1	2	1765	U
1	2	1766	U
1	2	1768	A

Continued on next page...

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Mol	Chain	Res	Type
1	2	1769	C
1	2	1770	G
1	2	1771	C
1	2	1772	A
1	2	1774	A
1	2	1800	G
1	2	1801	A
1	2	1802	A
1	2	1803	G
1	2	1804	U
1	2	1812	A
1	2	1814	G
1	2	1815	U
1	2	1826	G
1	2	1828	MA6
1	2	1829	C
1	2	1838	G
1	2	1839	G
1	2	1846	U

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	162	C
1	2	225	G
1	2	236	A
1	2	442	U
1	2	450	U
1	2	491	G
1	2	493	A
1	2	573	G
1	2	866	A
1	2	998	A
1	2	1117	U
1	2	1319	A
1	2	1430	A
1	2	1701	C
1	2	1705	C
1	2	1706	C
1	2	1726	U
1	2	1769	C
1	2	1773	U

Continued on next page...

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Mol	Chain	Res	Type
1	2	1802	A
1	2	1814	G

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

6 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	$\#\|Z\| > 2$
1	MA6	2	1827	1	23,26,27	0.32	0	34,38,41	0.68	1 (2%)
1	UR3	2	1807	1	19,22,23	0.34	0	26,32,35	0.83	1 (3%)
1	MA6	2	1828	1	23,26,27	0.33	0	34,38,41	0.66	1 (2%)
1	2MG	2	1825	1	23,26,27	0.31	0	32,38,41	0.57	0
1	G7M	2	525	1	23,26,27	0.64	0	35,39,42	0.57	0
1	4OC	2	1664	1	20,23,24	0.40	0	26,32,35	0.87	2 (7%)

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
1	MA6	2	1827	1	-	0/11/29/30	0/3/3/3
1	UR3	2	1807	1	-	2/7/25/26	0/2/2/2
1	MA6	2	1828	1	-	2/11/29/30	0/3/3/3
1	2MG	2	1825	1	-	0/9/27/28	0/3/3/3
1	G7M	2	525	1	-	3/7/25/26	0/3/3/3
1	4OC	2	1664	1	-	1/9/29/30	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1828	MA6	C2-N1-C6	3.00	118.83	111.75
1	2	1827	MA6	C2-N1-C6	2.95	118.72	111.75
1	2	1664	4OC	O2'-C2'-C1'	-2.73	103.75	109.08
1	2	1664	4OC	O3'-C3'-C2'	2.53	118.36	111.17
1	2	1807	UR3	C4-N3-C2	-2.07	122.61	124.56

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1664	4OC	C3'-C2'-O2'-CM2
1	2	525	G7M	C3'-C4'-C5'-O5'
1	2	525	G7M	O4'-C4'-C5'-O5'
1	2	1828	MA6	C4'-C5'-O5'-P
1	2	1828	MA6	C3'-C4'-C5'-O5'
1	2	1807	UR3	O4'-C4'-C5'-O5'
1	2	1807	UR3	C3'-C4'-C5'-O5'
1	2	525	G7M	C4'-C5'-O5'-P

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1827	MA6	1	0
1	2	1828	MA6	1	0
1	2	1825	2MG	1	0
1	2	1664	4OC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
40	ATP	W	501	-	29,33,33	0.65	0	44,52,52	0.50	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
40	ATP	W	501	-	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

