Full wwPDB EM Validation Report ⓘ

Oct 29, 2026 – 03:49 pm GMT

PDB ID	:	9TRS / pdb_00009trs
EMDB ID	:	EMD-56196
Title	:	Structure of the Plant mitochondrial pre-initiation complex 2, (SSU,mtIF3,mRNA)
Authors	:	Skaltsogiannis, V.; Giege, P.; Soufari, H.
Deposited on	:	2025-12-27
Resolution	:	2.55 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:

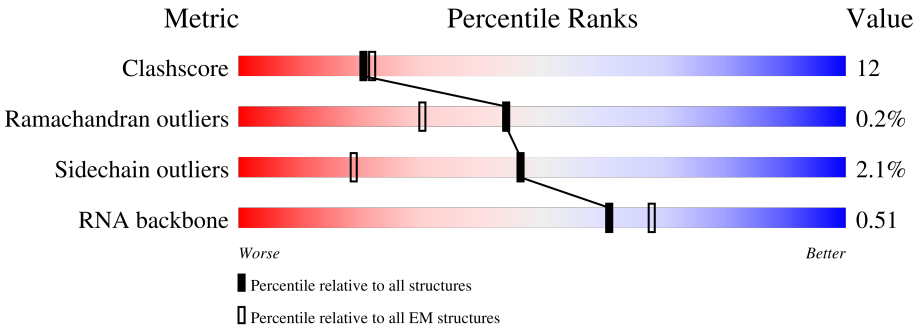
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

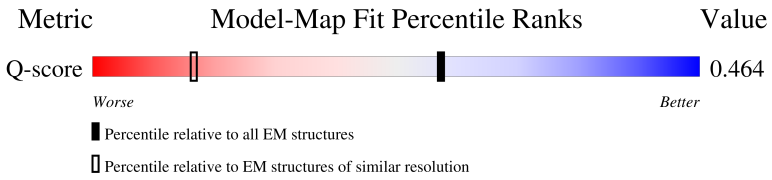
1 Overall quality at a glance

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

The reported resolution of this entry is 2.55 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.





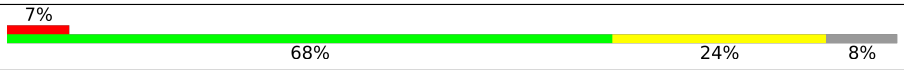
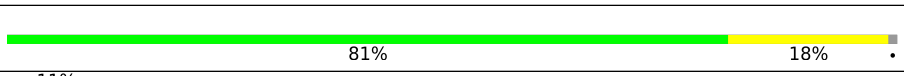
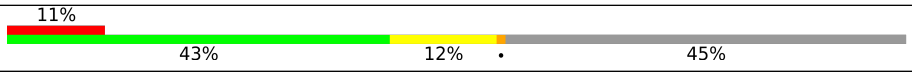
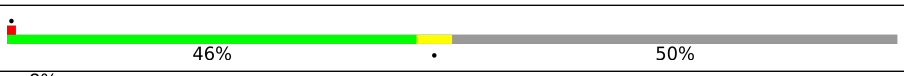
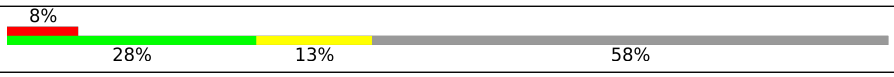
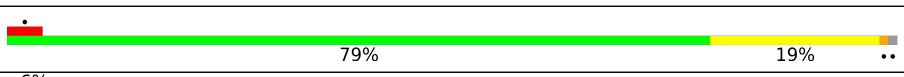
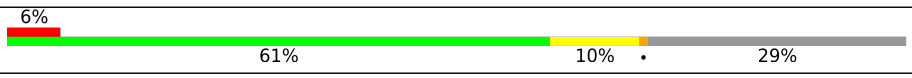
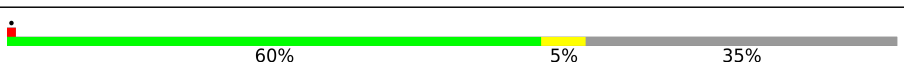
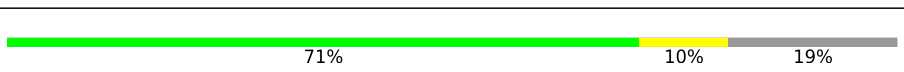
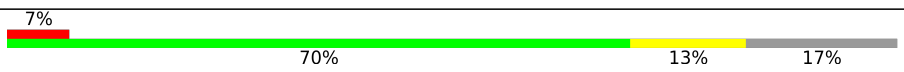
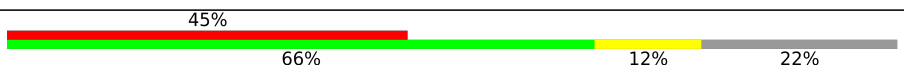
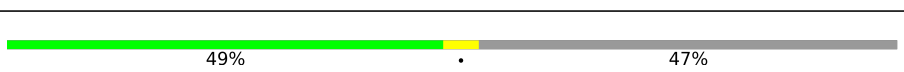
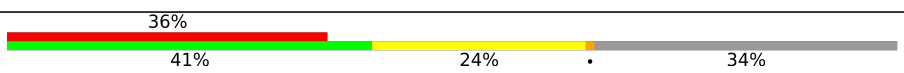
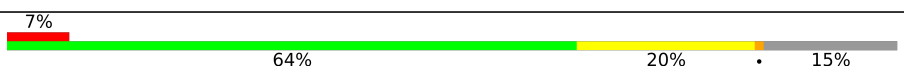
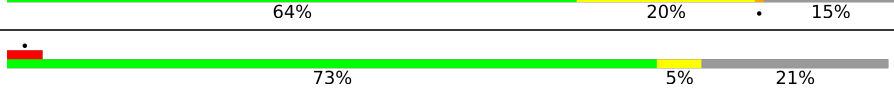
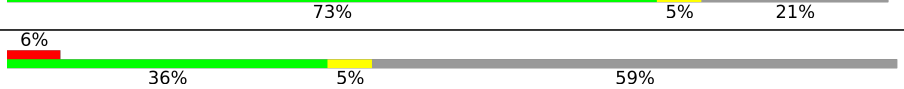
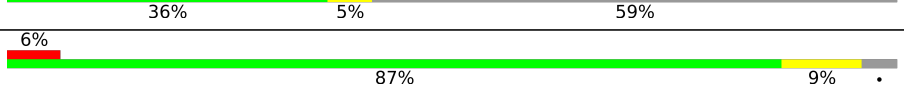
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7475 (2.05 - 3.05)

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	1613	8% 55% 35% 10%
2	6	6	67% 50% 50%
3	8	520	11% 13% 6% 79%

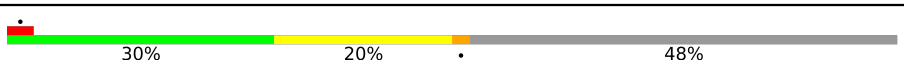
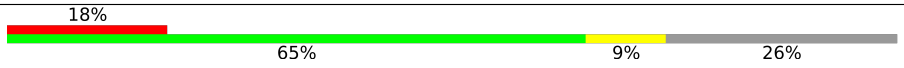
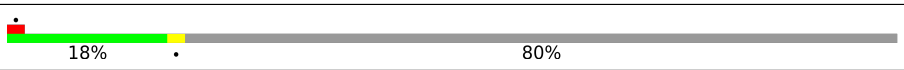
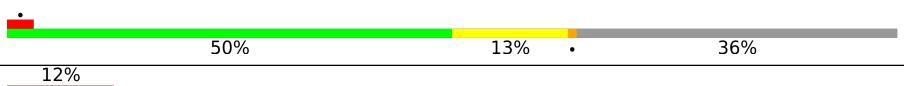
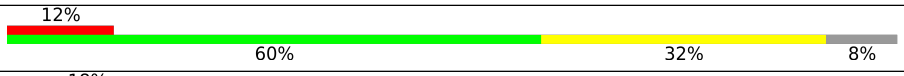
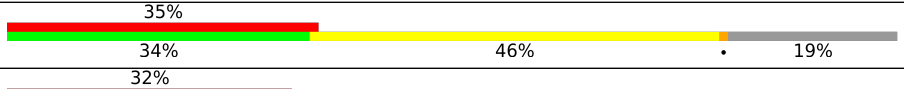
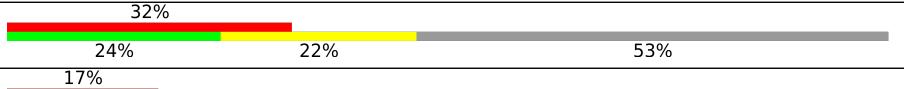
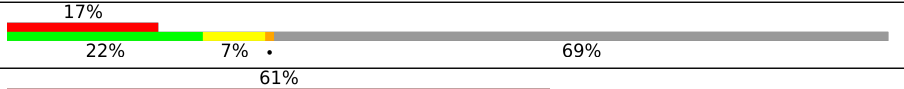
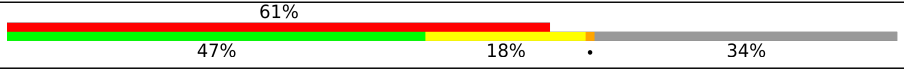
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Mol	Chain	Length	Quality of chain
4	A	212	
5	B	554	
6	C	362	
7	D	501	
8	E	138	
9	F	157	
10	G	129	
11	H	383	
12	I	228	
13	J	304	
14	K	125	
15	L	154	
16	M	155	
17	N	414	
18	O	136	
19	P	110	
20	Q	237	
21	R	212	
22	S	100	
23	T	94	
24	U	192	
25	V	193	
26	W	483	
27	X	496	
28	Y	102	

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Mol	Chain	Length	Quality of chain
29	Z	153	
30	a	424	
31	b	80	
32	c	128	
33	d	110	
34	e	383	
35	f	410	
36	g	668	
37	h	384	
38	i	725	
39	k	153	
40	l	576	

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 90102 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	1613	34549	15434	6299	11203	1613	0	0

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	6	6	120	54	12	48	6	0	0

- Molecule 3 is a protein called Translation initiation factor IF3-1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	8	109	1801	566	927	151	153	4	0	0

- Molecule 4 is a protein called Ribosomal protein S2.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 6 is a protein called Ribosomal protein S4.

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

- Molecule 7 is a protein called S5 DRBM domain-containing protein.

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

- Molecule 8 is a protein called bS6m.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS7m.

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

- Molecule 10 is a protein called 40S ribosomal protein S15a.

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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 12 is a protein called Small ribosomal subunit protein uS10 domain-containing protein.

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

- Molecule 13 is a protein called Ribosomal protein S11.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS12m.

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

- Molecule 15 is a protein called uS13m.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS14m.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS15c.

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

- Molecule 18 is a protein called 30S ribosomal protein S16.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS17c.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	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 21 is a protein called Small ribosomal subunit protein uS19m.

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

- Molecule 22 is a protein called Ribosomal protein S21.

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

- Molecule 23 is a protein called 30S ribosomal protein S31, mitochondrial.

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

- Molecule 24 is a protein called mS23.

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

- Molecule 25 is a protein called mS26.

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

- Molecule 26 is a protein called Small ribosomal subunit protein mS29.

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

- Molecule 27 is a protein called BnaC06g06470D protein.

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

- Molecule 28 is a protein called MOSC domain-containing protein.

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

- Molecule 29 is a protein called Mitochondrial 28S ribosomal protein S34.

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

- Molecule 30 is a protein called Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein.

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

- Molecule 31 is a protein called IMS import disulfide relay-system CHCH-CHCH-like Cx9C domain-containing protein.

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

- Molecule 32 is a protein called Small ribosomal subunit protein mS38.

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

- Molecule 33 is a protein called IGR domain-containing protein.

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

- Molecule 34 is a protein called mS45.

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

- Molecule 35 is a protein called mS47.

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

- Molecule 36 is a protein called Small ribosomal subunit protein mS81 (rPPR8).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	123	Total	C	N	O	S	0	0
			979	630	163	179	7		

- Molecule 37 is a protein called (rape) hypothetical protein.

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

- Molecule 38 is a protein called PROP1-like PPR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	338	Total	C	N	O	S	0	0
			2740	1728	460	537	15		

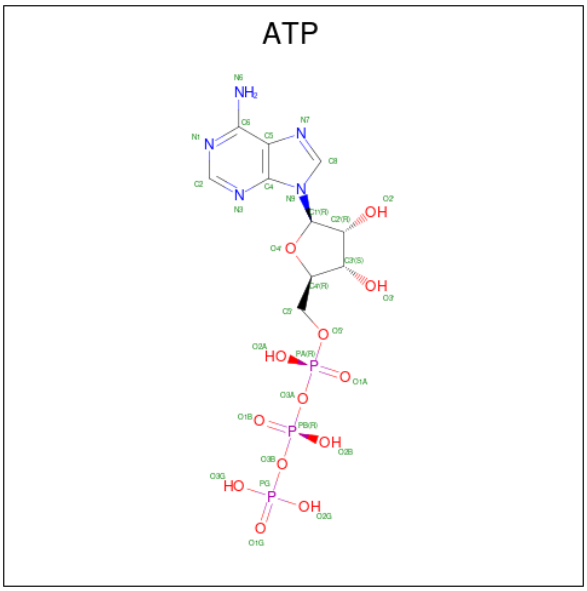
- Molecule 39 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	47	Total	C	N	O	S	0	0
			319	198	61	56	4		

- Molecule 40 is a protein called Small ribosomal subunit protein mS80 (rPPR6).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	378	Total	C	N	O	S	0	0
			2955	1882	489	561	23		

- Molecule 41 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
41	W	1	Total	C	N	O	P	0
			31	10	5	13	3	

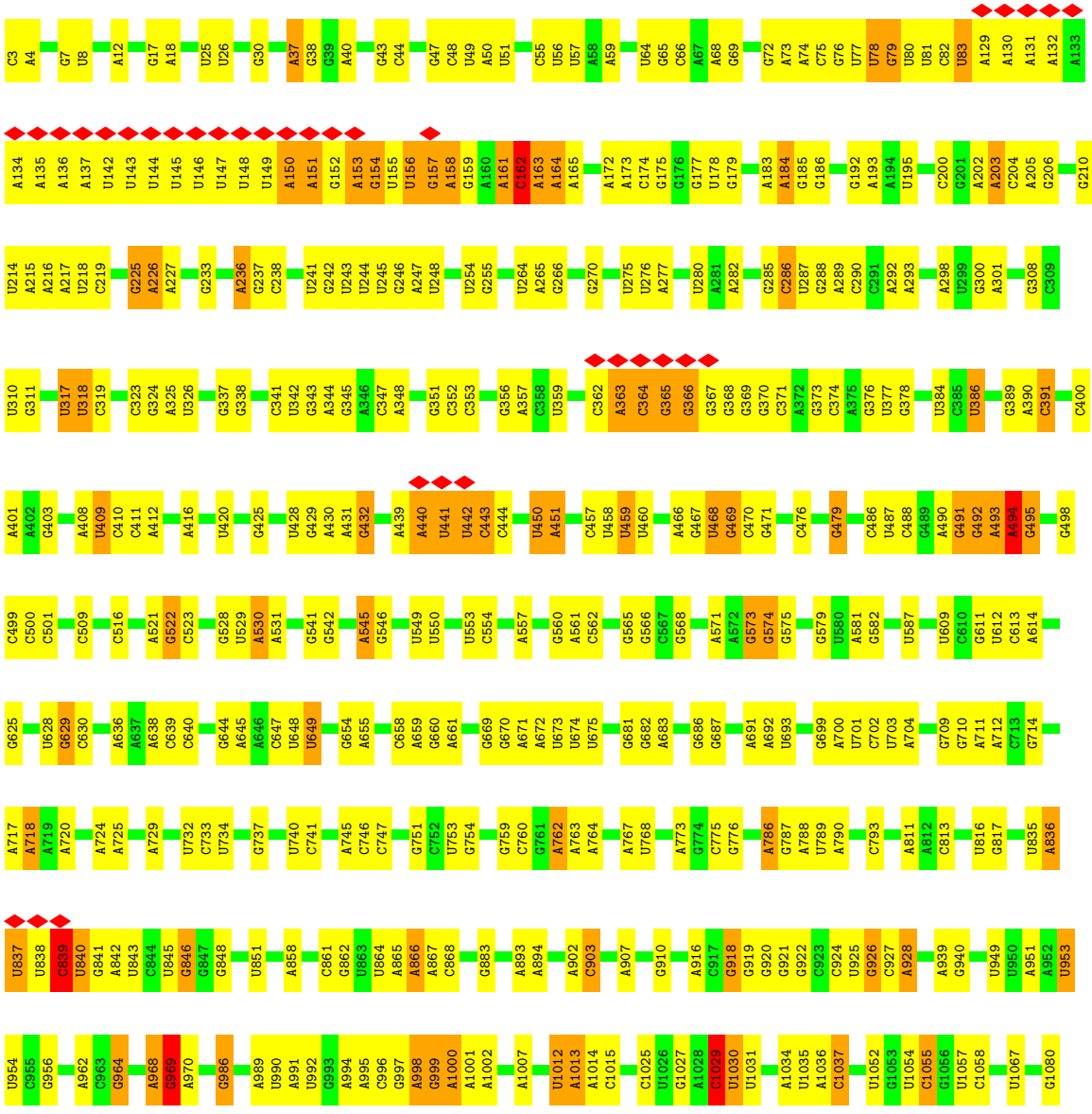
3 Residue-property plots (i)

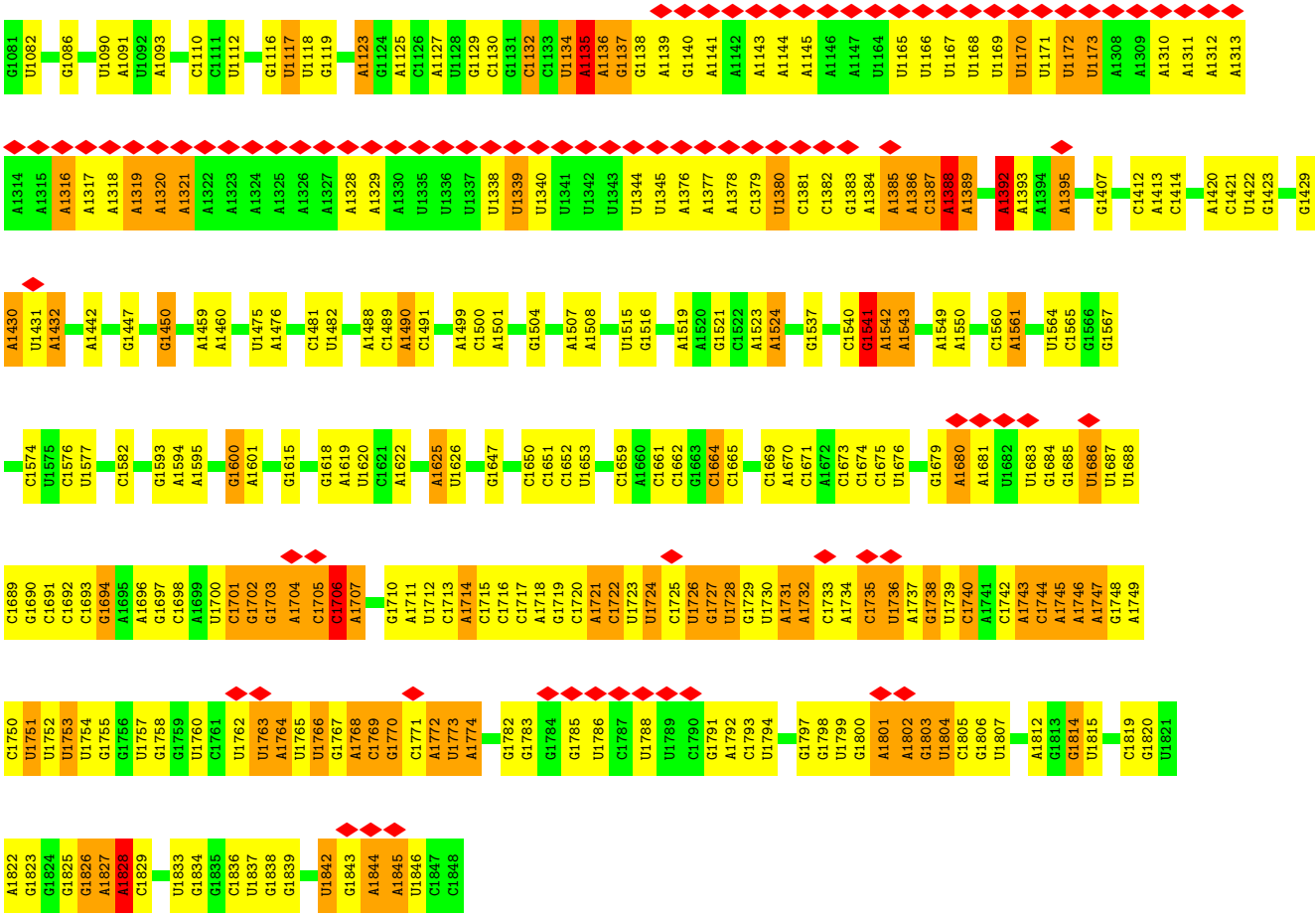
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