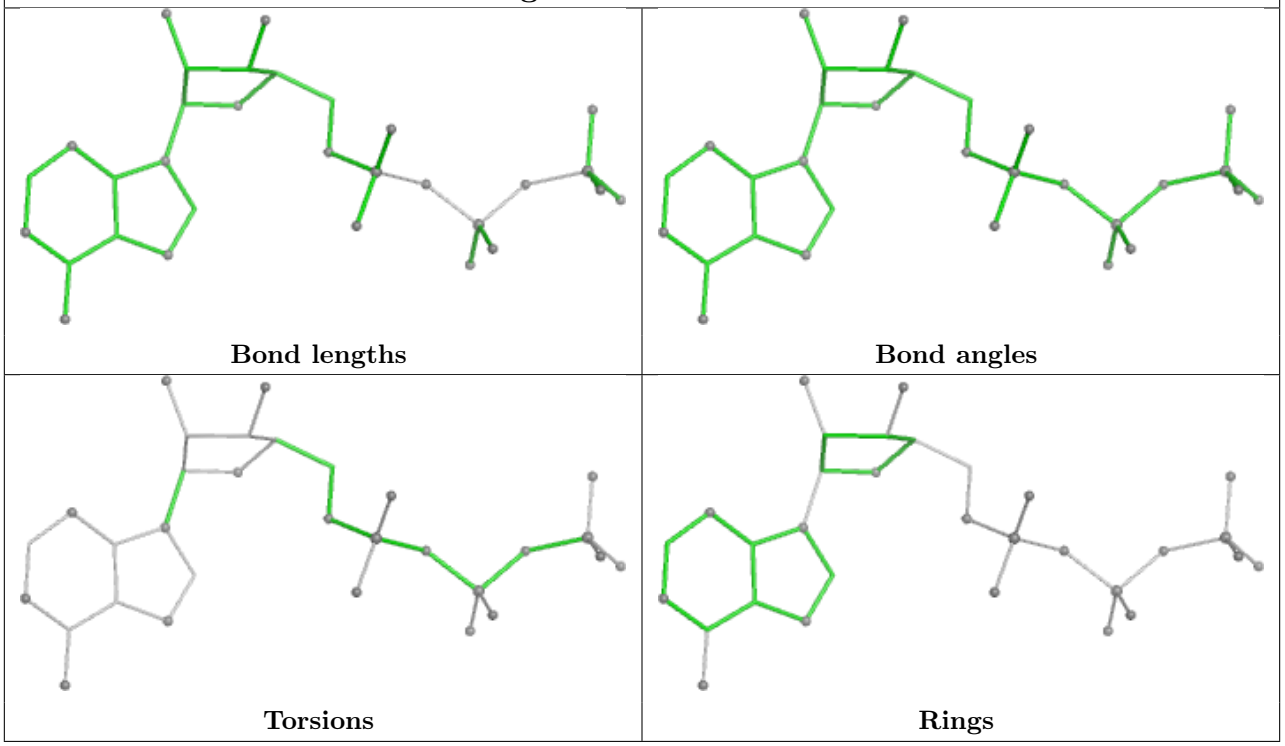
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand ATP W 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1172:U	O3'	1309:A	P	20.56
1	2	1330:A	O3'	1335:U	P	18.93
1	2	137:A	O3'	142:U	P	14.70
1	2	1345:U	O3'	1376:A	P	14.09
1	2	84:A	O3'	129:A	P	13.51
1	2	1842:U	O3'	1845:A	P	9.18

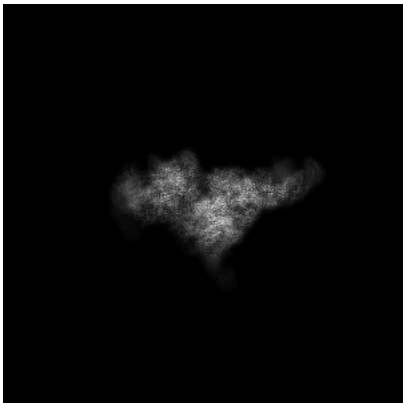
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56198. These allow visual inspection of the internal detail of the map and identification of artifacts.

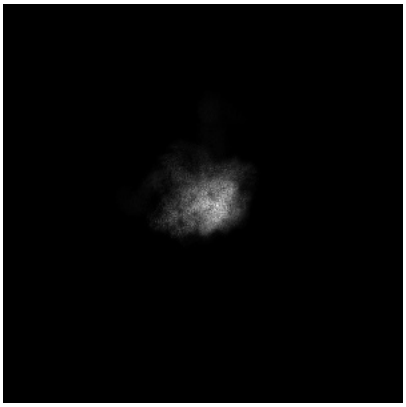
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

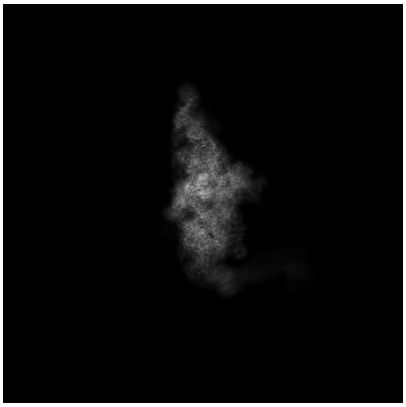
6.1.1 Primary map



X



Y

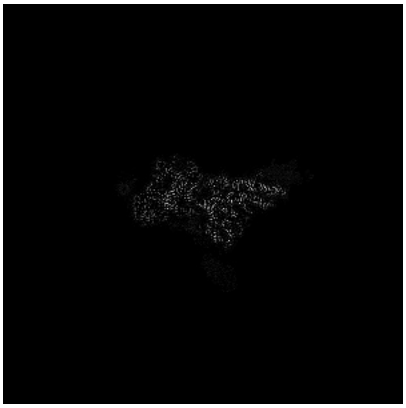


Z

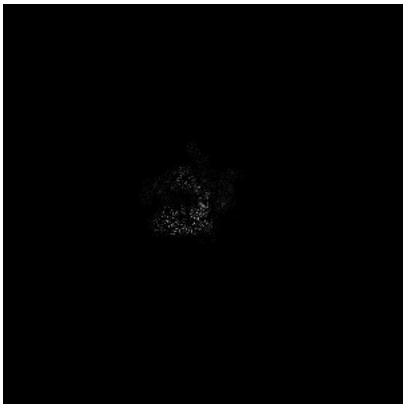
The images above show the map projected in three orthogonal directions.

6.2 Central slices

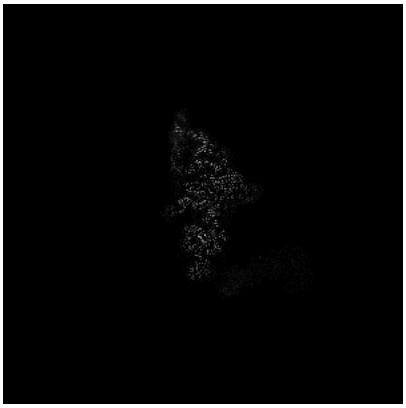
6.2.1 Primary map



X Index: 350



Y Index: 350

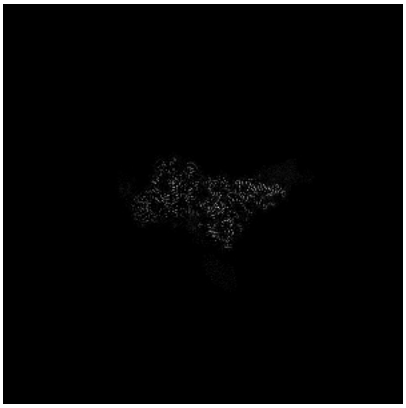


Z Index: 350

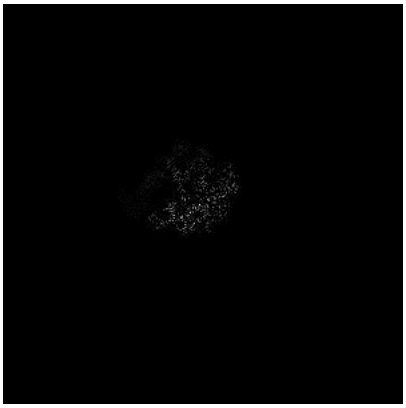
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

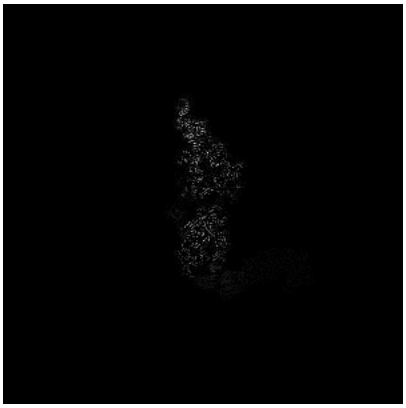
6.3.1 Primary map



X Index: 348



Y Index: 376

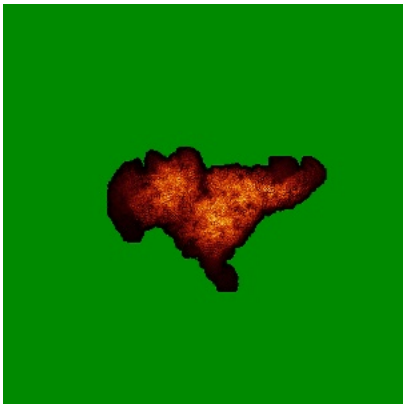


Z Index: 371

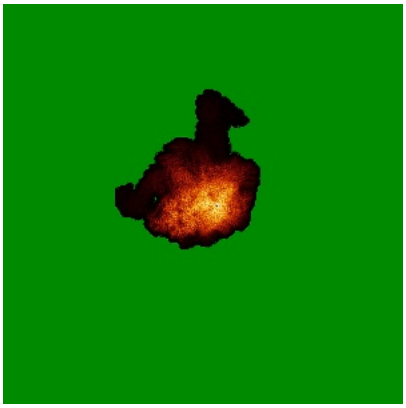
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