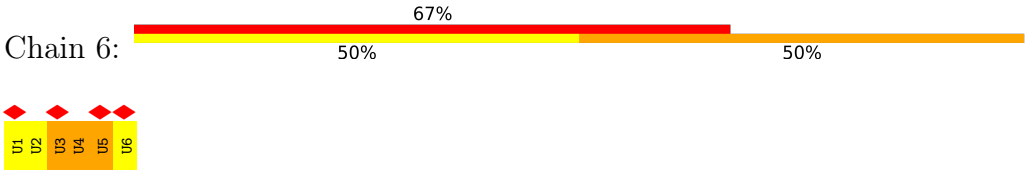
Chain 2:



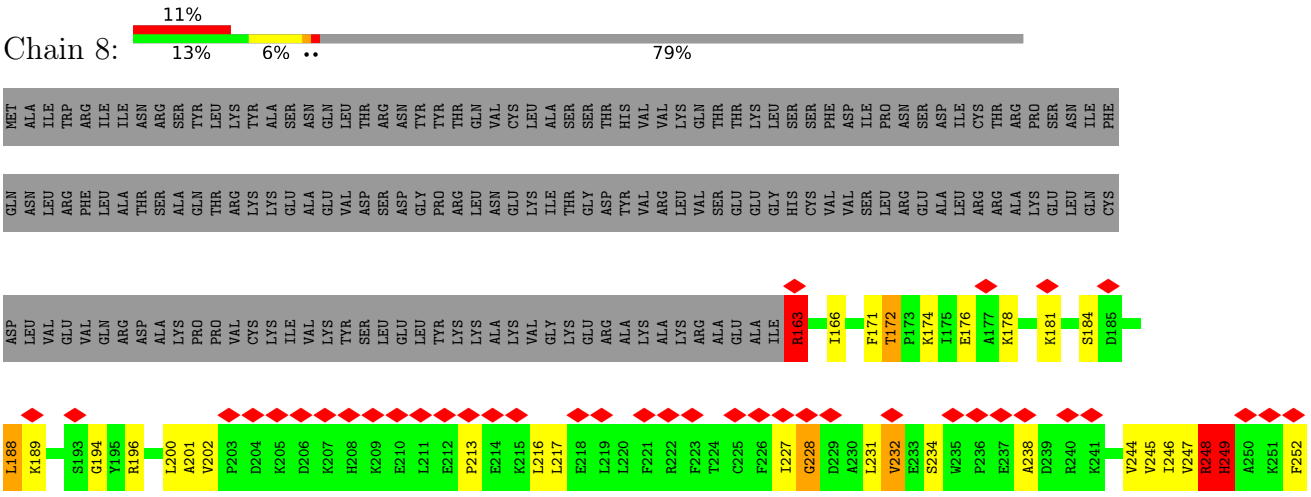


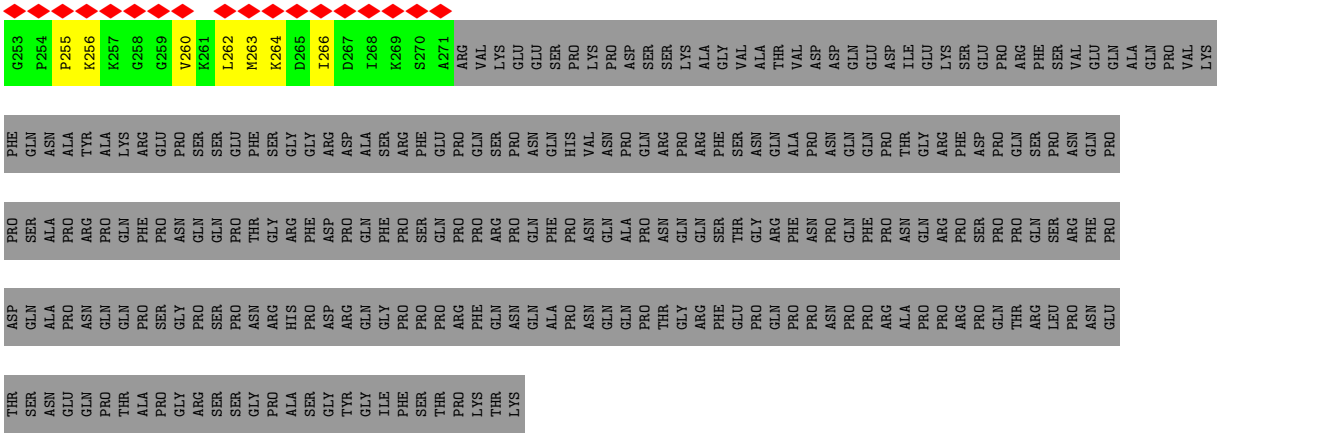


• Molecule 2: mRNA



• Molecule 3: Translation initiation factor IF3-1, mitochondrial

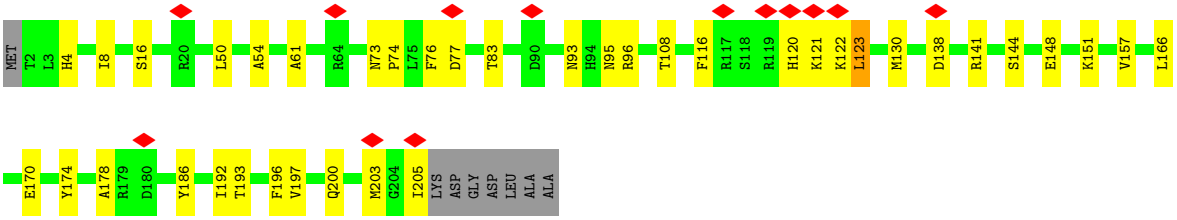




• Molecule 4: Ribosomal protein S2

Chain A:

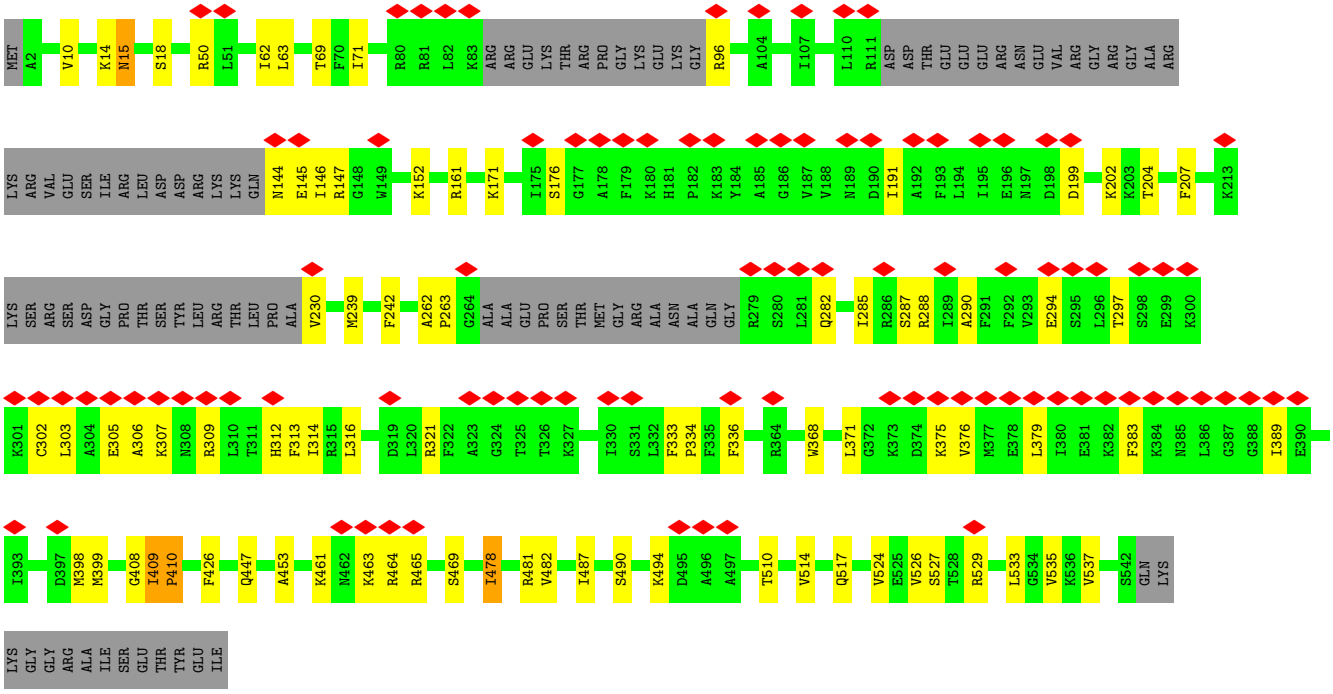




• Molecule 5: Small ribosomal subunit protein uS3m

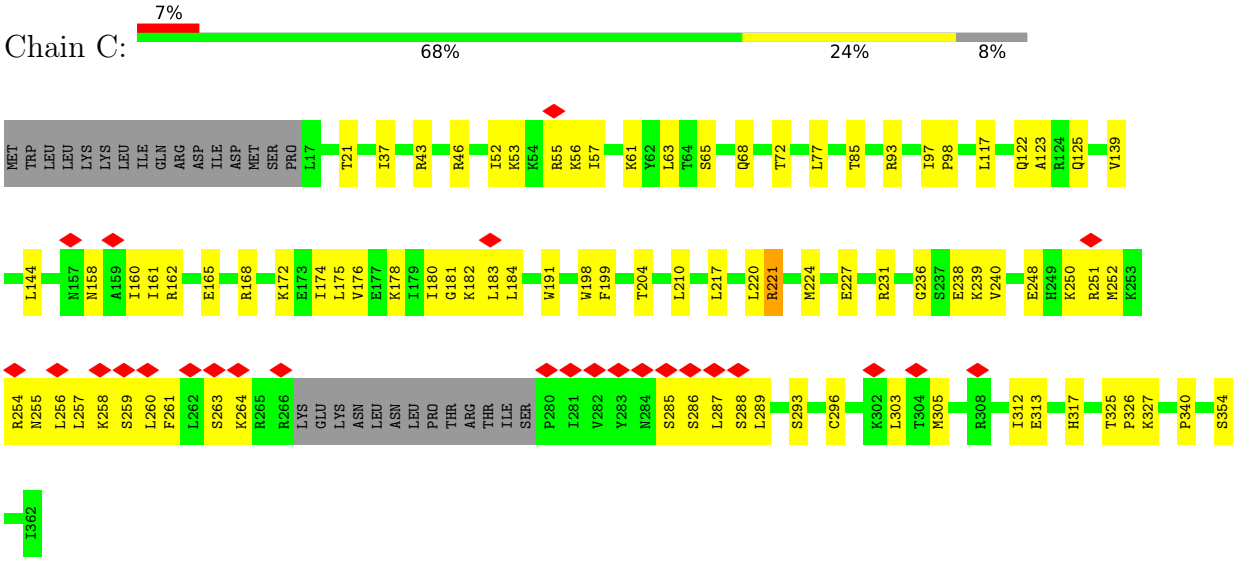
Chain B:





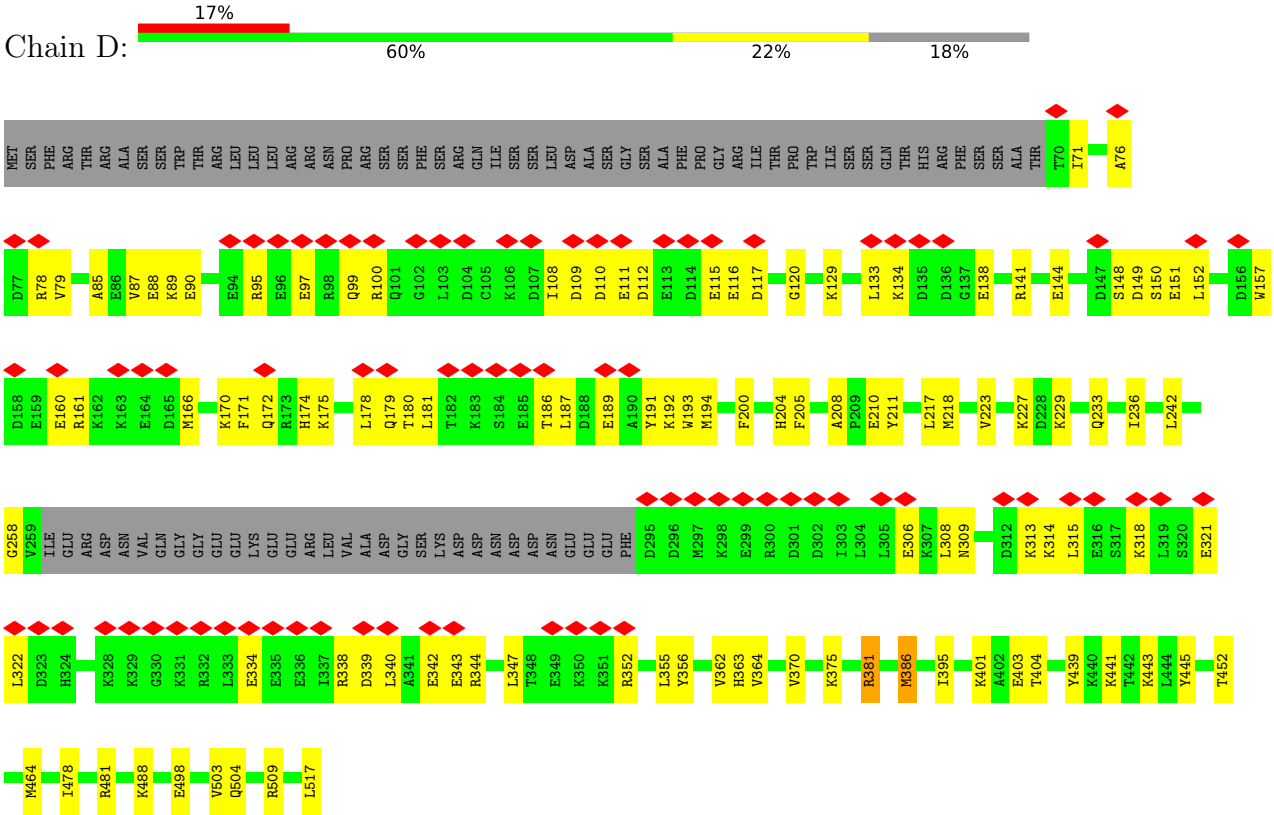
• Molecule 6: Ribosomal protein S4

Chain C:



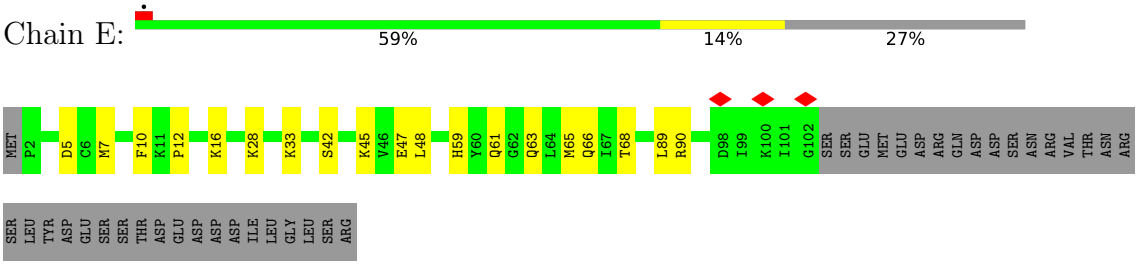
• Molecule 7: S5 DRBM domain-containing protein

Chain D:



• Molecule 8: bS6m

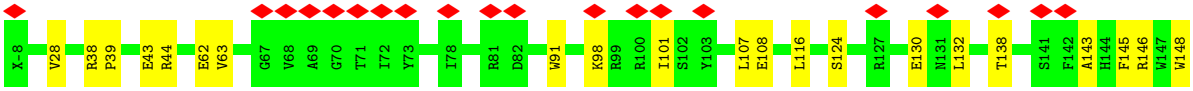
Chain E:



• Molecule 9: Small ribosomal subunit protein uS7m

Chain F:





• Molecule 10: 40S ribosomal protein S15a

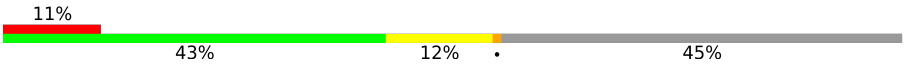
Chain G:

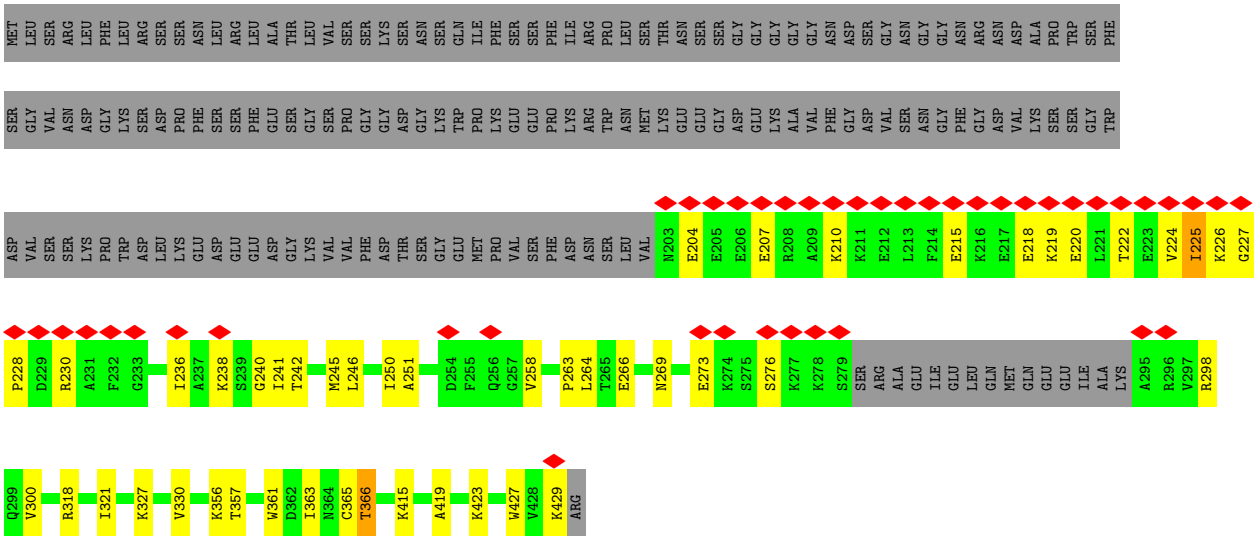




• Molecule 11: 30S ribosomal protein S9

Chain H:

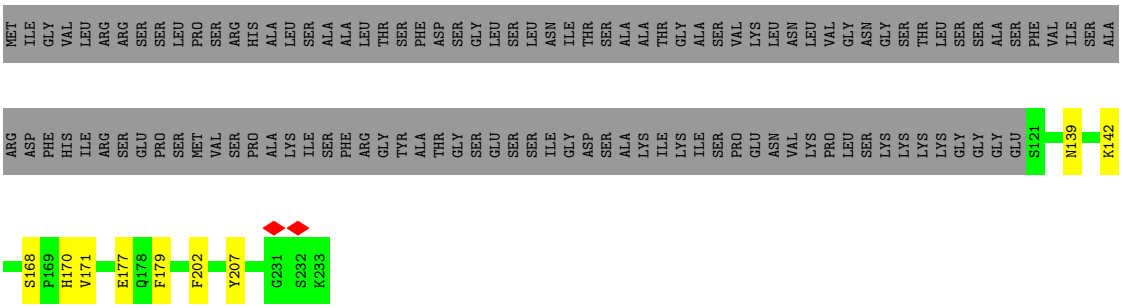




• Molecule 12: Small ribosomal subunit protein uS10 domain-containing protein

Chain I:

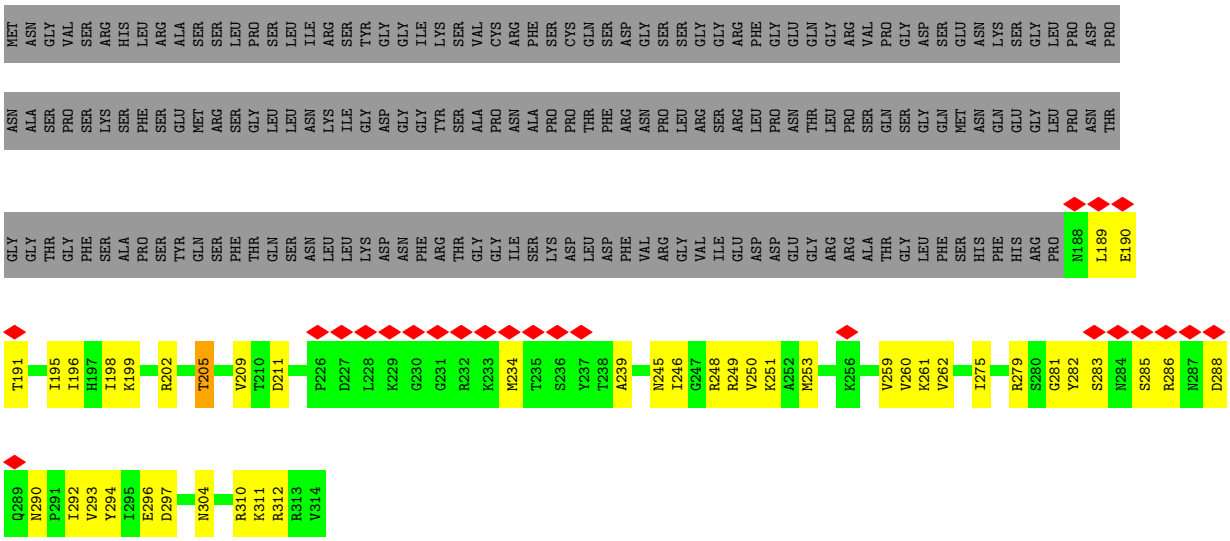




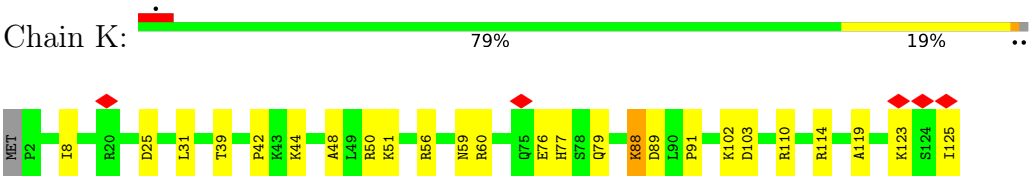
• Molecule 13: Ribosomal protein S11

Chain J:

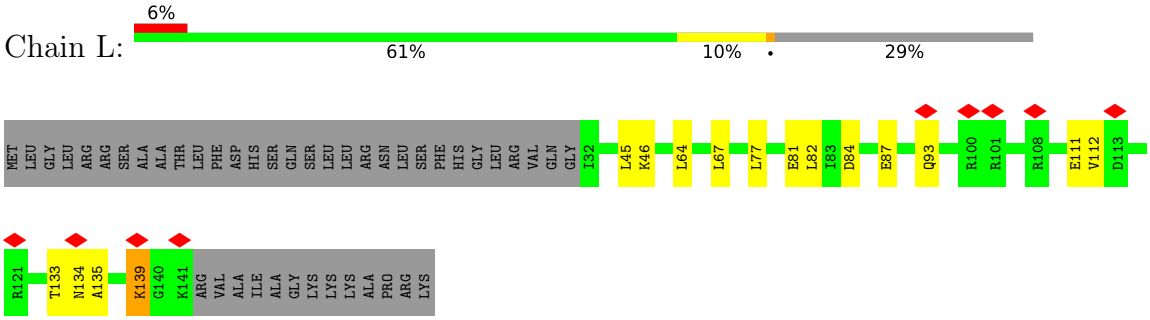




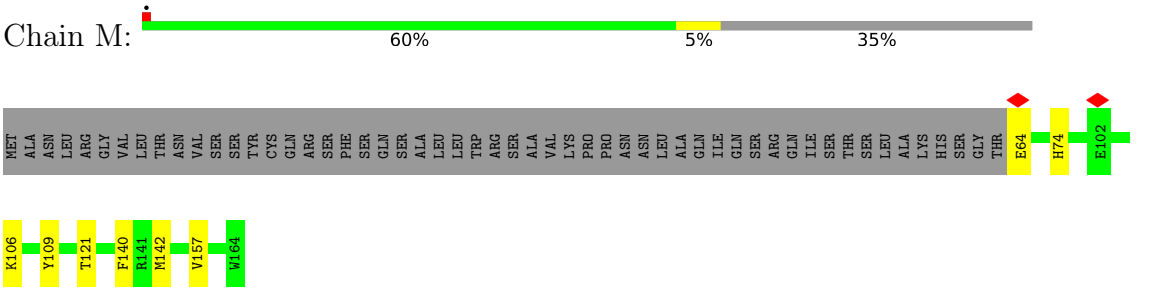
• Molecule 14: Small ribosomal subunit protein uS12m



• Molecule 15: uS13m

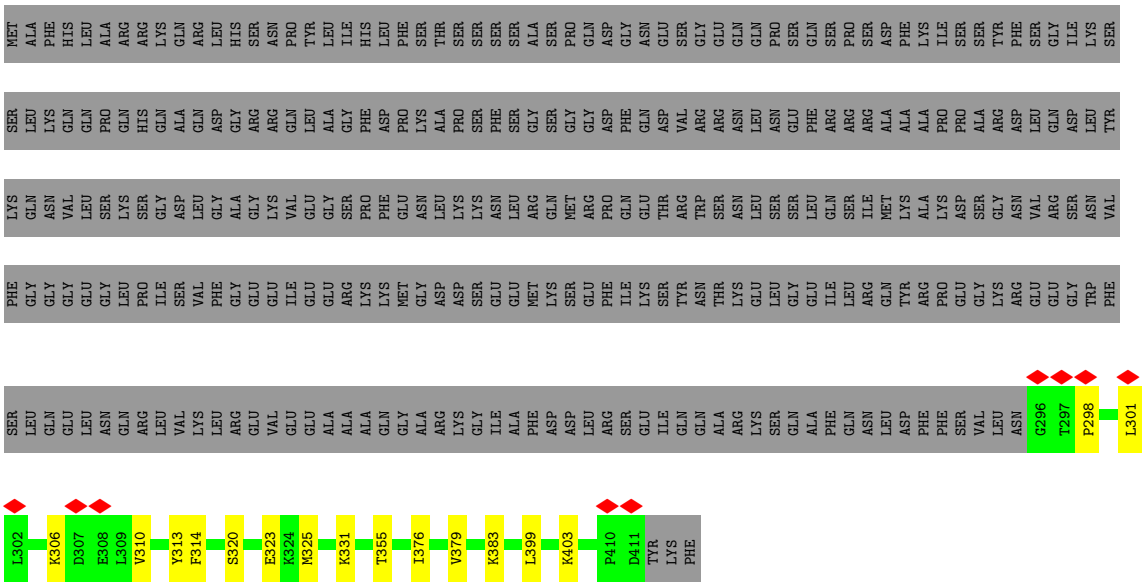


• Molecule 16: Small ribosomal subunit protein uS14m

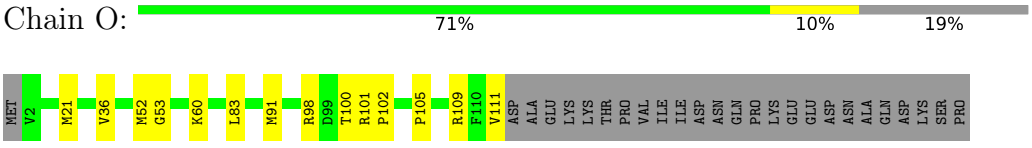


• Molecule 17: Small ribosomal subunit protein uS15c

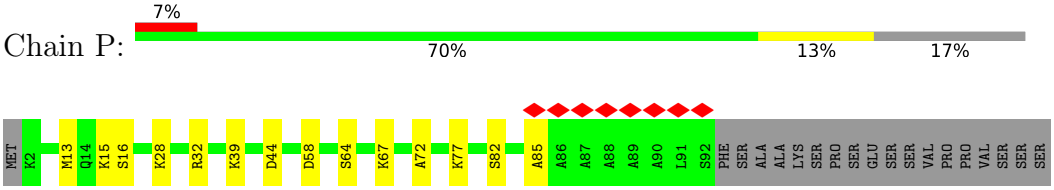




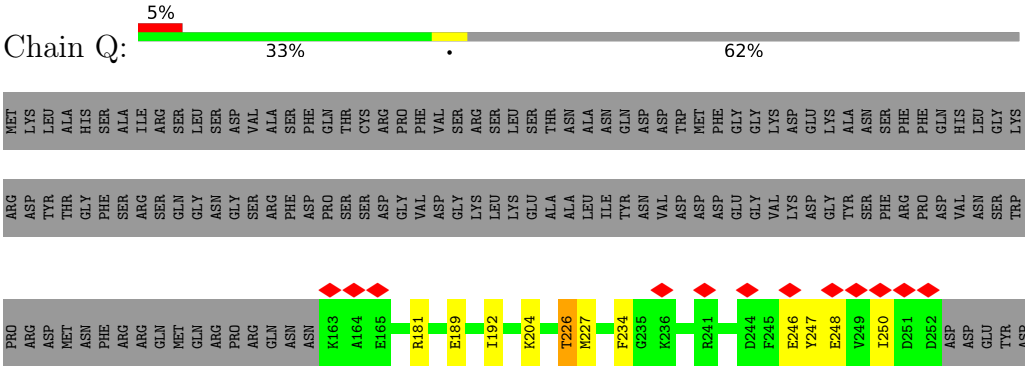
• Molecule 18: 30S ribosomal protein S16



• Molecule 19: Small ribosomal subunit protein uS17c

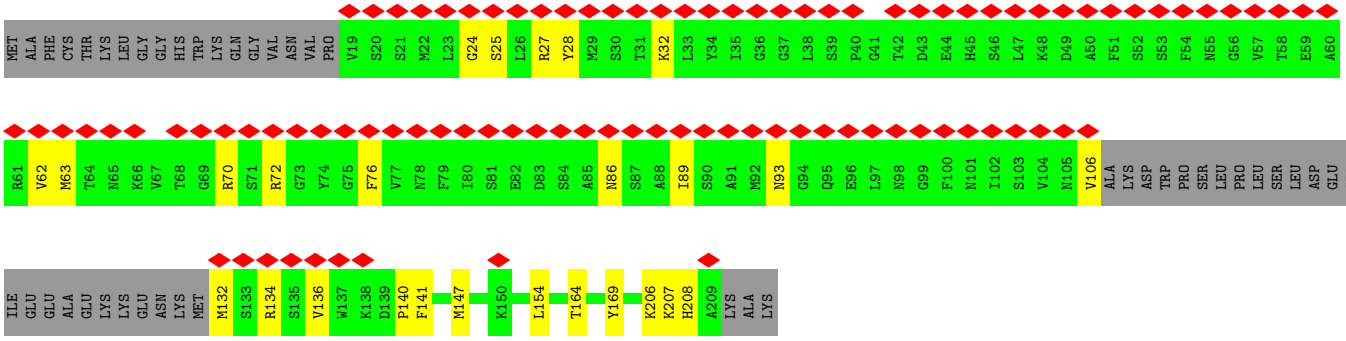


• Molecule 20: Small ribosomal subunit protein bS18c



• Molecule 21: Small ribosomal subunit protein uS19m

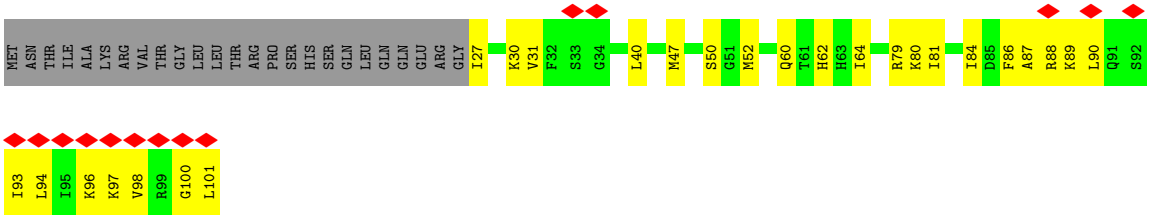




• Molecule 22: Ribosomal protein S21

Chain S:

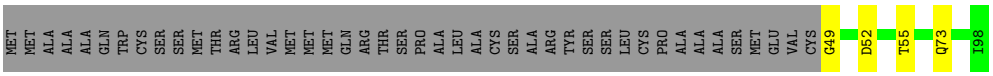




• Molecule 23: 30S ribosomal protein S31, mitochondrial

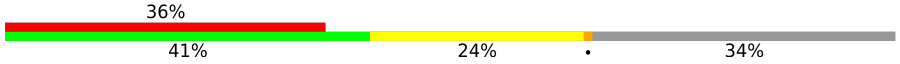
Chain T:

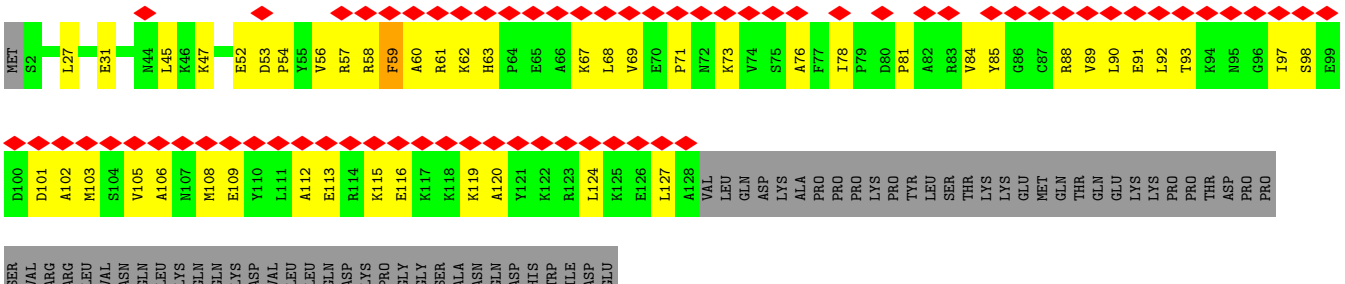




• Molecule 24: mS23

Chain U:

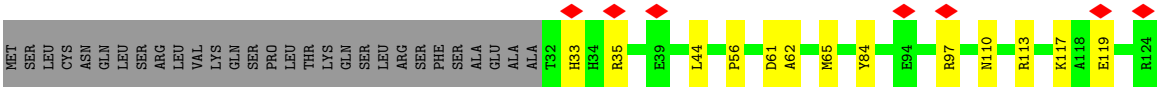


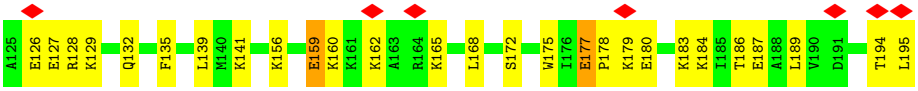


• Molecule 25: mS26

Chain V:



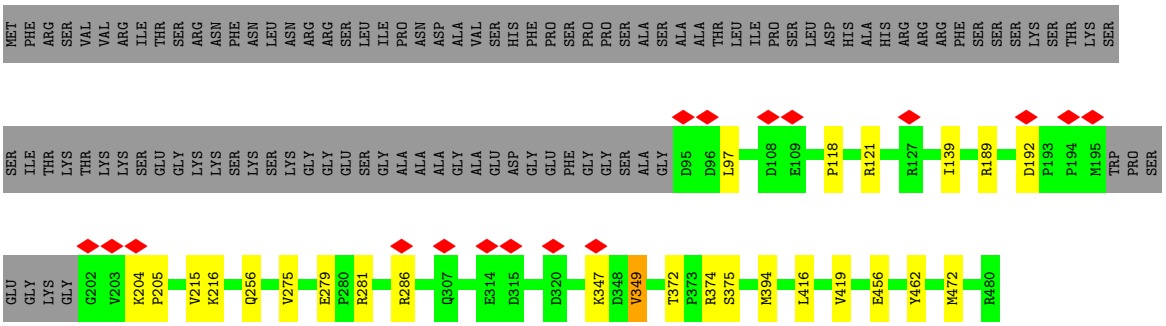




• Molecule 26: Small ribosomal subunit protein mS29

Chain W:

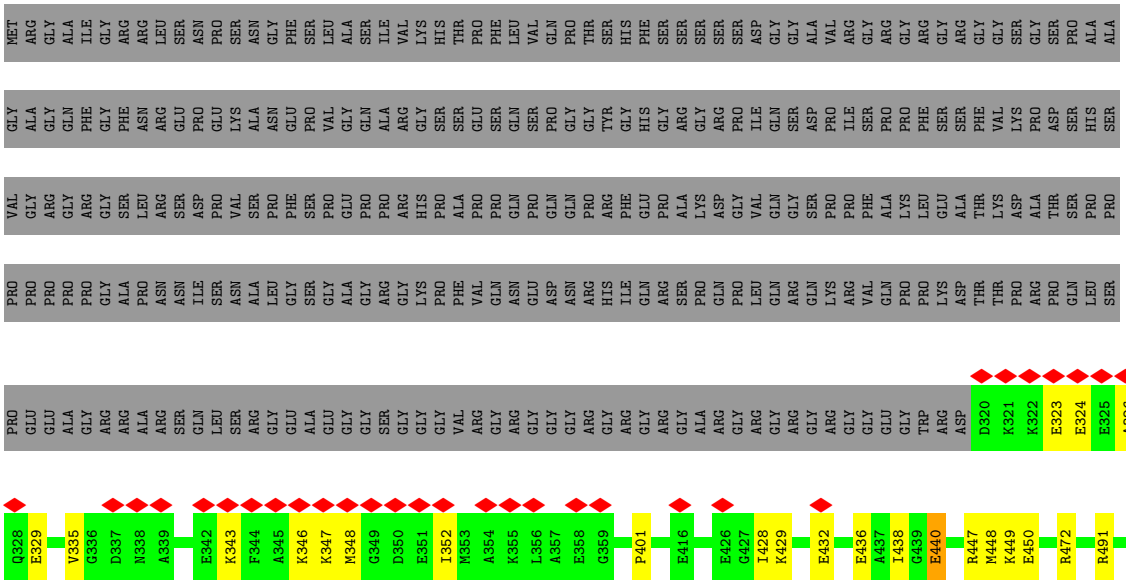




• Molecule 27: BnaC06g06470D protein

Chain X:

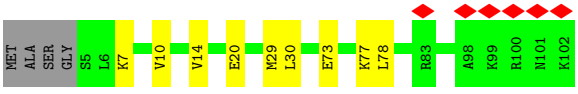




• Molecule 28: MOSC domain-containing protein

Chain Y:

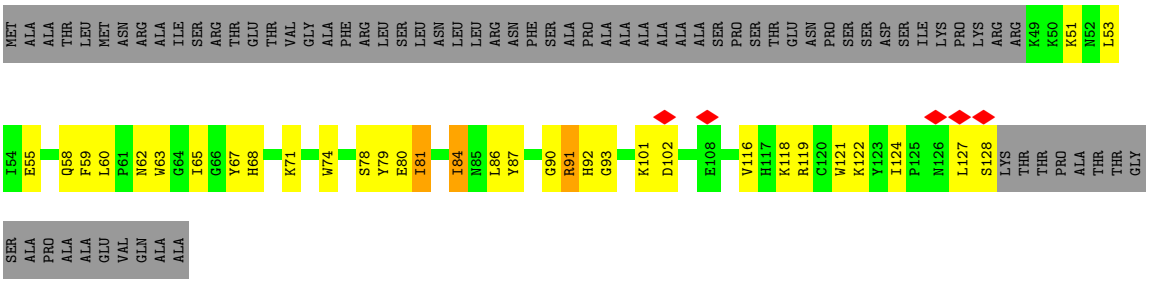




• Molecule 29: Mitochondrial 28S ribosomal protein S34

Chain Z:

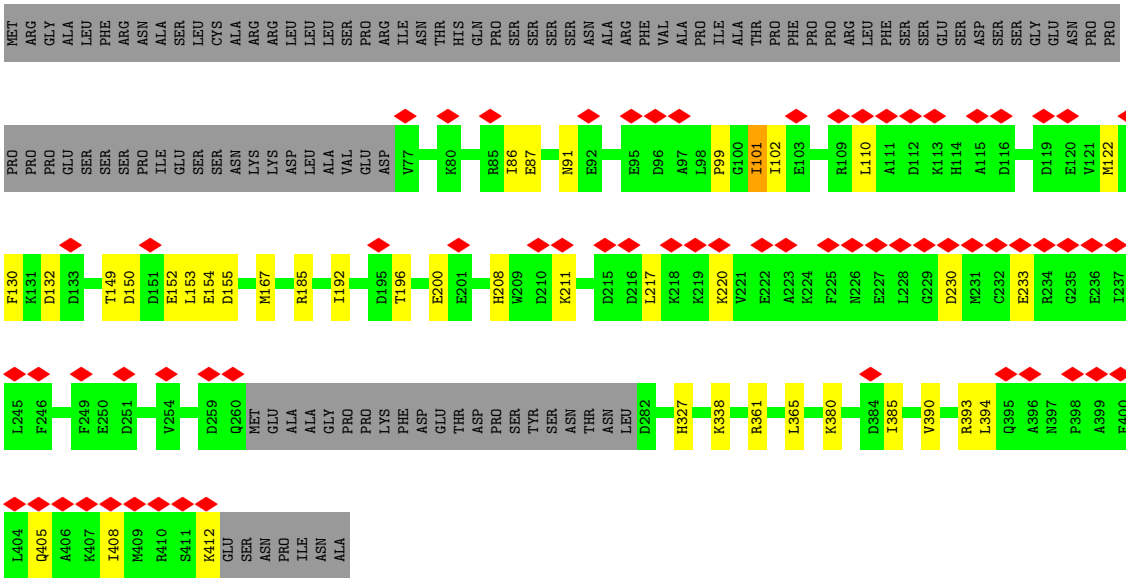




• Molecule 30: Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein

Chain a:

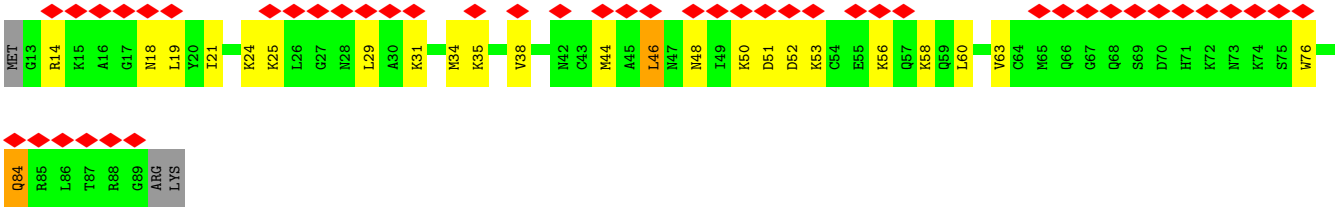




• Molecule 31: IMS import disulfide relay-system CHCH-CHCH-like Cx9C domain-containing protein

Chain b:



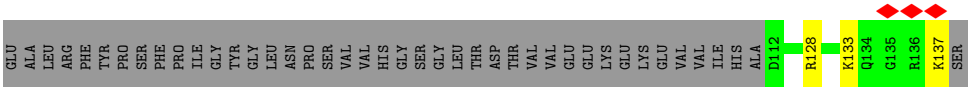


• Molecule 32: Small ribosomal subunit protein mS38

Chain c:





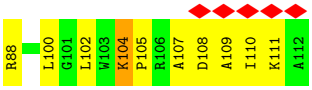


• Molecule 33: IGR domain-containing protein

Chain d:



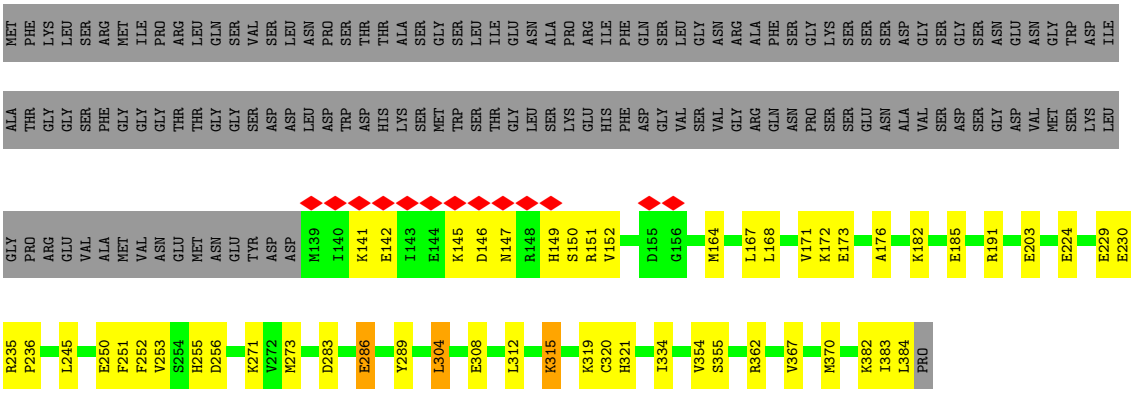




• Molecule 34: mS45

Chain e:

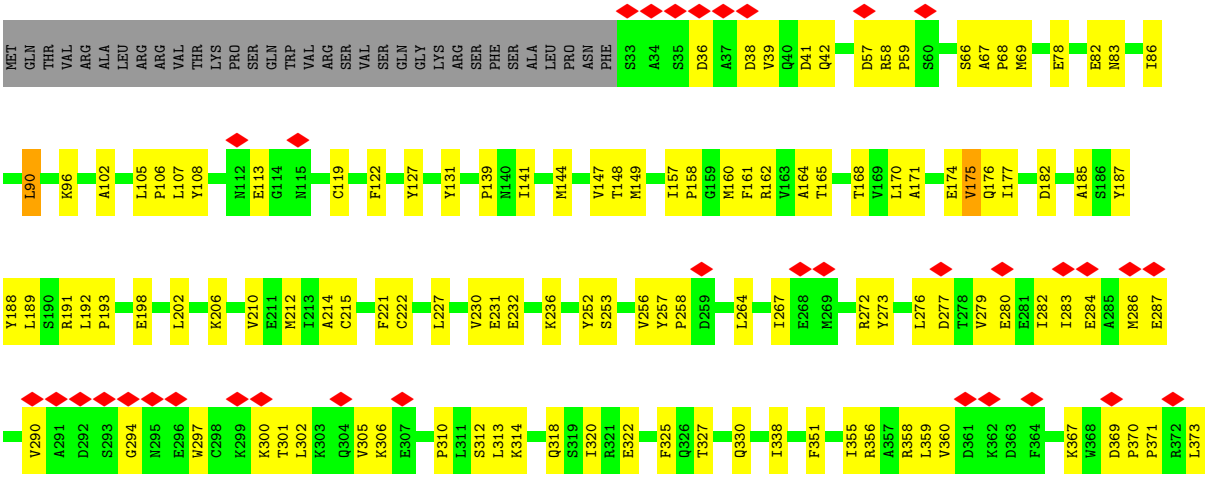


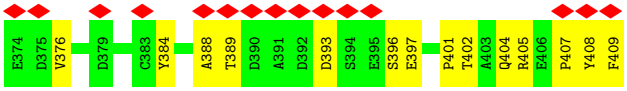


• Molecule 35: mS47

Chain f:

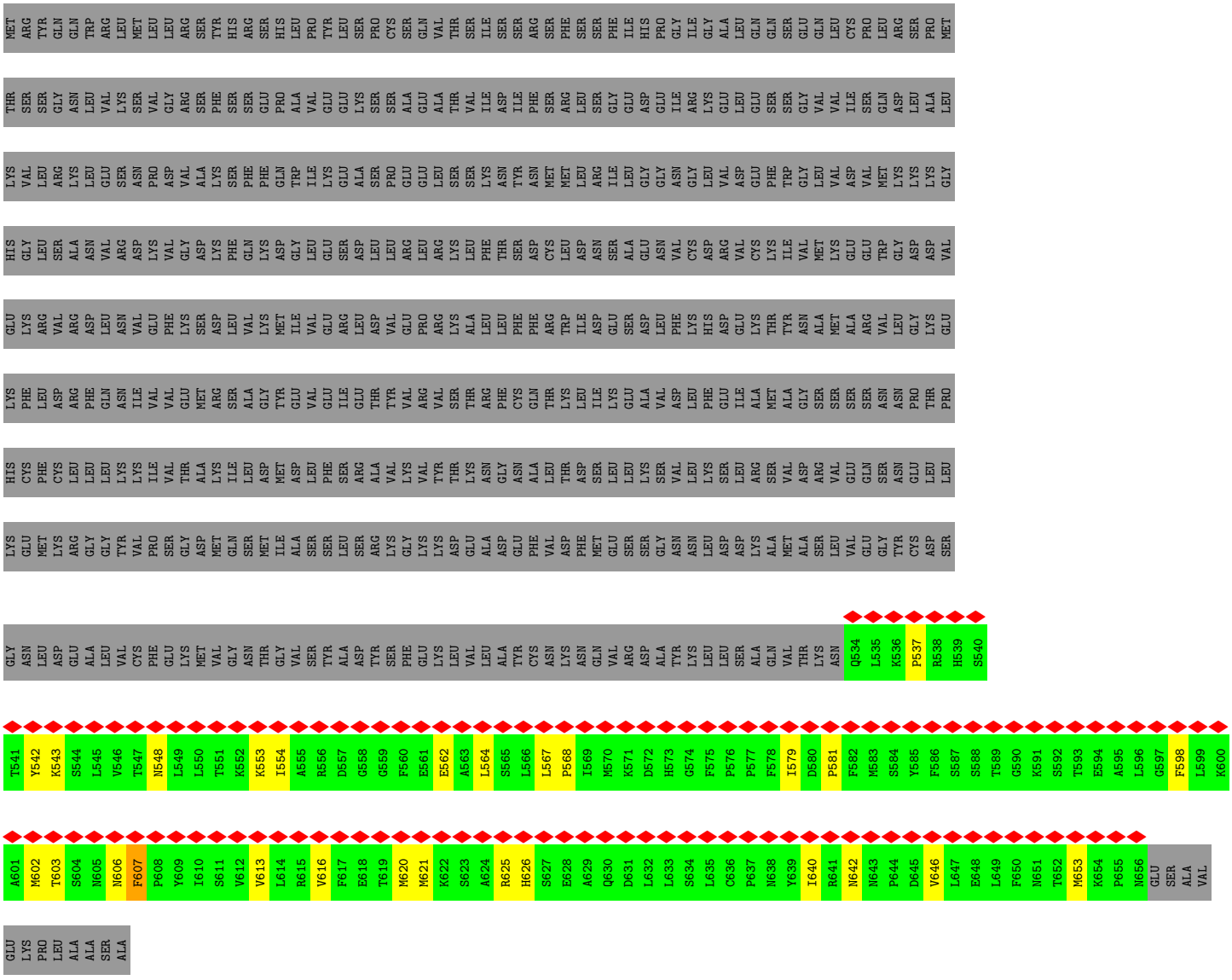






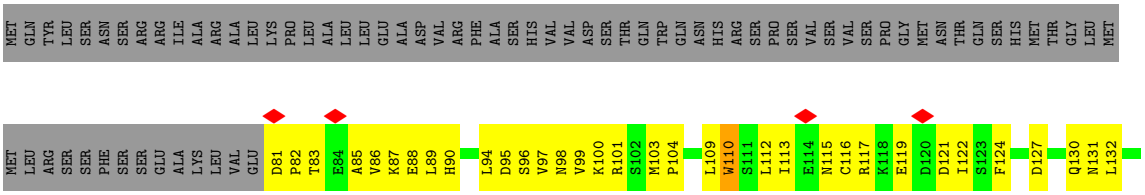
• Molecule 36: Small ribosomal subunit protein mS81 (rPPR8)

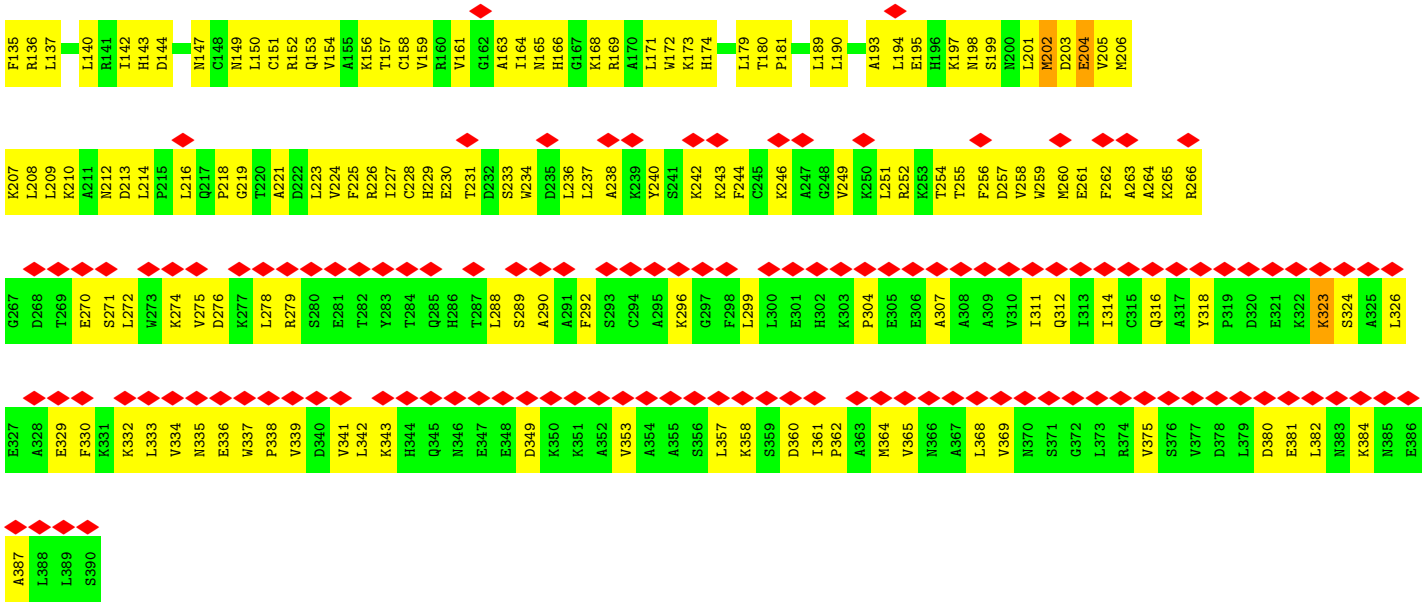




• Molecule 37: (rape) hypothetical protein



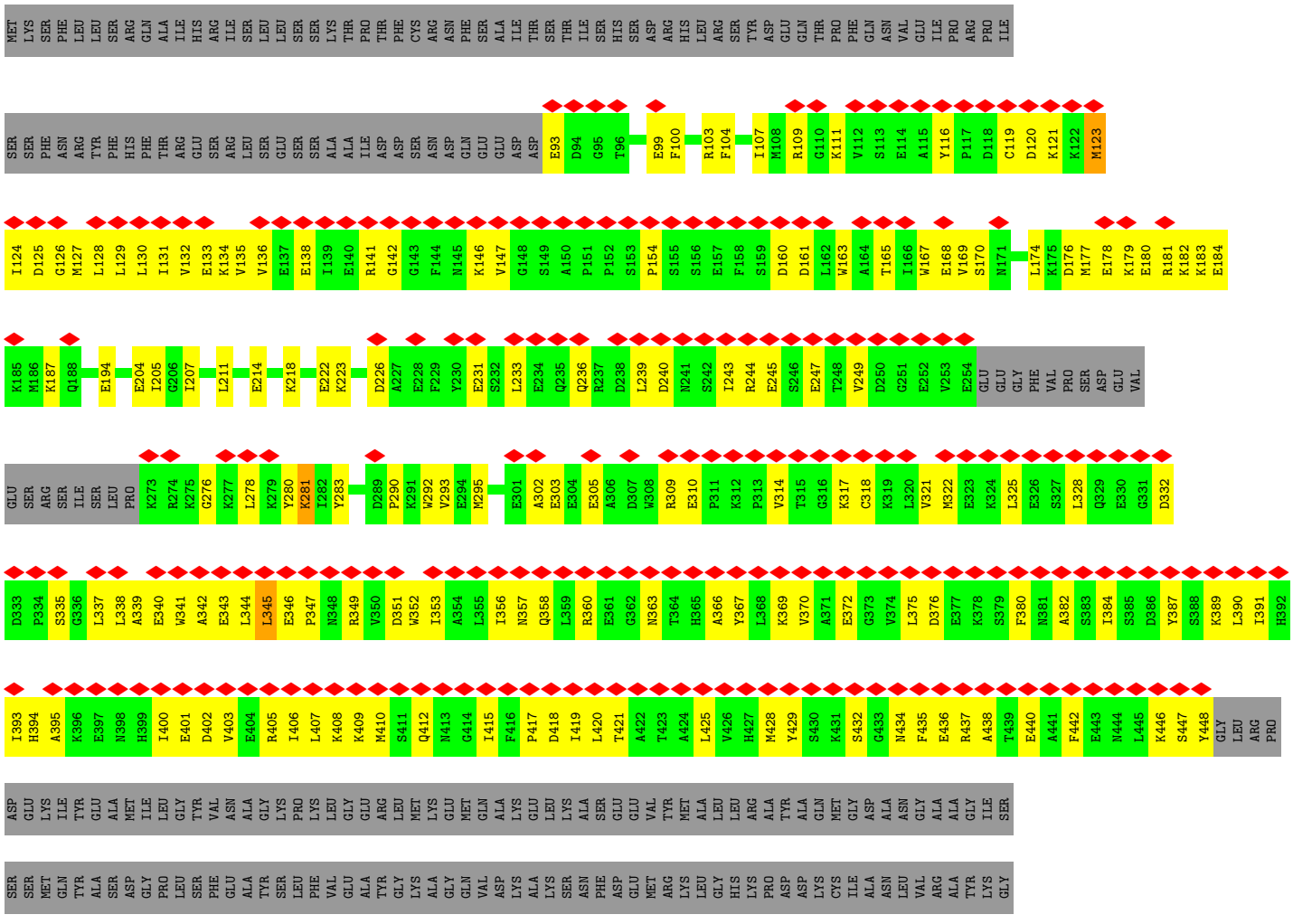


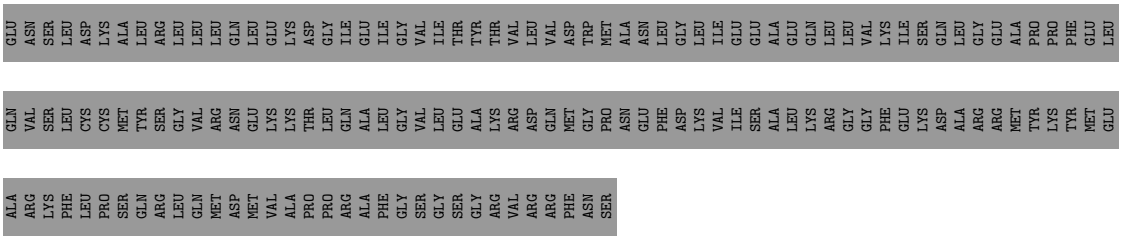


• Molecule 38: PROP1-like PPR domain-containing protein

Chain i:



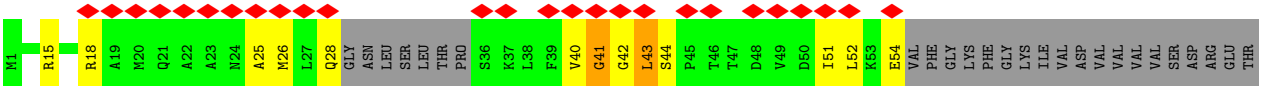


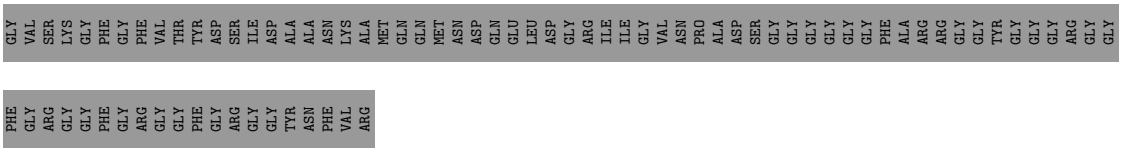


• Molecule 39: RRM domain-containing protein

Chain k:



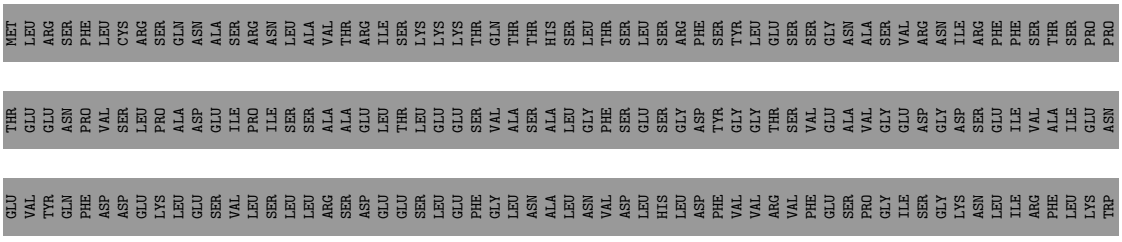




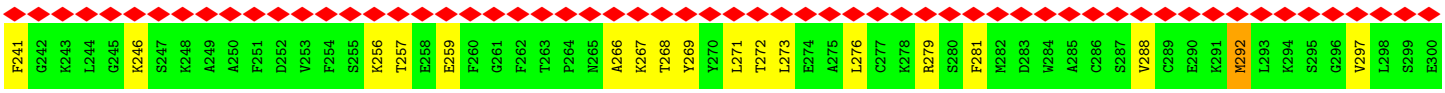
• Molecule 40: Small ribosomal subunit protein mS80 (rPPR6)