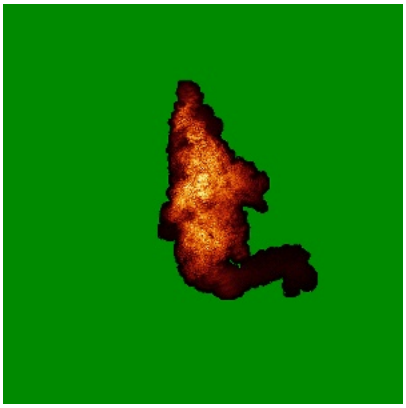
6.4.1 Primary map



X



Y

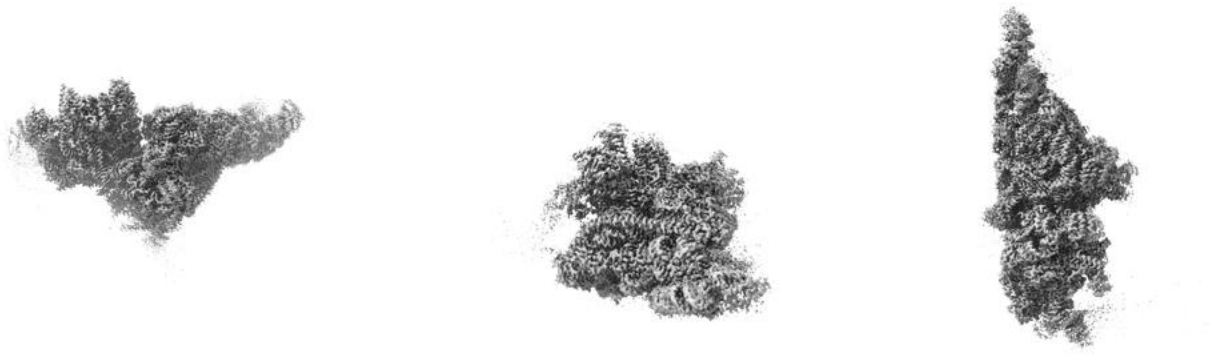


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

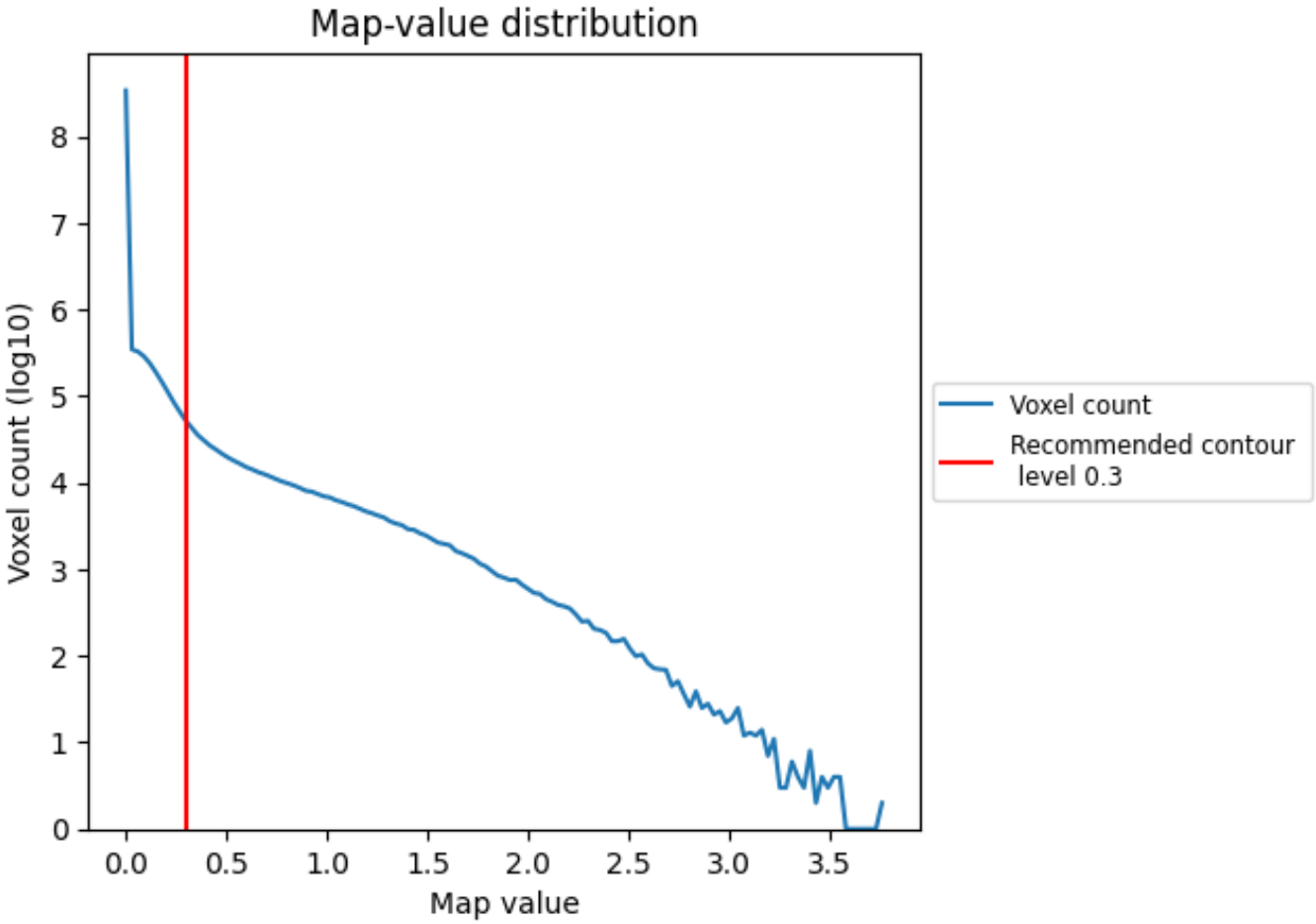
6.6 Mask visualisation (i)

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

7 Map analysis

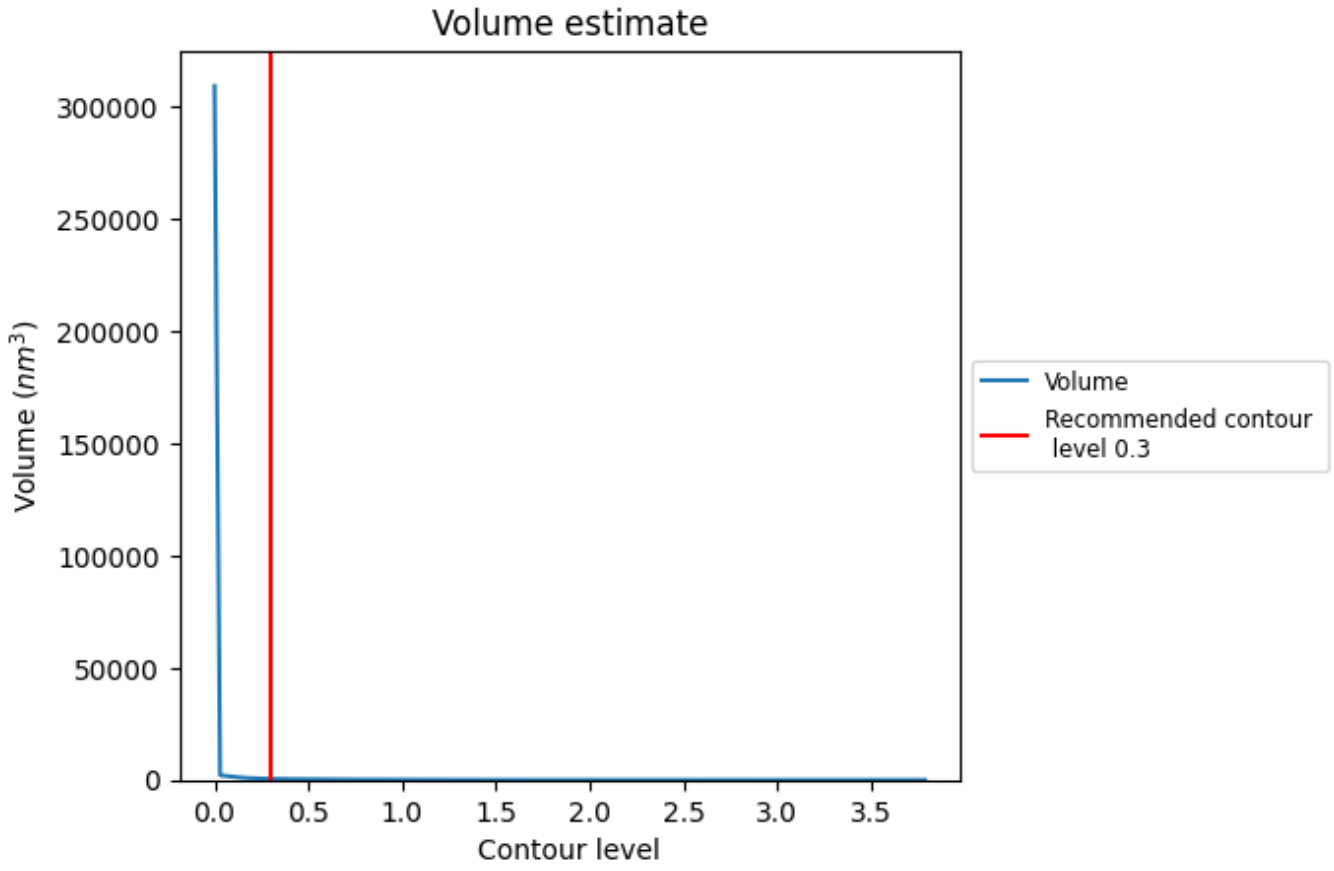
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