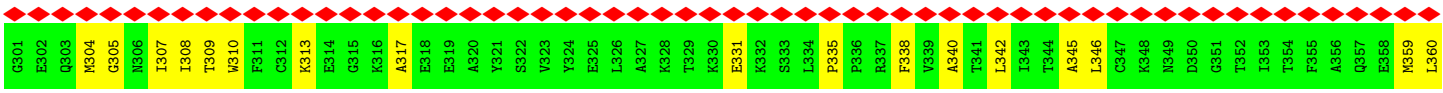
Chain l:

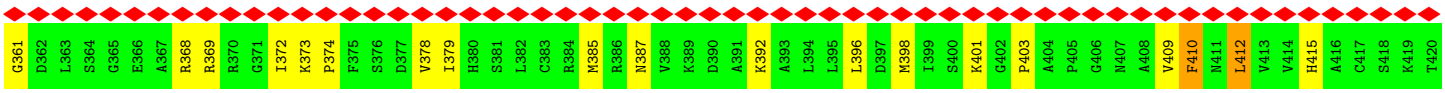


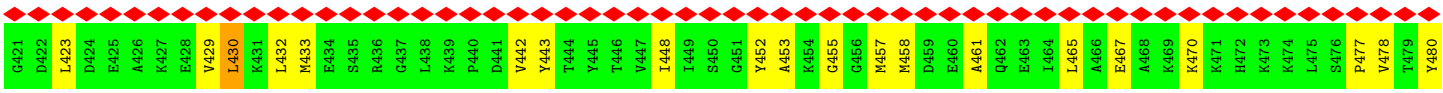


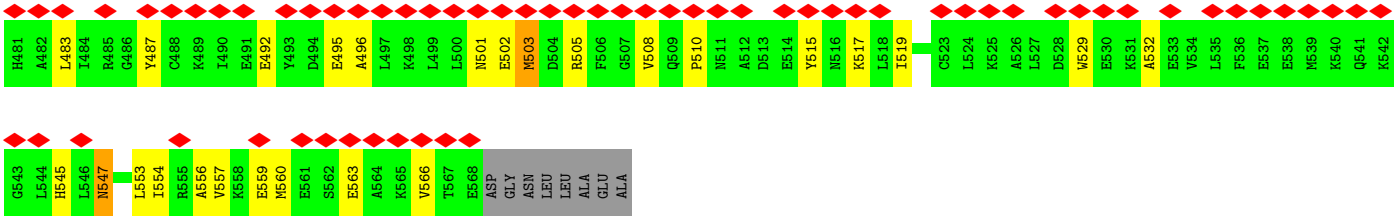











H481 A482 L483 I484 R485 G486 Y487 C488 K489 I490 E491 E492 Y493 D494 E495 A496 L497 K498 L499 L500 N501 E502 N503 D504 R505 F506 G507 V508 Q509 P510 N511 A512 D513 E514 Y515 N516 K517 L518 I519 C523 L524 K525 A526 L527 D528 W529 E530 K531 A532 E533 V534 L535 F536 E537 E538 M539 K540 Q541 K542
G543 L544 H545 L546 N547 L553 I554 R555 A556 V557 K558 E559 M560 E561 S562 E563 A564 K565 V566 T567 E568 ASP GLY ASN LEU LEU ALA GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62215	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	3.133	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	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: 2MG, MA6, ATP, G7M, 4OC, UR3

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	2/38519 (0.0%)	0.90	60/60046 (0.1%)
2	6	0.20	0/131	0.61	0/200
3	8	0.69	1/891 (0.1%)	0.90	1/1191 (0.1%)
4	A	0.19	0/1647	0.34	0/2227
5	B	0.41	0/3969	0.59	1/5320 (0.0%)
6	C	0.13	0/2859	0.32	0/3828
7	D	0.25	0/3438	0.39	1/4599 (0.0%)
8	E	0.12	0/838	0.29	0/1121
9	F	0.28	0/1225	0.47	0/1641
10	G	0.13	0/1054	0.26	0/1418
11	H	0.35	0/1696	0.46	0/2273
12	I	0.41	0/964	0.52	0/1293
13	J	0.26	0/1000	0.45	1/1340 (0.1%)
14	K	0.30	0/1010	0.48	0/1345
15	L	0.38	0/883	0.66	5/1176 (0.4%)
16	M	0.41	0/856	0.43	0/1134
17	N	0.12	0/958	0.25	0/1280
18	O	0.14	0/890	0.32	0/1196
19	P	0.12	0/730	0.28	0/984
20	Q	0.11	0/733	0.27	0/978
21	R	0.30	0/1323	0.42	0/1772
22	S	0.39	0/614	0.57	0/809
23	T	0.45	0/416	0.44	0/547
24	U	0.16	0/1036	0.35	0/1395
25	V	0.10	0/1423	0.24	0/1895
26	W	0.34	0/3139	0.44	0/4250
27	X	0.36	0/1644	0.54	0/2216
28	Y	0.36	0/807	0.43	0/1077
29	Z	0.11	0/669	0.34	0/900
30	a	0.39	0/2523	0.55	0/3386
31	b	0.47	0/618	0.73	0/822
32	c	0.35	0/233	0.58	0/296

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	d	0.26	0/628	0.47	1/840 (0.1%)
34	e	0.25	0/2118	0.45	1/2828 (0.0%)
35	f	0.11	0/2981	0.34	0/4033
36	g	0.17	0/1003	0.44	0/1355
37	h	0.11	0/2511	0.34	0/3391
38	i	0.12	0/2791	0.32	0/3751
39	k	0.52	0/322	0.75	0/431
40	l	0.20	0/3002	0.42	0/4033
All	All	0.48	3/94092 (0.0%)	0.69	71/134617 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	8	0	3
7	D	0	2
14	K	0	1
22	S	0	1
31	b	0	1
32	c	0	1
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	8	249	HIS	C-O	-15.33	1.06	1.23
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 (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	8	249	HIS	O-C-N	-15.14	103.01	121.79
1	2	1542	A	N7-C8-N9	11.76	119.68	113.80
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
15	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1388	A	O4'-C1'-N9	7.37	114.09	108.20
1	2	1173	U	C2-N1-C1'	6.80	125.86	117.70
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
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
5	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
33	d	104	LYS	O-C-N	-5.96	117.67	121.85
1	2	1173	U	N3-C2-O2	-5.90	118.07	122.20
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
13	J	286	ARG	N-CA-C	-5.71	105.71	114.16
1	2	1173	U	N1-C2-O2	5.65	126.76	122.80
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
15	L	134	ASN	CA-CB-CG	5.49	118.09	112.60
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	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
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
15	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
15	L	133	THR	CA-C-N	-5.09	114.83	122.47
15	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
7	D	370	VAL	CA-C-O	-5.06	117.68	121.68
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 (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	8	163	ARG	Sidechain
3	8	248	ARG	Sidechain
3	8	249	HIS	Mainchain
7	D	352	ARG	Sidechain
7	D	381	ARG	Sidechain
14	K	44	LYS	Peptide
22	S	79	ARG	Sidechain
31	b	18	ASN	Mainchain
32	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	34549	0	17413	549	0
2	6	120	0	61	14	0
3	8	874	927	926	29	0
4	A	1611	0	1633	34	0
5	B	3877	0	4008	64	0
6	C	2806	0	2971	108	0
7	D	3389	0	3419	110	0
8	E	823	0	879	14	0
9	F	1254	0	1268	12	0
10	G	1037	0	1058	15	0
11	H	1671	0	1713	57	0
12	I	941	0	970	6	0
13	J	988	0	1022	37	0
14	K	993	0	1052	15	0
15	L	873	0	904	5	0
16	M	843	0	884	6	0
17	N	941	0	978	18	0
18	O	869	0	898	9	0
19	P	717	0	755	9	0
20	Q	724	0	744	17	0
21	R	1299	0	1307	19	0
22	S	611	0	687	26	0
23	T	408	0	444	2	0
24	U	1014	0	1061	69	0
25	V	1399	0	1427	38	0
26	W	3062	0	3030	14	0
27	X	1613	0	1559	21	0
28	Y	793	0	834	7	0
29	Z	649	0	662	28	0
30	a	2486	0	2376	37	0
31	b	610	0	626	30	0
32	c	232	0	278	1	0
33	d	616	0	674	21	0
34	e	2074	0	2074	50	0
35	f	2922	0	2870	113	0
36	g	979	0	987	18	0
37	h	2463	0	2488	226	0
38	i	2740	0	2694	211	0
39	k	319	0	272	26	0
40	l	2955	0	3012	82	0
41	W	31	0	12	0	0
All	All	89175	927	72930	1948	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 (1948) 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)
16:M:64:GLU:OE1	16:M:74:HIS:CE1	1.88	1.25
31:b:24:LYS:HG2	31:b:29:LEU:HD11	1.21	1.20
37:h:166:HIS:HA	37:h:169:ARG:HD2	1.25	1.14
37:h:234:TRP:HA	37: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	4:A:121:LYS:HD2	1.50	1.11
37:h:193:ALA:HB2	37:h:201:LEU:HD22	1.32	1.11
38:i:124:ILE:HA	38:i:127:MET:HE1	1.12	1.11
39:k:51:ILE:HG22	39:k:52:LEU:H	1.18	1.09
35:f:369:ASP:HB3	35:f:370:PRO:HD3	1.36	1.07
1:2:202:A:H2'	1:2:203:A:H5"	1.33	1.06
4:A:200:GLN:HA	4:A:203:MET:HE2	1.35	1.05
37:h:85:ALA:HB1	37:h:115:ASN:ND2	1.70	1.04
24:U:73:LYS:HE2	39:k:18:ARG:HG2	1.35	1.03
1:2:1385:A:H4'	40:l:517:LYS:HE3	1.40	1.02
1:2:162:C:H3'	1:2:163:A:H5"	1.37	1.01
6:C:204:THR:HA	7:D:116:GLU:HG2	1.42	1.01
24:U:73:LYS:CE	39:k:18:ARG:CG	2.39	1.00
5:B:398:MET:HG3	30:a:122:MET:SD	2.02	1.00
37:h:85:ALA:CB	37:h:115:ASN:ND2	2.26	0.99
24:U:73:LYS:CE	39:k:18:ARG:HG2	1.91	0.99
6:C:287:LEU:HD22	7:D:178:LEU:HD23	1.45	0.99
4:A:203:MET:HE3	4:A:205:ILE:HD12	1.44	0.99
16:M:64:GLU:OE1	16:M:74:HIS:HE1	1.31	0.98
38:i:127:MET:HA	38:i:130:LEU:HD12	1.43	0.98
20:Q:227:MET:HE2	22:S:52:MET:HG2	1.46	0.98
39:k:51:ILE:HG22	39:k:52:LEU:N	1.75	0.97
1:2:1726:U:H3	1:2:1744:C:N4	1.62	0.97
37:h:197:LYS:HE2	37:h:230:GLU:HB2	1.45	0.97
39:k:51:ILE:CG2	39:k:52:LEU:H	1.78	0.96
1:2:1763:U:H4'	1:2:1764:A:H5'	1.47	0.95
31:b:24:LYS:HG2	31:b:29:LEU:CD1	1.97	0.95
37:h:85:ALA:CB	37:h:115:ASN:HD21	1.79	0.94
6:C:21:THR:HG21	6:C:77:LEU:HD11	1.48	0.94
24:U:58:ARG:HD2	24:U:103:MET:HE3	1.48	0.94
1:2:1745:A:OP1	37:h:149:ASN:HB3	1.68	0.94
1:2:669:G:H2'	1:2:670:G:C8	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:200:GLN:HG2	4:A:205:ILE:HB	1.47	0.93
37:h:311:ILE:HD11	37:h:368:LEU:HD21	1.49	0.93
1:2:458:U:H2'	1:2:459:U:H5"	1.48	0.93
1:2:922:G:H1	1:2:1650:C:H42	1.12	0.93
1:2:1726:U:H3	1:2:1744:C:H42	0.94	0.93
7:D:218:MET:HE3	34:e:167:LEU:HB3	1.52	0.92
1:2:1567:G:H21	1:2:1594:A:H2	1.17	0.91
38:i:363:ASN:HB3	38:i:366:ALA:HB3	1.53	0.91
1:2:200:C:H5	1:2:246:G:H1	1.19	0.89
6:C:257:LEU:HD12	7:D:194:MET:CE	2.01	0.89
24:U:61:ARG:C	24: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
6:C:180:ILE:HG22	6:C:191:TRP:CZ2	2.08	0.88
37:h:361:ILE:HG22	37:h:362:PRO:HD3	1.55	0.88
6:C:175:LEU:HD11	6:C:198:TRP:HB3	1.51	0.88
38:i:127:MET:O	38: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
1:2:163:A:H4'	1:2:164:A:H5'	1.54	0.87
38:i:165:THR:HA	38:i:168:GLU:HG2	1.56	0.87
38:i:429:TYR:HB3	38:i:438:ALA:HB2	1.54	0.87
1:2:835:U:H2'	1:2:836:A:O4'	1.74	0.86
6:C:252:MET:HE2	34:e:150:SER:HB3	1.57	0.86
7:D:138:GLU:HB2	7:D:141:ARG:HB2	1.57	0.86
35:f:157:ILE:HA	35:f:162:ARG:HD2	1.56	0.86
1:2:164:A:H2'	1:2:165:A:C8	2.10	0.86
34:e:230:GLU:HG3	34:e:236:PRO:HA	1.57	0.85
37:h:279:ARG:HH22	37:h:290:ALA:HB1	1.40	0.85
24:U:101:ASP:O	24:U:105:VAL:HG12	1.74	0.85
1:2:670:G:H2'	1:2:671:A:H8	1.41	0.84
11:H:225:ILE:HA	11:H:228:PRO:HG3	1.58	0.84
37:h:147:ASN:OD1	37:h:150:LEU:HD23	1.77	0.84
37:h:82:PRO:HB2	37:h:87:LYS:HD2	1.60	0.84
38:i:375:LEU:HD12	38:i:387:TYR:HE1	1.42	0.83
17:N:399:LEU:HD11	17:N:403:LYS:HD2	1.60	0.83
35:f:301:THR:O	35:f:305:VAL:HG23	1.78	0.83
6:C:289:LEU:HD21	34:e:151:ARG:HG2	1.59	0.83
6:C:257:LEU:HD12	7:D:194:MET:HE2	1.59	0.83
34:e:147:ASN:HB3	34:e:151:ARG:HH12	1.43	0.82
1:2:612:U:H2'	1:2:613:C:C6	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:24:LYS:CG	31:b:29:LEU:HD11	2.06	0.82
37:h:119:GLU:OE2	37:h:163:ALA:HB2	1.79	0.81
38:i:109:ARG:HH21	38:i:124:ILE:HG22	1.43	0.81
38:i:142:GLY:HA3	38:i:146:LYS:HD2	1.62	0.81
1:2:1664:4OC:HM23	1:2:1665:C:H5'	1.62	0.81
38:i:124:ILE:HA	38:i:127:MET:CE	2.03	0.81
38:i:132:VAL:O	38:i:136:VAL:HG12	1.79	0.81
1:2:3:C:O2'	1:2:4:A:H2'	1.79	0.81
24:U:73:LYS:HE3	39:k:18:ARG:HE	1.44	0.81
1:2:26:U:H3	1:2:910:G:H1	1.25	0.81
6:C:325:THR:HG21	6:C:327:LYS:HZ1	1.46	0.81
35:f:139:PRO:HA	35: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
11:H:207:GLU:HA	11:H:210:LYS:HD2	1.62	0.80
7:D:242:LEU:HD12	38:i:205:ILE:HD11	1.64	0.80
37:h:342:LEU:HD21	37:h:387:ALA:HB1	1.62	0.80
1:2:1737:A:H3'	1:2:1738:G:H21	1.46	0.80
1:2:25:U:H2'	1:2:26:U:C6	2.17	0.80
37:h:153:GLN:HA	37:h:156:LYS:HG2	1.63	0.79
18:O:91:MET:HE3	33:d:100:LEU:HD13	1.64	0.79
24:U:73:LYS:HE3	39:k:18:ARG:CG	2.10	0.79
11:H:225:ILE:HG22	11:H:226:LYS:H	1.48	0.79
24:U:106:ALA:HA	24:U:109:GLU:OE2	1.82	0.79
1:2:1734:A:H2'	1:2:1735:C:H4'	1.64	0.79
37:h:234:TRP:CZ2	37:h:266:ARG:HG3	2.17	0.79
29:Z:62:ASN:O	29:Z:65:ILE:HD12	1.81	0.79
1:2:1746:A:H2'	1:2:1747:A:H8	1.48	0.78
39:k:25:ALA:HA	39: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
21:R:140:PRO:HB2	21:R:164:THR:HG21	1.65	0.78
38:i:290:PRO:HA	38:i:293:VAL:HG22	1.62	0.78
34:e:147:ASN:HB3	34:e:151:ARG:NH1	1.98	0.78
38:i:134:LYS:HD2	38:i:134:LYS:O	1.83	0.78
38:i:421:THR:O	38:i:425:LEU:HD13	1.83	0.78
24:U:73:LYS:CE	39:k:18:ARG:HG3	2.12	0.78
38:i:391:ILE:HD13	38:i:425:LEU:HD11	1.66	0.78
17:N:325:MET:HE1	17:N:355:THR:HG22	1.67	0.77
40:l:373:LYS:HG3	40:l:374:PRO:HD3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:3:U:H2'	2:6:4:U:O4'	1.84	0.77
6:C:260:LEU:CD2	7:D:181:LEU:HG	2.14	0.77
7:D:97:GLU:HA	7:D:100:ARG:HH21	1.49	0.77
35:f:367:LYS:HD2	35:f:367:LYS:O	1.83	0.77
11:H:241:ILE:HG12	11:H:246:LEU:HD13	1.66	0.77
6:C:204:THR:HA	7:D:116:GLU:CG	2.14	0.77
11:H:225:ILE:HA	11:H:228:PRO:CG	2.14	0.77
37:h:339:VAL:O	37:h:343:LYS:HG2	1.84	0.77
1:2:163:A:H1'	1:2:165:A:OP2	1.85	0.77
37:h:96:SER:HA	37:h:100:LYS:HE2	1.67	0.77
38:i:375:LEU:HD12	38:i:387:TYR:CE1	2.19	0.77
14:K:123:LYS:HE3	14:K:125:ILE:HG12	1.66	0.77
38:i:303:GLU:HB3	38:i:309:ARG:HH21	1.50	0.77
37:h:204:GLU:HA	37:h:207:LYS:HG2	1.66	0.76
1:2:659:A:H5"	20:Q:204:LYS:HD2	1.68	0.76
35:f:276:LEU:HB2	35:f:282:ILE:CD1	2.15	0.76
38:i:131:ILE:O	38:i:135:VAL:HG23	1.85	0.76
6:C:325:THR:HG21	6:C:327:LYS:NZ	2.01	0.76
11:H:230:ARG:HH11	11:H:230:ARG:HG3	1.50	0.76
14:K:114:ARG:HB2	14:K:119:ALA:HB3	1.67	0.76
24:U:58:ARG:HD2	24:U:103:MET:CE	2.14	0.76
37:h:244:PHE:HD1	37:h:249:VAL:HG21	1.51	0.76
37:h:263:ALA:HB3	37:h:272:LEU:HD13	1.68	0.76
38:i:128:LEU:O	38:i:132:VAL:HG12	1.84	0.76
5:B:96:ARG:HH21	27:X:326:ALA:HB3	1.51	0.76
6:C:303:LEU:HB3	7:D:160:GLU:OE2	1.85	0.76
37:h:202:MET:C	37:h:206:MET:HE2	2.11	0.75
37:h:259:TRP:CZ3	37: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
6:C:260:LEU:HD21	7: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
34:e:142:GLU:HA	34:e:145:LYS:HD2	1.69	0.75
1:2:573:G:O2'	1:2:817:G:H5'	1.86	0.75
37:h:229:HIS:HA	37:h:262:PHE:CZ	2.21	0.75
7:D:403:GLU:HG2	7:D:404:THR:HG23	1.69	0.74
37:h:137:LEU:HD21	37:h:143:HIS:CD2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:710:G:H2'	1:2:711:A:C8	2.22	0.74
37:h:97:VAL:HG13	37:h:135:PHE:CD1	2.21	0.74
37:h:361:ILE:CG2	37:h:362:PRO:HD3	2.17	0.74
1:2:1797:G:H2'	1:2:1798:G:H8	1.50	0.74
6:C:182:LYS:CE	6:C:220:LEU:HB3	2.18	0.74
38:i:245:GLU:O	38: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
6:C:210:LEU:HD12	7:D:87:VAL:HG22	1.69	0.74
6:C:183:LEU:HD12	6: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
34:e:168:LEU:O	34:e:172:LYS:HG2	1.88	0.73
1:2:323:C:C2'	1:2:324:G:H5'	2.19	0.73
6:C:285:SER:HB2	34:e:151:ARG:HH21	1.53	0.73
35:f:131:TYR:OH	35:f:407:PRO:HG3	1.87	0.73
37:h:103:MET:HE1	37:h:132:LEU:HD22	1.69	0.73
37:h:365:VAL:O	37:h:369:VAL:HG23	1.89	0.73
6:C:261:PHE:HB3	38:i:236:GLN:OE1	1.89	0.73
38:i:218:LYS:O	38:i:222:GLU:HG2	1.88	0.73
37:h:122:ILE:HD11	37:h:161:VAL:HG21	1.71	0.73
8:E:42:SER:HB2	8:E:65:MET:HE3	1.71	0.73
35:f:257:TYR:OH	38:i:293:VAL:HG12	1.89	0.73
35:f:369:ASP:HB3	35:f:370:PRO:CD	2.18	0.73
37:h:90:HIS:HE1	37:h:127:ASP:HB3	1.52	0.73
7:D:191:TYR:O	7:D:194:MET:HB2	1.88	0.72
38:i:176:ASP:O	38:i:180:GLU:HG2	1.89	0.72
1:2:660:G:H22	1:2:737:G:H1	1.37	0.72
37:h:203:ASP:O	37: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
22:S:93:ILE:CD1	31:b:19:LEU:HD12	2.19	0.72
1:2:997:G:H1	1:2:1029:C:H5	1.37	0.72
35:f:409:PHE:HD1	38:i:187:LYS:HZ1	1.38	0.72
10:G:17:GLU:HG3	10: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
36:g:642:ASN:HB3	40: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:f:165:THR:O	35:f:168:THR:HG22	1.89	0.72
38:i:142:GLY:CA	38:i:146:LYS:HD2	2.20	0.72
1:2:458:U:C2'	1:2:459:U:H5"	2.20	0.71
6:C:252:MET:HE2	34:e:150:SER:CB	2.19	0.71
38:i:322:MET:HA	38:i:325:LEU:HG	1.69	0.71
1:2:1540:C:O2'	1:2:1542:A:H8	1.71	0.71
13:J:249:ARG:O	13:J:253:MET:HG2	1.90	0.71
37:h:103:MET:SD	37:h:104:PRO:HD2	2.30	0.71
37:h:193:ALA:CB	37:h:201:LEU:HD22	2.16	0.71
24:U:105:VAL:O	24:U:108:MET:HG2	1.90	0.71
1:2:323:C:H2'	1:2:324:G:H5'	1.73	0.71
25:V:178:PRO:HG2	25:V:179:LYS:HE2	1.73	0.71
13:J:283:SER:CB	13:J:288:ASP:HB3	2.21	0.71
22:S:97:LYS:HE2	39:k:54:GLU:HA	1.71	0.71
38:i:134:LYS:HD2	38:i:134:LYS:C	2.14	0.71
37:h:274:LYS:O	37:h:278:LEU:HG	1.90	0.71
38:i:417:PRO:HB3	38:i:421:THR:CG2	2.20	0.71
7:D:217:LEU:HD11	38:i:207:ILE:HD11	1.71	0.71
4:A:203:MET:HE3	4:A:205:ILE:CD1	2.19	0.71
37:h:197:LYS:HD2	37:h:230:GLU:O	1.91	0.71
1:2:457:C:H2'	1:2:458:U:O2	1.90	0.70
34:e:141:LYS:HB3	34:e:145:LYS:HE3	1.73	0.70
37:h:244:PHE:CD1	37: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
4:A:116:PHE:HD1	4:A:123:LEU:HD23	1.56	0.70
7:D:187:LEU:HB2	38:i:244:ARG:NH2	2.07	0.70
38:i:180:GLU:O	38:i:184:GLU:HG2	1.90	0.70
27:X:429:LYS:HA	27:X:429:LYS:HE3	1.72	0.70
5:B:144:ASN:HA	5:B:147:ARG:HB2	1.73	0.70
35:f:107:LEU:HD11	35:f:119:CYS:HA	1.72	0.70
19:P:58:ASP:OD2	19:P:72:ALA:HB2	1.91	0.70
24:U:73:LYS:HE3	39:k:18:ARG:HG3	1.72	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
38:i:339:ALA:O	38:i:343:GLU:HG2	1.91	0.70
38:i:429:TYR:CB	38: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
5:B:161:ARG:HH12	5:B:426:PHE:HB2	1.57	0.69
13:J:189:LEU:HD23	20:Q:246:GLU:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:h:194:LEU:HD11	37:h:226:ARG:HG2	1.73	0.69
37:h:335:ASN:OD1	37:h:381:GLU:HG2	1.93	0.69
4:A:74:PRO:HA	4:A:77:ASP:OD1	1.93	0.69
35:f:297:TRP:O	35:f:301:THR:HG23	1.92	0.69
1:2:1702:G:H2'	1:2:1703:G:C8	2.28	0.69
6:C:260:LEU:O	6:C:264:LYS:HB3	1.91	0.69
37:h:86:VAL:HG21	37:h:121:ASP:HB2	1.74	0.69
38:i:337:LEU:O	38:i:340:GLU:HG3	1.93	0.69
1:2:1801:A:O2'	1:2:1802:A:H5'	1.93	0.69
37:h:227:ILE:O	37:h:230:GLU:HG3	1.92	0.69
38:i:400:ILE:O	38:i:403:VAL:HG12	1.93	0.69
6:C:176:VAL:HA	6: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
5:B:461:LYS:HE2	5:B:526:VAL:HG13	1.73	0.69
6:C:180:ILE:HG13	6:C:181:GLY:N	2.07	0.69
6:C:43:ARG:HB2	7:D:144:GLU:HG3	1.74	0.68
37:h:150:LEU:O	37:h:154:VAL:HG12	1.93	0.68
37:h:227:ILE:HD12	37:h:228:CYS:N	2.08	0.68
1:2:359:U:H3	1:2:368:G:H1	1.40	0.68
7:D:78:ARG:HB3	7:D:78:ARG:NH1	2.08	0.68
24:U:68:LEU:O	24:U:71:PRO:HD2	1.93	0.68
35:f:227:LEU:O	35:f:231:GLU:HG2	1.93	0.68
6:C:257:LEU:HD12	7:D:194:MET:HE1	1.73	0.68
1:2:1693:C:O2'	1:2:1694:G:H5'	1.93	0.68
6:C:305:MET:HG3	7:D:157:TRP:CH2	2.29	0.68
6:C:313:GLU:HG3	6:C:340:PRO:HB3	1.75	0.68
11:H:269:ASN:O	11:H:273:GLU:HG3	1.94	0.68
37:h:90:HIS:CE1	37: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
35:f:277:ASP:HB3	38: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
24:U:62:LYS:HD2	24:U:62:LYS:N	2.08	0.68
37:h:193:ALA:HB2	37:h:201:LEU:CD2	2.19	0.68
1:2:1752:U:H2'	1:2:1753:U:C6	2.29	0.68
7:D:236:ILE:HG22	34:e:171:VAL:HG11	1.74	0.68
29:Z:81:ILE:HD11	29:Z:84:ILE:CG2	2.24	0.68
3:8:200:LEU:HG	3:8:202:VAL:HG23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:477:PRO:HG3	40:l:508:VAL:HG13	1.76	0.68
37:h:209:LEU:HD12	37:h:214:LEU:HB2	1.76	0.67
35:f:108:TYR:HE2	35:f:360:VAL:HG21	1.59	0.67
40:l:467:GLU:HA	40:l:470:LYS:HD3	1.74	0.67
1:2:48:C:H2'	1:2:49:U:C6	2.30	0.67
37:h:157:THR:O	37: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
9:F:62:GLU:HA	9:F:132:LEU:HD11	1.76	0.67
25:V:180:GLU:O	25:V:184:LYS:HG2	1.94	0.67
38:i:179:LYS:HE2	38:i:183:LYS:HE3	1.77	0.67
24:U:68:LEU:C	24:U:71:PRO:HD2	2.19	0.67
37:h:330:PHE:HA	37:h:333:LEU:HD13	1.76	0.67
40:l:452:TYR:HB3	40:l:461:ALA:HB2	1.77	0.67
37:h:194:LEU:HG	37:h:230:GLU:OE2	1.94	0.67
37:h:260:MET:HE1	37:h:279:ARG:CZ	2.24	0.67
37:h:97:VAL:O	37:h:101:ARG:HD2	1.95	0.67
37:h:204:GLU:HA	37:h:207:LYS:CG	2.23	0.67
37:h:236:LEU:HD22	37:h:240:TYR:CE2	2.30	0.67
1:2:409:U:H2'	1:2:410:C:C6	2.30	0.67
1:2:1710:G:O2'	1:2:1711:A:H5'	1.95	0.67
5:B:514:VAL:HB	5:B:517:GLN:HG3	1.77	0.67
11:H:225:ILE:HG23	11:H:228:PRO:HG3	1.77	0.67
19:P:82:SER:HB3	19:P:85:ALA:HB3	1.76	0.67
38:i:417:PRO:HB3	38:i:421:THR:HG21	1.75	0.67