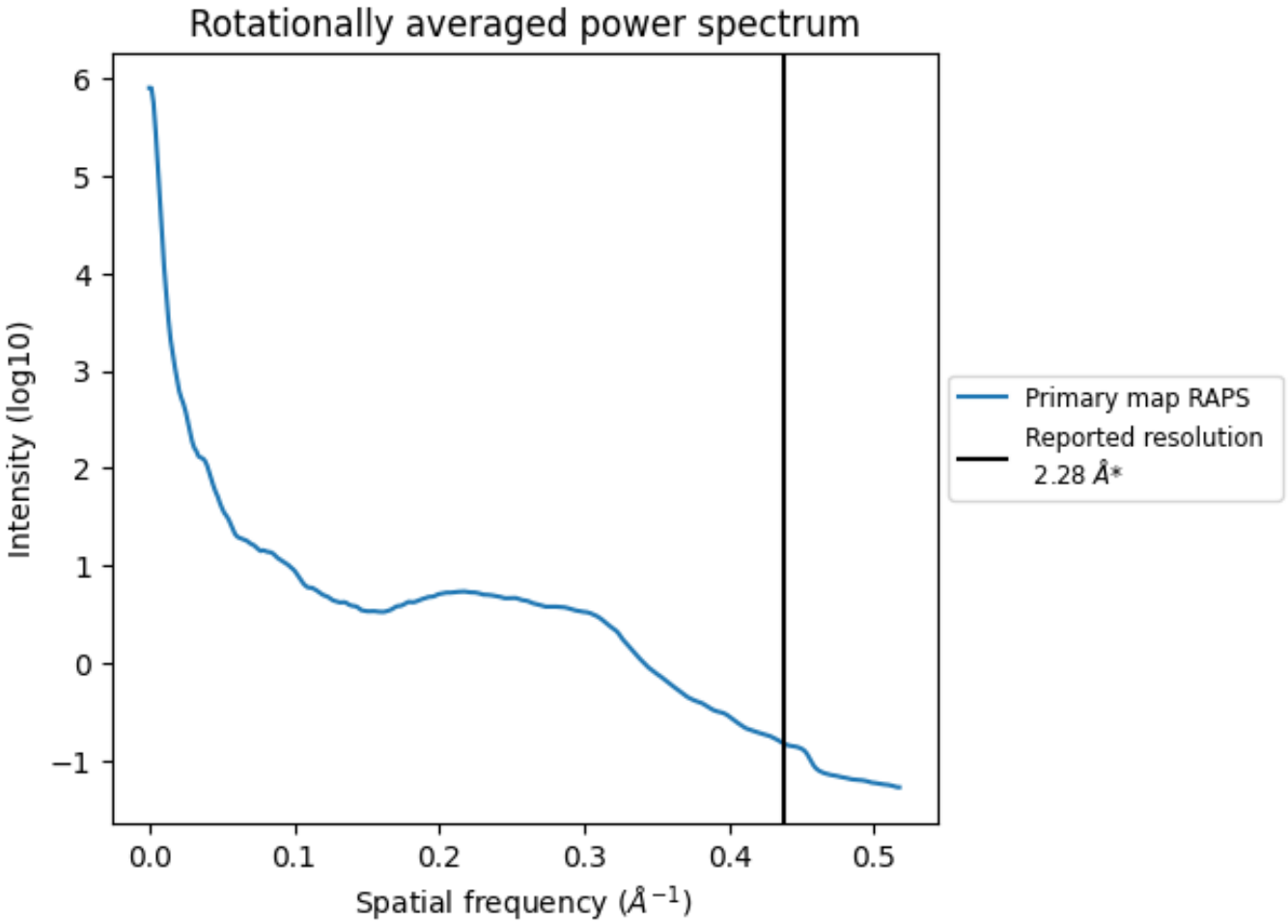
7.2 Volume estimate



The volume at the recommended contour level is 481 nm^3; this corresponds to an approximate mass of 435 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 (i)



*Reported resolution corresponds to spatial frequency of 0.439 Å^{-1}

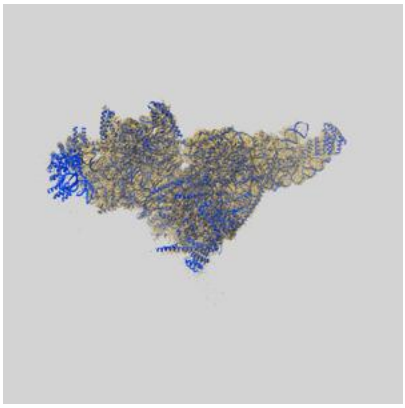
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

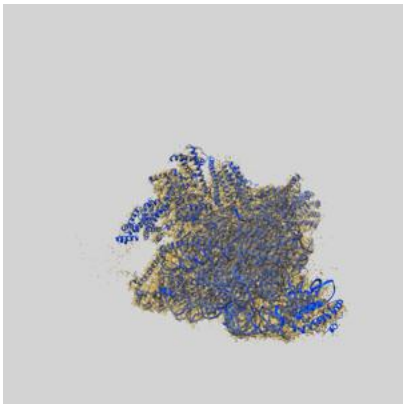
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56198 and PDB model 9TRV. Per-residue inclusion information can be found in section 3 on page 12.