1:2:647:C:O2'	1:2:648:U:H5'	1.94	0.66
6:C:182:LYS:HE3	6:C:220:LEU:HB3	1.77	0.66
17:N:399:LEU:CD1	17:N:403:LYS:HD2	2.24	0.66
21:R:86:ASN:HA	21:R:89:ILE:HD12	1.76	0.66
37:h:213:ASP:O	37:h:213:ASP:OD1	2.13	0.66
37:h:115:ASN:OD1	37:h:115:ASN:O	2.14	0.66
37:h:216:LEU:HD12	37:h:244:PHE:CE1	2.31	0.66
38:i:341:TRP:CH2	38:i:345:LEU:HG	2.30	0.66
3:8:227:ILE:HG22	3:8:227:ILE:O	1.93	0.66
22:S:93:ILE:HD12	31:b:19:LEU:CD1	2.25	0.66
37:h:259:TRP:CH2	37:h:275:VAL:HG12	2.29	0.66
33:d:66:ASP:OD2	33:d:68:SER:HB2	1.95	0.66
13:J:251:LYS:O	13:J:251:LYS:HD3	1.96	0.66
1:2:1744:C:H3'	1:2:1745:A:C5'	2.26	0.66
6:C:158:ASN:HD21	6:C:162:ARG:HH11	1.42	0.66
6:C:180:ILE:HG22	6:C:191:TRP:HZ2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:372:THR:HG22	26: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
24:U:76:ALA:HA	39:k:15:ARG:HH21	1.61	0.66
1:2:654:G:H2'	1:2:655:A:H8	1.60	0.66
35:f:171:ALA:HB2	35:f:206:LYS:HD2	1.76	0.66
1:2:718:A:H2	1:2:729:A:H61	1.43	0.66
38:i:407:LEU:O	38:i:410:MET:HG3	1.96	0.66
1:2:154:G:C6	37:h:172:TRP:CD1	2.83	0.65
1:2:673:U:H3	1:2:709:G:H22	1.41	0.65
6:C:46:ARG:CZ	7:D:148:SER:HB3	2.26	0.65
26:W:215:VAL:HG22	26:W:216:LYS:HG2	1.78	0.65
38:i:141:ARG:NH1	38:i:141:ARG:HA	2.11	0.65
38:i:356:ILE:HD12	38:i:357:ASN:N	2.11	0.65
3:8:217:LEU:HD11	3:8:238:ALA:HB2	1.79	0.65
38:i:165:THR:HA	38:i:168:GLU:CG	2.25	0.65
38:i:314:VAL:HG13	38:i:318:CYS:HB3	1.77	0.65
34:e:191:ARG:HG2	34:e:191:ARG:HH11	1.61	0.65
35:f:90:LEU:HD12	35:f:141:ILE:HB	1.77	0.65
1:2:968:A:H4'	1:2:969:G:H5"	1.77	0.65
5:B:399:MET:HE3	30:a:102:ILE:HB	1.77	0.65
24:U:52:GLU:O	24:U:56:VAL:HG23	1.95	0.65
35:f:185:ALA:HA	35:f:188:TYR:CE2	2.32	0.65
40:l:317:ALA:HB1	40:l:346:LEU:HD22	1.79	0.65
1:2:1687:U:H2'	1:2:1688:U:C6	2.32	0.65
6:C:261:PHE:CD2	38:i:233:LEU:HD22	2.31	0.65
24:U:73:LYS:HE3	39:k:18:ARG:NE	2.10	0.65
24:U:85:TYR:HE1	24:U:106:ALA:HB3	1.61	0.65
6:C:53:LYS:O	6:C:56:LYS:HG2	1.97	0.65
13:J:283:SER:HB3	13:J:288:ASP:HB3	1.79	0.65
24:U:115:LYS:HZ2	24:U:116:GLU:HG3	1.61	0.65
38:i:366:ALA:HA	38:i:369:LYS:HG2	1.78	0.65
1:2:816:U:H4'	1:2:817:G:OP2	1.97	0.65
2:6:1:U:H3'	2:6:2:U:C6	2.31	0.65
37:h:202:MET:SD	37:h:227:ILE:HD13	2.37	0.65
38:i:363:ASN:HD22	38:i:366:ALA:HB2	1.60	0.65
1:2:1318:A:H3'	1:2:1319:A:H8	1.61	0.65
39:k:51:ILE:CG2	39:k:52:LEU:N	2.42	0.65
1:2:1744:C:H2'	1:2:1746:A:N7	2.12	0.65
25:V:128:ARG:HE	25:V:132:GLN:HE21	1.44	0.65
37:h:234:TRP:CH2	37:h:266:ARG:HG3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:134:A:O2'	1:2:135:A:H5'	1.96	0.64
26:W:372:THR:HB	26:W:375:SER:HB3	1.79	0.64
1:2:837:U:O2'	24:U:61:ARG:HG2	1.97	0.64
31:b:21:ILE:HG23	31:b:25:LYS:HD3	1.79	0.64
37:h:296:LYS:HE3	37:h:333:LEU:HG	1.79	0.64
4:A:144:SER:O	4:A:148:GLU:HG3	1.96	0.64
8:E:7:MET:HE1	8:E:66:GLN:HB2	1.79	0.64
24:U:115:LYS:HD2	24:U:115:LYS:C	2.22	0.64
35:f:280:GLU:O	35:f:284:GLU:HG2	1.97	0.64
37:h:279:ARG:HH22	37: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
35:f:276:LEU:HB2	35:f:282:ILE:HD12	1.78	0.64
6:C:255:ASN:ND2	34:e:146:ASP:HB3	2.12	0.64
7:D:452:THR:HG22	7:D:452:THR:O	1.96	0.64
35:f:157:ILE:HA	35:f:162:ARG:CD	2.26	0.64
1:2:1703:G:H3'	1:2:1704:A:C8	2.32	0.64
35:f:58:ARG:HH12	35:f:66:SER:HB3	1.62	0.64
1:2:1574:C:H5'	21:R:136:VAL:HG22	1.80	0.64
5:B:239:MET:HB2	27:X:448:MET:HE2	1.80	0.64
38:i:111:LYS:HD2	38:i:111:LYS:C	2.23	0.64
1:2:212:G:O2'	1:2:213:C:H5'	1.98	0.64
11:H:263:PRO:HB2	11:H:266:GLU:OE2	1.97	0.64
38:i:322:MET:HE3	38:i:358:GLN:CD	2.23	0.64
37:h:228:CYS:HA	37:h:231:THR:OG1	1.98	0.64
2:6:2:U:H2'	2:6:3:U:O4'	1.98	0.63
1:2:991:A:H2'	1:2:992:U:C6	2.33	0.63
13:J:250:VAL:O	13: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
13:J:190:GLU:HB2	20:Q:247:TYR:CZ	2.33	0.63
17:N:298:PRO:HD2	17:N:301:LEU:HD12	1.81	0.63
35:f:113:GLU:HG3	35:f:113:GLU:O	1.97	0.63
37:h:171:LEU:HD11	37:h:189:LEU:HD12	1.81	0.63
13:J:189:LEU:HD23	20:Q:246:GLU:CG	2.28	0.63
26:W:118:PRO:O	26:W:121:ARG:HG3	1.98	0.63
1:2:922:G:H1	1:2:1650:C:N4	1.90	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
37:h:169:ARG:HH11	37:h:169:ARG:HG3	1.63	0.63
37:h:299:LEU:HB3	37:h:337:TRP:HH2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:240:ASP:HA	38:i:243:ILE:HG22	1.81	0.63
1:2:147:U:H2'	1:2:148:U:C6	2.33	0.63
6:C:256:LEU:HD12	6:C:286:SER:HB2	1.81	0.63
35:f:280:GLU:OE2	35:f:373:LEU:HG	1.99	0.63
24:U:47:LYS:NZ	24:U:47:LYS:HB3	2.13	0.63
40:l:517:LYS:O	40: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	40:l:545:HIS:HB3	2.34	0.63
14:K:39:THR:HG22	14:K:51:LYS:HD3	1.80	0.63
29:Z:68:HIS:HA	29:Z:79:TYR:O	1.99	0.63
37:h:316:GLN:OE1	37: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
5:B:399:MET:HE1	30:a:101:ILE:HB	1.81	0.62
6:C:287:LEU:CD2	7:D:178:LEU:HD23	2.25	0.62
35:f:356:ARG:HA	35:f:360:VAL:HB	1.80	0.62
13:J:294:TYR:OH	22:S:30:LYS:HD2	2.00	0.62
38:i:335:SER:HA	38:i:338:LEU:CD2	2.29	0.62
38:i:99:GLU:O	38:i:103:ARG:HG3	2.00	0.62
40:l:217:VAL:HG11	40:l:237:LEU:HD11	1.81	0.62
24:U:88:ARG:NH1	38:i:420:LEU:HD22	2.15	0.62
33:d:60:LEU:HD21	33:d:83:ILE:HD11	1.82	0.62
34:e:149:HIS:HA	34:e:152:VAL:HG12	1.80	0.62
37:h:288:LEU:HB2	37:h:318:TYR:HE2	1.64	0.62
38:i:400:ILE:HD13	38:i:429:TYR:HE1	1.64	0.62
1:2:81:U:H2'	1:2:82:C:C1'	2.29	0.62
5:B:62:ILE:HD13	5:B:71:ILE:HG12	1.80	0.62
7:D:318:LYS:HA	7:D:321:GLU:OE2	1.99	0.62
1:2:1135:A:HO2'	1:2:1136:A:H8	1.48	0.62
38:i:401:GLU:O	38: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
37:h:296:LYS:HD2	37:h:337:TRP:CE2	2.35	0.62
37:h:323:LYS:HG2	37:h:324:SER:N	2.13	0.62
38:i:177:MET:HB3	38:i:181:ARG:NH2	2.14	0.62
37:h:358:LYS:O	37:h:362:PRO:HG2	2.00	0.62
38:i:366:ALA:O	38: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
5:B:282:GLN:HA	5:B:285:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:73:LYS:HB2	39:k:18:ARG:HH21	1.64	0.62
35:f:367:LYS:HD2	35:f:367:LYS:C	2.24	0.62
1:2:644:G:O2'	1:2:645:A:H5'	2.00	0.61
11:H:225:ILE:HA	11:H:228:PRO:CB	2.28	0.61
35:f:164:ALA:HB1	35: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
7:D:76:ALA:O	7:D:79:VAL:HG12	2.00	0.61
11:H:240:GLY:C	38:i:295:MET:HE1	2.25	0.61
22:S:90:LEU:HD11	31:b:21:ILE:HD11	1.82	0.61
37:h:90:HIS:CD2	37:h:94:LEU:HD13	2.35	0.61
37:h:165:ASN:HA	37: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
25:V:61:ASP:O	25:V:65:MET:HG3	2.01	0.61
35:f:210:VAL:HG22	35:f:256:VAL:HG21	1.82	0.61
38:i:290:PRO:HA	38: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
7:D:180:THR:HG21	7:D:193:TRP:CZ2	2.35	0.61
24:U:113:GLU:HA	24:U:116:GLU:OE1	1.99	0.61
37:h:81:ASP:HB2	37:h:82:PRO:HD3	1.83	0.61
11:H:204:GLU:HA	11:H:207:GLU:HG3	1.82	0.61
24:U:115:LYS:NZ	24:U:116:GLU:HG3	2.15	0.61
39:k:42:GLY:O	39:k:43:LEU:C	2.43	0.61
35:f:272:ARG:HD2	35:f:273:TYR:HE1	1.66	0.61
38:i:341:TRP:NE1	38:i:347:PRO:HG3	2.15	0.61
1:2:1791:G:H5"	1:2:1792:A:OP1	2.01	0.61
7:D:504:GLN:HG3	7:D:509:ARG:O	2.01	0.61
38:i:322:MET:HE3	38: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
6:C:72:THR:HG21	6:C:85:THR:OG1	2.01	0.61
10:G:68:VAL:HG21	10:G:71:CYS:SG	2.40	0.61
2:6:1:U:H3'	2:6:2:U:H6	1.66	0.61
6:C:117:LEU:HD13	6:C:123:ALA:HA	1.81	0.61
22:S:93:ILE:CD1	31:b:19:LEU:CD1	2.78	0.61
40:l:465:LEU:HD22	40:l:483:LEU:HD23	1.83	0.61
1:2:150:A:H3'	1:2:151:A:C8	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1797:G:H2'	1:2:1798:G:C8	2.34	0.60
38:i:435:PHE:HD1	38:i:436:GLU:N	1.99	0.60
36:g:564:LEU:HD11	36:g:598:PHE:HA	1.83	0.60
37:h:229:HIS:HA	37:h:262:PHE:CE2	2.36	0.60
1:2:1392:A:H2	40:l:545:HIS:HB3	1.66	0.60
5:B:176:SER:HG	5:B:230:VAL:N	1.99	0.60
24:U:73:LYS:NZ	39:k:18:ARG:HG3	2.15	0.60
37:h:171:LEU:HA	37:h:181:PRO:HB3	1.82	0.60
1:2:1726:U:H4'	1:2:1727:G:OP1	2.00	0.60
29:Z:86:LEU:HD21	29:Z:90:GLY:HA2	1.81	0.60
30:a:86:ILE:HD13	30:a:101:ILE:HD12	1.84	0.60
35:f:232:GLU:OE2	35: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	5:B:529:ARG:NE	2.49	0.60
1:2:969:G:H22	1:2:1625:A:H5'	1.65	0.60
17:N:306:LYS:O	17:N:310:VAL:HG23	2.01	0.60
35:f:108:TYR:CE2	35:f:360:VAL:HG21	2.35	0.60
38:i:100:PHE:O	38:i:104:PHE:HB2	2.02	0.60
38:i:129:LEU:HA	38:i:132:VAL:CG1	2.31	0.60
1:2:545:A:H4'	1:2:546:G:O5'	2.01	0.60
7:D:306:GLU:OE1	7:D:306:GLU:HA	2.02	0.60
24:U:81:PRO:HA	24:U:84:VAL:HG12	1.83	0.60
38:i:408:LYS:N	38:i:408:LYS:HD2	2.17	0.60
1:2:386:U:H5	1:2:412:A:N1	1.99	0.60
4:A:200:GLN:HG2	4:A:205:ILE:CB	2.28	0.60
38:i:109:ARG:O	38:i:109:ARG:HD3	2.01	0.60
1:2:866:A:H5'	1:2:866:A:H8	1.67	0.60
35:f:389:THR:CG2	35:f:397:GLU:HG3	2.32	0.60
37:h:171:LEU:HD11	37:h:189:LEU:CD1	2.30	0.60
37:h:197:LYS:CE	37:h:230:GLU:HB2	2.27	0.60
38:i:347:PRO:HA	38:i:351:ASP:OD2	2.02	0.60
1:2:1167:U:H2'	1:2:1168:U:C6	2.37	0.60
34:e:173:GLU:HG2	34:e:176:ALA:HB2	1.84	0.60
1:2:714:G:N2	20:Q:192:ILE:HG22	2.17	0.59
6:C:176:VAL:HA	6:C:180:ILE:HG23	1.84	0.59
7:D:138:GLU:HB2	7:D:141:ARG:CB	2.31	0.59
24:U:88:ARG:HA	24:U:91:GLU:CD	2.27	0.59
34:e:354:VAL:HG21	34:e:362:ARG:NH1	2.17	0.59
37:h:236:LEU:HD22	37:h:240:TYR:HE2	1.66	0.59
1:2:1560:C:H4'	1:2:1561:A:H5"	1.84	0.59
6:C:204:THR:CA	7:D:116:GLU:HG2	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:80:LYS:O	22:S:84:ILE:HG12	2.01	0.59
26:W:347:LYS:H	26:W:347:LYS:HD2	1.68	0.59
36:g:621:MET:HG2	36:g:653:MET:HE2	1.84	0.59
13:J:283:SER:HB2	13:J:288:ASP:HB3	1.84	0.59
38:i:204:GLU:HG3	38:i:204:GLU:O	2.02	0.59
38:i:335:SER:O	38:i:338:LEU:HG	2.02	0.59
1:2:242:G:O2'	1:2:243:U:H5'	2.01	0.59
3:8:200:LEU:HD13	3:8:244:VAL:HG22	1.84	0.59
6:C:46:ARG:NH2	7:D:148:SER:HB3	2.18	0.59
7:D:175:LYS:O	7:D:179:GLN:HG2	2.02	0.59
37:h:83:THR:O	37:h:86:VAL:HG22	2.02	0.59
37:h:271:SER:HA	37:h:274:LYS:HB2	1.84	0.59
6:C:256:LEU:HD22	6:C:257:LEU:HD22	1.85	0.59
7:D:343:GLU:O	7:D:347:LEU:HD12	2.02	0.59
35:f:192:LEU:HB3	35: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
6:C:256:LEU:CD2	6:C:257:LEU:HD22	2.32	0.59
7:D:174:HIS:HB2	7:D:200:PHE:HE2	1.67	0.59
37:h:223:LEU:O	37:h:227:ILE:HG13	2.02	0.59
38:i:303:GLU:HB3	38:i:309:ARG:NH2	2.18	0.59
7:D:452:THR:O	7:D:452:THR:CG2	2.50	0.59
38:i:408:LYS:HA	38:i:408:LYS:HE2	1.82	0.59
1:2:1727:G:H1'	1:2:1728:U:H5'	1.84	0.59
6:C:178:LYS:NZ	6:C:224:MET:HE1	2.18	0.59
11:H:238:LYS:HD2	38:i:302:ALA:HB2	1.85	0.59
37:h:225:PHE:HA	37:h:228:CYS:SG	2.43	0.59
38:i:244:ARG:HA	38:i:247:GLU:OE1	2.01	0.59
1:2:842:A:O2'	1:2:843:U:H5'	2.03	0.59
11:H:222:THR:OG1	24:U:120:ALA:HB1	2.02	0.59
35:f:177:ILE:HD12	35:f:358:ARG:HG3	1.85	0.59
36:g:621:MET:HE1	36:g:626:HIS:CD2	2.37	0.59
1:2:1450:G:H5'	11:H:415:LYS:HE2	1.85	0.58
1:2:1687:U:H2'	1:2:1688:U:H6	1.65	0.58
11:H:222:THR:HA	11:H:225:ILE:HD12	1.85	0.58
11:H:236:ILE:HG23	11:H:241:ILE:CG2	2.32	0.58
39:k:41:GLY:O	39:k:42:GLY:C	2.46	0.58
1:2:1730:U:H2'	1:2:1731:A:H8	1.68	0.58
7:D:227:LYS:HE3	34:e:286:GLU:HG2	1.85	0.58
30:a:124:SER:HB2	30:a:128:GLN:CD	2.29	0.58
38:i:170:SER:O	38:i:174:LEU:HD23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:197:VAL:CG1	11:H:258:VAL:HG13	2.33	0.58
7:D:403:GLU:HG2	7:D:404:THR:CG2	2.31	0.58
25:V:56:PRO:HG3	25:V:65:MET:SD	2.43	0.58
29:Z:124:ILE:HG22	29:Z:127:LEU:H	1.68	0.58
35:f:127:TYR:OH	35:f:182:ASP:HB2	2.03	0.58
37:h:82:PRO:HB2	37:h:87:LYS:CD	2.32	0.58
40:l:272:THR:HG21	40:l:288:VAL:HG11	1.85	0.58
11:H:241:ILE:HA	38:i:295:MET:HE2	1.84	0.58
27:X:447:ARG:HA	27:X:450:GLU:HG3	1.85	0.58
35:f:402:THR:O	35:f:407:PRO:HD3	2.04	0.58
35:f:408:TYR:O	38:i:187:LYS:HD3	2.04	0.58
37:h:330:PHE:CD2	37:h:375:VAL:HG11	2.38	0.58
1:2:1729:G:H2'	1:2:1730:U:C6	2.39	0.58
7:D:258:GLY:HA3	7:D:356:TYR:CE2	2.37	0.58
11:H:225:ILE:HG22	11:H:226:LYS:N	2.18	0.58
38:i:109:ARG:HD3	38:i:109:ARG:C	2.28	0.58
1:2:998:A:H4'	1:2:999:G:O5'	2.02	0.58
37:h:296:LYS:HD2	37:h:337:TRP:CD2	2.39	0.58
38:i:178:GLU:OE1	38:i:178:GLU:HA	2.03	0.58
38:i:335:SER:HA	38: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
4:A:197:VAL:HG12	11:H:258:VAL:HG13	1.85	0.58
1:2:1757:U:O2'	1:2:1758:G:H5'	2.04	0.58
3:8:213:PRO:HA	3:8:216:LEU:HD13	1.85	0.58
33:d:107:ALA:O	33:d:109:ALA:N	2.37	0.58
35:f:393:ASP:HB3	35:f:396:SER:OG	2.03	0.58
1:2:1490:A:OP2	15:L:139:LYS:HE3	2.04	0.58
7:D:308:LEU:HD22	7:D:344:ARG:NH1	2.19	0.58
7:D:339:ASP:HA	7:D:342:GLU:OE1	2.04	0.58
35:f:105:LEU:HB3	35:f:106:PRO:HD3	1.86	0.58
38:i:154:PRO:HG3	38:i:160:ASP:OD2	2.04	0.58
40:l:379:ILE:HG13	40: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
6:C:57:ILE:O	7:D:364:VAL:HG23	2.04	0.57
9:F:146:ARG:NH2	31:b:31:LYS:HB2	2.19	0.57
37:h:86:VAL:HG21	37:h:121:ASP:CB	2.33	0.57
38:i:328:LEU:HD23	38:i:369:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:345:LEU:O	38:i:345:LEU:HD13	2.04	0.57
1:2:1430:A:H2'	1:2:1432:A:N7	2.19	0.57
31:b:51:ASP:HB3	31: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
14:K:123:LYS:HE3	14:K:125:ILE:CG1	2.34	0.57
34:e:304:LEU:O	34:e:308:GLU:HG2	2.03	0.57
35:f:272:ARG:HD2	35:f:273:TYR:CE1	2.38	0.57
37:h:221:ALA:HA	37:h:224:VAL:HG12	1.86	0.57
38:i:419:ILE:HD11	38:i:448:TYR:HE2	1.68	0.57
4:A:121:LYS:O	4:A:122:LYS:HB2	2.04	0.57
5:B:306:ALA:HA	5:B:309:ARG:HG2	1.87	0.57
36:g:613:VAL:HG11	36:g:640:ILE:HD13	1.86	0.57
37:h:258:VAL:O	37:h:261:GLU:HG2	2.05	0.57
37:h:304:PRO:O	37:h:364:MET:HE1	2.04	0.57
40:l:342:LEU:O	40:l:346:LEU:HD23	2.05	0.57
1:2:553:U:H2'	1:2:554:C:C6	2.40	0.57
37:h:121:ASP:HA	37:h:124:PHE:CD1	2.40	0.57
37:h:270:GLU:H	37:h:270:GLU:CD	2.13	0.57
37:h:307:ALA:HB3	37:h:364:MET:CE	2.35	0.57
38:i:278:LEU:HD12	38:i:278:LEU:O	2.03	0.57
38:i:356:ILE:HB	38:i:367:TYR:HE1	1.69	0.57
40:l:385:MET:SD	40:l:387:ASN:HB2	2.45	0.57
1:2:298:A:H5"	1:2:300:G:O4'	2.04	0.57
1:2:439:A:H2'	1:2:441:U:H1'	1.87	0.57
2:6:3:U:C2'	2:6:4:U:H5'	2.34	0.57
12:I:139:ASN:HB2	12:I:142:LYS:HE3	1.87	0.57
37:h:229:HIS:CD2	37:h:258:VAL:HG13	2.40	0.57
1:2:1622:A:C8	16: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
38:i:305:GLU:O	38:i:305:GLU:HG2	2.04	0.57
1:2:148:U:H2'	1:2:149:U:C6	2.40	0.57
25:V:129:LYS:HB3	25:V:129:LYS:HZ2	1.70	0.57
37:h:153:GLN:OE1	37:h:156:LYS:HD3	2.03	0.57
38:i:418:ASP:H	38:i:421:THR:HB	1.69	0.57
1:2:1731:A:H5'	37:h:218:PRO:HD2	1.86	0.56
6:C:161:ILE:O	6:C:165:GLU:HG3	2.05	0.56
35:f:369:ASP:O	35:f:371:PRO:HD3	2.05	0.56
1:2:236:A:OP1	1:2:236:A:H4'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1169:U:H2'	1:2:1170:U:H6	1.70	0.56
3:8:200:LEU:HD12	3:8:201:ALA:H	1.69	0.56
7:D:229:LYS:O	7:D:233:GLN:HG3	2.05	0.56
26:W:281:ARG:HD2	26: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
11:H:250:ILE:O	11:H:251:ALA:HB3	2.06	0.56
24:U:73:LYS:CB	39:k:18:ARG:HH21	2.18	0.56
34:e:382:LYS:HB3	34:e:382:LYS:NZ	2.19	0.56
37:h:227:ILE:O	37:h:231:THR:HG23	2.05	0.56
37:h:357:LEU:O	37:h:361:ILE:HG22	2.06	0.56
38:i:389:LYS:O	38:i:393:ILE:HG22	2.05	0.56
40:l:308:ILE:HG21	40:l:338:PHE:HB3	1.87	0.56
40:l:415:HIS:HE2	40:l:443:TYR:HE2	1.53	0.56
1:2:163:A:H4'	1:2:164:A:C5'	2.33	0.56
25:V:194:THR:HG22	25:V:195:LEU:H	1.69	0.56
35:f:36:ASP:O	35: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
2:6:5:U:H2'	2:6:6:U:O4'	2.05	0.56
35:f:215:CYS:SG	35: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
4:A:83:THR:HG23	4:A:193:THR:OG1	2.05	0.56
6:C:183:LEU:O	6:C:184:LEU:HD12	2.06	0.56
7:D:181:LEU:HD13	7:D:193:TRP:CB	2.36	0.56
18:O:21:MET:HE1	18:O:36:VAL:HG22	1.86	0.56
25:V:110:ASN:O	25:V:113:ARG:HG2	2.06	0.56
37:h:151:CYS:SG	37:h:179:LEU:HA	2.45	0.56
37:h:380:ASP:O	37:h:384:LYS:HG3	2.06	0.56
38:i:124:ILE:CA	38:i:127:MET:HE1	2.08	0.56
38:i:328:LEU:HD23	38:i:369:LYS:CD	2.35	0.56
38:i:436:GLU:HG2	38:i:437:ARG:N	2.19	0.56
1:2:1793:C:O2'	1:2:1794:U:H5'	2.06	0.56
7:D:186:THR:HG23	38:i:244:ARG:HH12	1.70	0.56
7:D:309:ASN:O	7:D:313:LYS:HG2	2.06	0.56
13:J:260:VAL:HG11	13:J:275:ILE:HD13	1.87	0.56