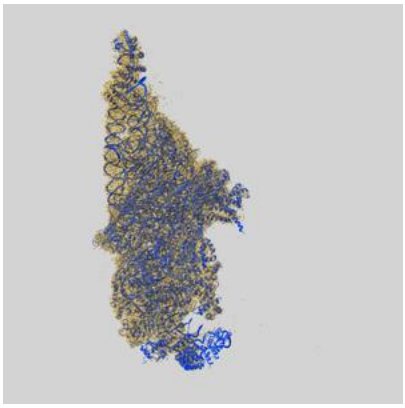
9.1 Map-model overlay



X



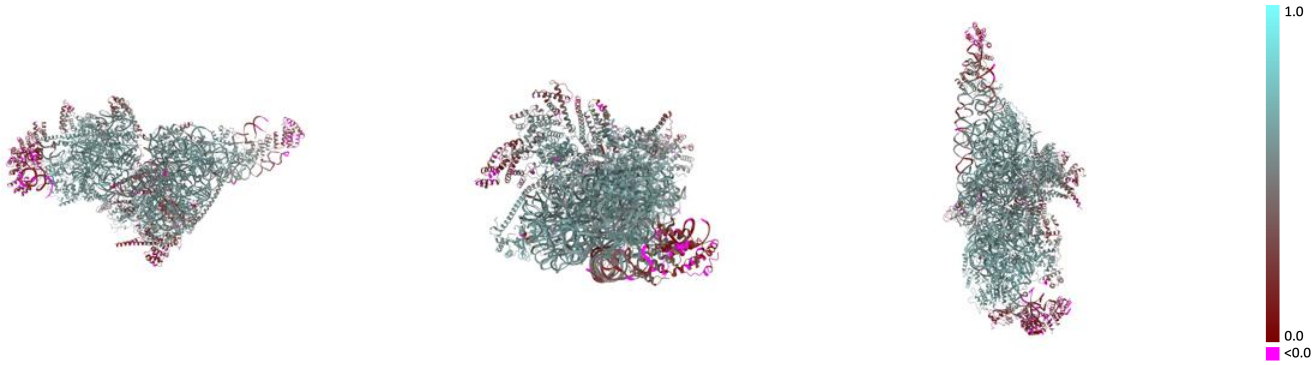
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

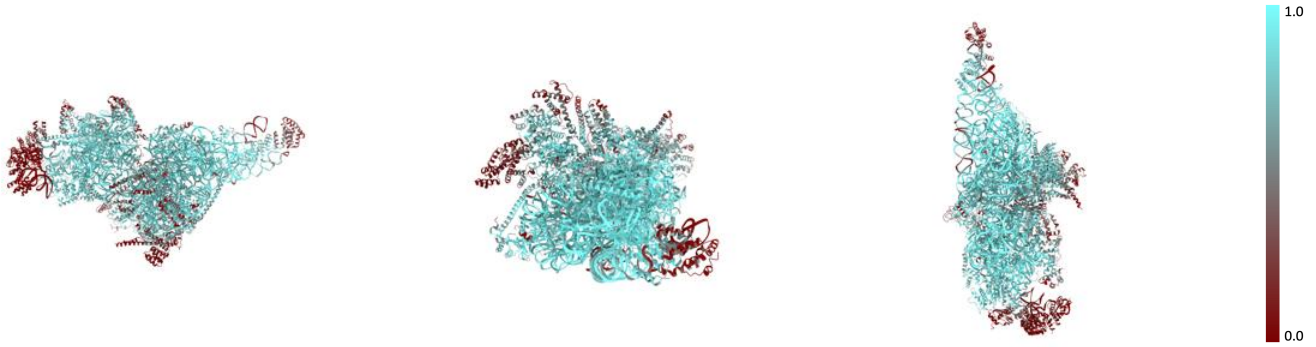
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

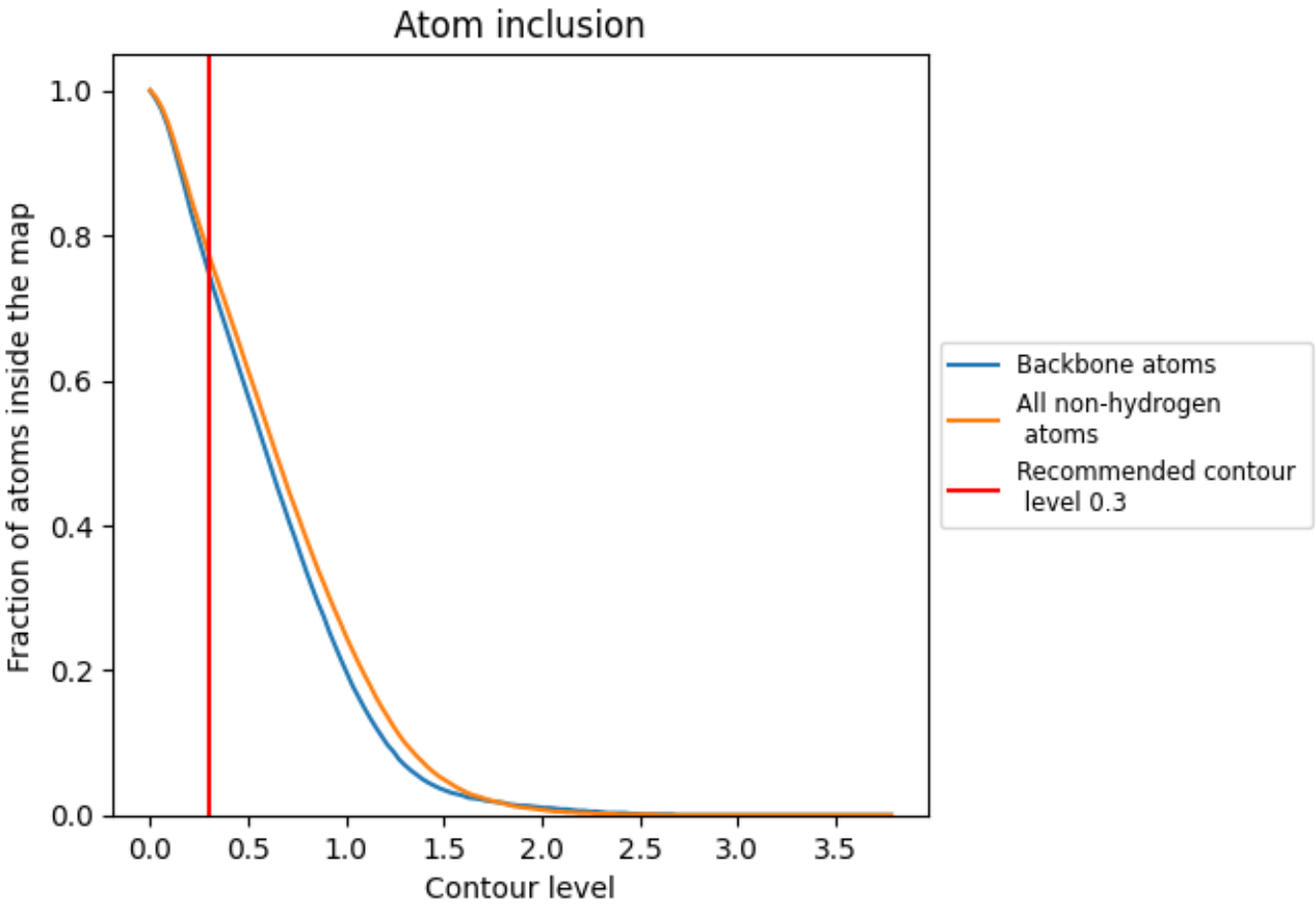
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 77% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7740	0.5230
2	0.8940	0.5540
8	0.3770	0.3240
A	0.8640	0.5960
B	0.7500	0.5360
C	0.8410	0.5680
D	0.7240	0.5220
E	0.9070	0.6270
F	0.7330	0.5760
G	0.9560	0.6400
H	0.7430	0.5480
I	0.9430	0.6440
J	0.7570	0.5260
K	0.9140	0.6130
L	0.8000	0.6110
M	0.9630	0.6610
N	0.8910	0.6160
O	0.9620	0.6240
P	0.8830	0.6050
Q	0.8320	0.5970
R	0.4300	0.3650
S	0.7370	0.5430
T	0.9550	0.6460
U	0.4920	0.3920
V	0.7850	0.5510
W	0.8870	0.6260
X	0.7740	0.5580
Y	0.8310	0.6070
Z	0.9100	0.5280
a	0.7250	0.5410
b	0.2030	0.3040
c	0.8120	0.5560
d	0.8650	0.5560
e	0.8520	0.5750
f	0.7490	0.5380



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Chain	Atom inclusion	Q-score
g	0.0000	0.1080
h	0.5230	0.2660
i	0.2920	0.3180
k	0.4900	0.4280
l	0.1100	0.1910