24:U:88:ARG:HA	24:U:91:GLU:OE2	2.06	0.56
29:Z:67:TYR:O	29:Z:80:GLU:HA	2.05	0.56
38:i:407:LEU:HD12	38:i:410:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:A:93:ASN:HB3	4:A:96:ARG:HB3	1.88	0.56
6:C:139:VAL:HG11	6:C:144:LEU:HD22	1.86	0.56
13:J:248:ARG:HG2	13:J:281:GLY:O	2.05	0.56
16:M:64:GLU:OE1	16:M:74:HIS:ND1	2.35	0.56
24:U:90:LEU:C	24:U:90:LEU:HD13	2.31	0.56
35:f:284:GLU:HA	35:f:284:GLU:OE2	2.06	0.56
37:h:116:CYS:O	37:h:117:ARG:HD2	2.06	0.56
1:2:1166:U:H2'	1:2:1167:U:C6	2.40	0.56
7:D:95:ARG:O	7:D:99:GLN:HB2	2.06	0.56
35:f:96:LYS:O	35:f:96:LYS:HD3	2.06	0.56
40:l:331:GLU:HG2	40:l:331:GLU:O	2.05	0.56
28:Y:20:GLU:H	28:Y:20:GLU:CD	2.14	0.55
34:e:354:VAL:O	34:e:355:SER:HB3	2.05	0.55
35:f:210:VAL:CG2	35:f:256:VAL:HG21	2.36	0.55
35:f:302:LEU:O	35:f:306:LYS:HG2	2.06	0.55
1:2:211:G:O2'	1:2:212:G:H5'	2.05	0.55
37:h:337:TRP:HB3	37:h:338:PRO:HD3	1.88	0.55
40:l:234:LEU:HD13	40:l:257:THR:HG23	1.87	0.55
1:2:1705:C:H4'	1:2:1706:C:OP2	2.05	0.55
22:S:94:LEU:O	22:S:98:VAL:HG12	2.05	0.55
37:h:83:THR:HG23	37:h:86:VAL:HG13	1.88	0.55
37:h:136:ARG:O	37:h:140:LEU:HB2	2.06	0.55
38:i:419:ILE:HD11	38:i:448:TYR:CE2	2.41	0.55
1:2:1711:A:H2'	1:2:1712:U:O4'	2.07	0.55
27:X:348:MET:HE1	27:X:352:ILE:CG2	2.37	0.55
37:h:292:PHE:CE1	37:h:333:LEU:HD11	2.42	0.55
4:A:130:MET:HA	4:A:130:MET:HE2	1.88	0.55
30:a:405:GLN:HA	30:a:408:ILE:HG12	1.87	0.55
35:f:401:PRO:HG2	35:f:405:ARG:HG3	1.87	0.55
38:i:239:LEU:HD13	38:i:239:LEU:C	2.31	0.55
1:2:64:U:H2'	1:2:65:G:C8	2.42	0.55
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
31:b:56:LYS:HE2	31:b:56:LYS:HA	1.89	0.55
35:f:214:ALA:HB1	35:f:264:LEU:HD22	1.89	0.55
37:h:121:ASP:O	37:h:124:PHE:HB2	2.07	0.55
1:2:376:G:O2'	1:2:377:U:H5'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1688:U:O2'	1:2:1689:C:H5'	2.06	0.55
3:8:227:ILE:O	3:8:227:ILE:CG2	2.55	0.55
6:C:158:ASN:HD21	6:C:162:ARG:NH1	2.05	0.55
7:D:117:ASP:OD1	7:D:120:GLY:HA2	2.06	0.55
30:a:230:ASP:O	30:a:233:GLU:HG2	2.07	0.55
1:2:1388:A:H4'	30:a:393:ARG:NE	2.22	0.55
1:2:1805:C:H2'	1:2:1806:G:O4'	2.07	0.55
5:B:63:LEU:HD13	30:a:167:MET:HE1	1.88	0.55
25:V:97:ARG:HB3	25: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
11:H:238:LYS:HD2	38:i:302:ALA:CB	2.37	0.55
1:2:1845:A:O5'	39:k:41:GLY:HA3	2.07	0.54
17:N:331:LYS:HB2	17:N:331:LYS:NZ	2.22	0.54
34:e:283:ASP:HB3	34:e:286:GLU:HB2	1.89	0.54
6:C:93:ARG:HD2	6:C:98:PRO:HG2	1.89	0.54
6:C:224:MET:HE2	34:e:251:PHE:CE1	2.42	0.54
11:H:225:ILE:H	11:H:228:PRO:HA	1.72	0.54
24:U:57:ARG:O	24:U:60:ALA:HB3	2.07	0.54
34:e:182:LYS:HB2	34:e:185:GLU:HG3	1.88	0.54
40:l:346:LEU:HG	40: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
6:C:97:ILE:HD11	6:C:354:SER:HB3	1.89	0.54
6:C:182:LYS:HD2	6:C:224:MET:SD	2.48	0.54
30:a:124:SER:HA	30:a:128:GLN:HG3	1.90	0.54
11:H:241:ILE:HD12	11:H:245:MET:HE2	1.90	0.54
24:U:52:GLU:OE2	24:U:52:GLU:N	2.35	0.54
13:J:292:ILE:O	22:S:31:VAL:HG11	2.07	0.54
37:h:234:TRP:CH2	37:h:266:ARG:CG	2.91	0.54
38:i:133:GLU:HA	38:i:136:VAL:CG1	2.38	0.54
1:2:247:A:O2'	1:2:248:U:H5'	2.07	0.54
6:C:178:LYS:HZ1	6:C:224:MET:HE1	1.71	0.54
37:h:171:LEU:O	37:h:181:PRO:HB3	2.08	0.54
38:i:321:VAL:HG11	38:i:340:GLU:OE1	2.07	0.54
1:2:568:G:H1'	1:2:816:U:C4	2.42	0.54
6:C:256:LEU:HD12	6:C:286:SER:CB	2.38	0.54
28:Y:10:VAL:HG22	30:a:385:ILE:HD11	1.89	0.54
29:Z:68:HIS:ND1	29:Z:128:SER:HA	2.23	0.54
35:f:198:GLU:HG3	35:f:320:ILE:HG21	1.89	0.54
40:l:368:ARG:HH21	40:l:401:LYS:HB2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:491:G:H4'	1:2:492:G:OP1	2.07	0.54
5:B:309:ARG:HA	5:B:312:HIS:HB2	1.88	0.54
7:D:97:GLU:HA	7:D:100:ARG:NH2	2.20	0.54
4:A:116:PHE:CD1	4:A:123:LEU:HD23	2.41	0.54
8:E:7:MET:CE	8:E:66:GLN:HB2	2.37	0.54
31:b:52:ASP:O	31:b:53:LYS:HG2	2.08	0.54
37:h:380:ASP:HB3	37:h:384:LYS:HE3	1.89	0.54
40:l:410:PHE:CE1	40: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
15:L:46:LYS:HE3	15:L:64:LEU:HD12	1.90	0.54
35:f:277:ASP:HB3	38:i:121:LYS:HZ1	1.73	0.54
37:h:83:THR:O	37:h:87:LYS:HG3	2.08	0.54
37:h:227:ILE:HD12	37:h:228:CYS:H	1.71	0.54
40:l:379:ILE:HG23	40:l:412:LEU:HD21	1.90	0.54
7:D:315:LEU:HG	7:D:340:LEU:HD13	1.90	0.53
31:b:35:LYS:HA	31:b:38:VAL:HG12	1.89	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"	31:b:76:TRP:CZ2	2.43	0.53
7:D:150:SER:OG	7:D:152:LEU:HD23	2.08	0.53
7:D:181:LEU:HD13	7:D:193:TRP:HB2	1.88	0.53
18:O:52:MET:HG3	18:O:53:GLY:N	2.23	0.53
22:S:100:GLY:O	22:S:101:LEU:HD23	2.09	0.53
29:Z:71:LYS:HD2	29:Z:74:TRP:CZ2	2.43	0.53
38:i:314:VAL:HG13	38:i:318:CYS:CB	2.38	0.53
40:l:266:ALA:HB2	40:l:297:VAL:HG22	1.89	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
34:e:383:ILE:O	34:e:384:LEU:HG	2.08	0.53
7:D:85:ALA:O	7:D:89:LYS:HD3	2.08	0.53
10:G:97:GLN:HA	10:G:97:GLN:NE2	2.23	0.53
13:J:196:ILE:HD12	13:J:209:VAL:HG22	1.90	0.53
33:d:107:ALA:C	33:d:109:ALA:N	2.66	0.53
38:i:369:LYS:HA	38: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'	28:Y:78:LEU:HD21	1.91	0.53
1:2:1054:U:H2'	1:2:1055:C:C6	2.43	0.53
38:i:342:ALA:HA	38:i:347:PRO:CD	2.37	0.53
7:D:318:LYS:HA	7:D:321:GLU:HG2	1.91	0.53
5:B:464:ARG:HG3	5:B:465:ARG:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:148:TRP:OXT	31:b:31:LYS:NZ	2.19	0.53
1:2:1757:U:H2'	1:2:1758:G:C8	2.43	0.53
5:B:481:ARG:HG3	30:a:154:GLU:HB3	1.91	0.53
22:S:27:ILE:HD12	22:S:47:MET:SD	2.49	0.53
34:e:149:HIS:HA	34:e:152:VAL:CG1	2.39	0.53
38:i:407:LEU:HG	38:i:410:MET:HE3	1.90	0.53
40:l:201:ILE:HD12	40:l:213:LEU:HD13	1.91	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
6:C:293:SER:HA	6:C:296:CYS:SG	2.48	0.53
26:W:462:TYR:HA	26:W:472:MET:HE2	1.91	0.53
33:d:45:PHE:CE2	33:d:49:ILE:HD11	2.44	0.53
35:f:66:SER:OG	35:f:69:MET:HG3	2.09	0.53
35:f:276:LEU:HB2	35:f:282:ILE:HD11	1.91	0.53
37:h:97:VAL:HG13	37:h:135:PHE:HD1	1.74	0.53
37:h:311:ILE:HD11	37:h:368:LEU:CD2	2.31	0.53
7:D:242:LEU:HD12	38:i:205:ILE:CD1	2.37	0.53
7:D:314:LYS:O	7:D:318:LYS:HD2	2.08	0.53
13:J:198:ILE:HB	13:J:262:VAL:HG12	1.91	0.53
37:h:228:CYS:SG	37:h:237:LEU:HD23	2.49	0.53
38:i:93:GLU:O	38:i:93:GLU:HG2	2.09	0.53
38:i:352:TRP:HB3	38: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
11:H:219:LYS:HD2	24:U:127:LEU:HD11	1.91	0.52
24:U:73:LYS:NZ	39:k:18:ARG:CG	2.71	0.52
37:h:332:LYS:HD2	37:h:336:GLU:HB2	1.91	0.52
1:2:866:A:H5'	1:2:866:A:C8	2.44	0.52
1:2:921:G:O2'	1:2:1842:U:OP1	2.26	0.52
7:D:334:GLU:O	7:D:338:ARG:HG3	2.09	0.52
11:H:218:GLU:N	11:H:218:GLU:OE2	2.43	0.52
11:H:245:MET:HB2	38:i:292:TRP:CH2	2.45	0.52
13:J:260:VAL:HG11	13:J:275:ILE:CD1	2.38	0.52
35:f:280:GLU:HA	35:f:283:ILE:CG2	2.39	0.52
37:h:203:ASP:HA	37: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
30:a:217:LEU:HA	30:a:220:LYS:HE3	1.91	0.52
36:g:640:ILE:HG23	36:g:646:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:h:265:LYS:O	37:h:341:VAL:HA	2.10	0.52
37:h:329:GLU:O	37:h:332:LYS:HB2	2.09	0.52
1:2:530:A:N7	5:B:529:ARG:CZ	2.73	0.52
1:2:956:G:N2	12: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
7:D:189:GLU:HA	7:D:192:LYS:HD2	1.92	0.52
37:h:224:VAL:HG11	37:h:244:PHE:HE2	1.74	0.52
38:i:127:MET:O	38:i:130:LEU:HB2	2.10	0.52
5:B:478:ILE:HD12	5:B:482:VAL:HG21	1.92	0.52
25:V:128:ARG:O	25:V:132:GLN:HG2	2.08	0.52
25:V:159:GLU:OE2	25:V:162:LYS:HE2	2.08	0.52
32:c:133:LYS:O	32:c:137:LYS:HE3	2.08	0.52
38:i:429:TYR:HA	38:i:432:SER:OG	2.10	0.52
9:F:146:ARG:HH21	31:b:31:LYS:HB2	1.75	0.52
18:O:98:ARG:O	18:O:100:THR:HG23	2.10	0.52
24:U:112:ALA:HA	24:U:115:LYS:HE3	1.90	0.52
34:e:233:LEU:HD11	34:e:235:ARG:NH1	2.24	0.52
35:f:171:ALA:HB2	35:f:206:LYS:CD	2.38	0.52
37:h:88:GLU:HA	37:h:88:GLU:OE2	2.09	0.52
37:h:89:LEU:HB3	37:h:112:LEU:HG	1.91	0.52
38:i:442:PHE:CE2	38:i:446:LYS:HE3	2.44	0.52
5:B:313:PHE:HD2	5:B:316:LEU:HB2	1.73	0.52
6:C:183:LEU:HD12	6:C:220:LEU:CD2	2.36	0.52
17:N:313:TYR:CE1	25:V:168:LEU:HD21	2.44	0.52
25:V:156:LYS:NZ	25:V:156:LYS:HB3	2.24	0.52
33:d:84:PRO:O	33:d:88:ARG:HG3	2.08	0.52
37:h:158:CYS:SG	37:h:166:HIS:HB2	2.49	0.52
37:h:204:GLU:CA	37:h:207:LYS:HG2	2.38	0.52
37:h:311:ILE:HA	37:h:314:ILE:HG22	1.90	0.52
1:2:4:A:OP1	25: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
4:A:54:ALA:HA	4:A:192:ILE:CD1	2.40	0.52
13:J:202:ARG:O	13:J:234:MET:HG3	2.09	0.52
37:h:166:HIS:HA	37:h:169:ARG:CD	2.17	0.52
37:h:339:VAL:O	37:h:342:LEU:HD23	2.09	0.52
17:N:325:MET:CE	17:N:355:THR:HG22	2.39	0.52
36:g:543:LYS:NZ	36:g:581:PRO:HG3	2.25	0.52
37:h:219:GLY:O	37:h:223:LEU:HD13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:h:271:SER:O	37:h:275:VAL:HG13	2.09	0.52
38:i:184:GLU:OE1	38:i:184:GLU:HA	2.10	0.52
11:H:238:LYS:CD	38:i:302:ALA:HB2	2.40	0.52
29:Z:68:HIS:HB3	29:Z:78:SER:HB2	1.92	0.52
35:f:82:GLU:HA	35:f:82:GLU:OE1	2.10	0.52
37:h:121:ASP:HA	37:h:124:PHE:HD1	1.73	0.52
37:h:165:ASN:HA	37:h:168:LYS:HZ1	1.74	0.52
37:h:203:ASP:HA	37:h:206:MET:HE3	1.92	0.52
2:6:4:U:H5"	2:6:5:U:P	2.50	0.51
6:C:183:LEU:C	6:C:184:LEU:HD12	2.35	0.51
7:D:108:ILE:O	7:D:112:ASP:HB2	2.10	0.51
7:D:148:SER:O	7:D:149:ASP:HB2	2.10	0.51
1:2:488:C:OP1	18:O:109:ARG:HD3	2.09	0.51
1:2:1804:U:H5"	3:8:174:LYS:O	2.09	0.51
6:C:303:LEU:O	6:C:303:LEU:HD23	2.10	0.51
11:H:219:LYS:O	24:U:124:LEU:HD21	2.10	0.51
1:2:364:C:H4'	1:2:365:G:C4	2.45	0.51
7:D:78:ARG:HB3	7:D:78:ARG:HH11	1.75	0.51
7:D:227:LYS:HD2	34:e:289:TYR:CD2	2.46	0.51
11:H:227:GLY:HA3	11:H:230:ARG:CZ	2.40	0.51
35:f:310:PRO:HB3	35:f:373:LEU:HA	1.93	0.51
35:f:325:PHE:CD1	38:i:103:ARG:HG2	2.46	0.51
37:h:233:SER:OG	37:h:236:LEU:HG	2.10	0.51
38:i:352:TRP:HB3	38:i:380:PHE:HE1	1.75	0.51
1:2:365:G:H2'	1:2:366:G:H5'	1.92	0.51
6:C:158:ASN:O	6:C:161:ILE:HG22	2.10	0.51
6:C:176:VAL:O	6:C:180:ILE:HG12	2.10	0.51
7:D:171:PHE:O	7:D:175:LYS:HG3	2.11	0.51
9:F:146:ARG:HG3	9:F:148:TRP:CE2	2.45	0.51
37:h:202:MET:CE	37:h:236:LEU:HD13	2.41	0.51
38:i:179:LYS:HE2	38:i:183:LYS:CE	2.39	0.51
38:i:394:HIS:CE1	38:i:402:ASP:HB3	2.46	0.51
1:2:153:A:C2	29:Z:59:PHE:HZ	2.28	0.51
1:2:636:A:OP1	25:V:117:LYS:HE3	2.11	0.51
1:2:1766:U:H2'	1:2:1767:G:C8	2.45	0.51
2:6:4:U:H5"	2:6:5:U:OP1	2.11	0.51
6:C:227:GLU:O	6:C:231:ARG:HG3	2.11	0.51
38:i:328:LEU:HG	38: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	37:h:150:LEU:HD22	2.09	0.51
6:C:259:SER:O	6:C:263:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:85:TYR:HE1	24:U:106:ALA:CB	2.22	0.51
24:U:98:SER:OG	24:U:101:ASP:HB2	2.10	0.51
35:f:273:TYR:CD2	35:f:286:MET:HG2	2.45	0.51
6:C:61:LYS:HB3	6:C:65:SER:OG	2.10	0.51
6:C:162:ARG:NH1	6:C:162:ARG:HG2	2.25	0.51
11:H:427:TRP:HZ3	11:H:429:LYS:HD3	1.76	0.51
24:U:73:LYS:CE	39:k:18:ARG:HE	2.19	0.51
38:i:342:ALA:HA	38:i:347:PRO:HD3	1.93	0.51
6:C:175:LEU:O	6:C:180:ILE:HG23	2.11	0.51
7:D:381:ARG:HE	7:D:401:LYS:HD2	1.75	0.51
13:J:297:ASP:OD2	22:S:47:MET:HE2	2.11	0.51
34:e:191:ARG:HG2	34:e:191:ARG:NH1	2.25	0.51
37:h:89:LEU:HB2	37:h:112:LEU:CD2	2.40	0.51
40:l:430:LEU:HA	40:l:433:MET:SD	2.51	0.51
1:2:1742:C:H2'	1:2:1743:A:H1'	1.91	0.51
3:8:200:LEU:CG	3:8:202:VAL:HG23	2.40	0.51
38:i:369:LYS:O	38:i:372:GLU:HG2	2.11	0.51
38:i:407:LEU:HG	38:i:410:MET:CE	2.41	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
8:E:16:LYS:CE	25:V:186:THR:HG23	2.40	0.51
35:f:279:VAL:O	35:f:283:ILE:HG22	2.11	0.51
40:l:272:THR:O	40: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
2:6:5:U:H3'	2:6:6:U:C6	2.46	0.50
9:F:43:GLU:O	9:F:44:ARG:HG2	2.10	0.50
10:G:17:GLU:OE1	10:G:66:GLY:HA2	2.12	0.50
14:K:76:GLU:O	14:K:77:HIS:HB2	2.10	0.50
24:U:88:ARG:O	24:U:91:GLU:HG2	2.10	0.50
24:U:89:VAL:O	24:U:93:THR:HG23	2.11	0.50
34:e:334:ILE:O	34: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
5:B:297:THR:HG21	5:B:312:HIS:NE2	2.26	0.50
21:R:206:LYS:HZ1	21:R:208:HIS:CE1	2.29	0.50
35:f:284:GLU:O	35:f:287:GLU:HG3	2.11	0.50
1:2:839:C:O2'	1:2:840:U:O5'	2.28	0.50
37:h:292:PHE:CE1	37:h:329:GLU:HB3	2.46	0.50
11:H:241:ILE:CA	38:i:295:MET:HE2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:625:ARG:CZ	36:g:625:ARG:HB2	2.41	0.50
37:h:83:THR:HG23	37:h:86:VAL:HG22	1.94	0.50
37:h:206:MET:O	37:h:209:LEU:HB3	2.12	0.50
40:l:304:MET:HE1	40:l:308:ILE:HD13	1.92	0.50
24:U:47:LYS:HB3	24:U:47:LYS:HZ1	1.75	0.50
38:i:165:THR:O	38:i:168:GLU:HG3	2.11	0.50
1:2:1012:U:H5'	1:2:1013:A:OP2	2.12	0.50
6:C:162:ARG:HH11	6:C:162:ARG:HG2	1.77	0.50
7:D:340:LEU:O	7:D:343:GLU:HG2	2.11	0.50
1:2:763:A:H2'	1:2:764:A:C8	2.47	0.50
6:C:217:LEU:HD23	6:C:220:LEU:HD12	1.94	0.50
6:C:305:MET:HG3	7:D:157:TRP:CZ3	2.47	0.50
37:h:156:LYS:HA	37:h:159:VAL:HG12	1.94	0.50
1:2:868:C:H4'	10:G:18:ARG:HH12	1.76	0.50
6:C:238:GLU:HG2	6:C:239:LYS:N	2.27	0.50
6:C:317:HIS:HB3	34:e:255:HIS:O	2.11	0.50
7:D:347:LEU:HD12	7:D:347:LEU:H	1.76	0.50
29:Z:81:ILE:HD11	29:Z:84:ILE:HG22	1.93	0.50
35:f:286:MET:HE1	35:f:301:THR:OG1	2.12	0.50
35:f:404:GLN:H	35:f:404:GLN:CD	2.20	0.50
37:h:136:ARG:HA	37:h:140:LEU:HD12	1.92	0.50
37:h:238:ALA:O	37: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
4:A:108:THR:HG23	4:A:148:GLU:HB3	1.94	0.50
7:D:174:HIS:O	7:D:178:LEU:HD13	2.12	0.50
27:X:346:LYS:HB3	27:X:347:LYS:NZ	2.27	0.50
31:b:44:MET:HE1	31:b:51:ASP:HA	1.94	0.50
35:f:157:ILE:O	35:f:162:ARG:HD3	2.11	0.50
38:i:400:ILE:CD1	38:i:429:TYR:HE1	2.25	0.50
1:2:57:U:O4	1:2:384:U:H5	1.94	0.49
20:Q:248:GLU:HG2	20:Q:250:ILE:H	1.77	0.49
35:f:267:ILE:HG12	38:i:276:GLY:O	2.11	0.49
38:i:322:MET:HA	38:i:325:LEU:CG	2.40	0.49
38:i:429:TYR:CD1	38: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
1:2:1388:A:H4'	30: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:246:ILE:HD12	3:8:246:ILE:N	2.26	0.49
7:D:186:THR:CG2	38:i:244:ARG:HH12	2.25	0.49
33:d:37:ALA:N	33:d:107:ALA:HB2	2.27	0.49
35:f:161:PHE:C	35:f:162:ARG:HG3	2.36	0.49
37:h:169:ARG:HG3	37:h:169:ARG:NH1	2.26	0.49
1:2:1134:U:C2'	1:2:1135:A:H5'	2.42	0.49
7:D:403:GLU:CG	7:D:404:THR:HG23	2.41	0.49
37:h:82:PRO:HG3	37:h:124:PHE:CZ	2.46	0.49
37:h:338:PRO:O	37:h:342:LEU:HD22	2.12	0.49
1:2:522:G:H2'	1:2:523:C:C6	2.47	0.49
3:8:188:LEU:CD2	3:8:227:ILE:HG23	2.42	0.49
6:C:176:VAL:HA	6:C:180:ILE:HG21	1.95	0.49
11:H:427:TRP:CZ3	11:H:429:LYS:HD3	2.47	0.49
37:h:136:ARG:CG	37:h:140:LEU:HD12	2.42	0.49
37:h:209:LEU:HD12	37:h:214:LEU:CB	2.41	0.49
1:2:848:G:OP2	1:2:864:U:H5	1.96	0.49
11:H:219:LYS:HD2	24:U:127:LEU:CD1	2.43	0.49
24:U:102:ALA:HA	24:U:105:VAL:CG1	2.43	0.49
31:b:51:ASP:HB3	31:b:58:LYS:HZ3	1.77	0.49
37:h:204:GLU:O	37:h:208:LEU:HB2	2.11	0.49
1:2:638:A:N3	10:G:104:THR:HG22	2.27	0.49
1:2:1430:A:P	31:b:76:TRP:HH2	2.34	0.49
1:2:1754:U:C2'	1:2:1755:G:H5'	2.42	0.49
35:f:355:ILE:O	35:f:359:LEU:HB2	2.13	0.49
35:f:389:THR:HG23	35:f:397:GLU:HG3	1.94	0.49
40:l:559:GLU:O	40:l:563:GLU:HG2	2.13	0.49
1:2:1524:A:H8	30: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
3:8:172:THR:HG23	3:8:174:LYS:H	1.77	0.49
38:i:134:LYS:NZ	38:i:138:GLU:HB2	2.27	0.49
38:i:243:ILE:HG12	38: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
2:6:3:U:O2'	2:6:4:U:H5'	2.12	0.49
5:B:376:VAL:HG13	5:B:379:LEU:HD23	1.95	0.49
6:C:93:ARG:CD	6:C:98:PRO:HG2	2.42	0.49
13:J:205:THR:HG21	13:J:239:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:346:LYS:HB3	27:X:347:LYS:HZ2	1.78	0.49
37:h:342:LEU:HD11	37:h:387:ALA:O	2.13	0.49
38:i:194:GLU:OE1	38:i:223:LYS:HD3	2.13	0.49
40:l:515:TYR:O	40: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
5:B:453:ALA:O	5:B:524:VAL:HG11	2.13	0.49
6:C:117:LEU:HD13	6:C:123:ALA:CA	2.42	0.49
10:G:49:PHE:HA	10:G:61:THR:O	2.13	0.49
15:L:45:LEU:HD11	15:L:77:LEU:HD11	1.94	0.49
35:f:58:ARG:NH1	35:f:66:SER:HB3	2.27	0.49
35:f:258:PRO:HD3	38:i:280:TYR:CZ	2.48	0.49
38:i:420:LEU:HD12	38:i:421:THR:N	2.28	0.49
5:B:302:CYS:SG	5:B:305:GLU:HB2	2.52	0.48
5:B:371:LEU:HA	5:B:375:LYS:HE3	1.93	0.48
14:K:59:ASN:O	14:K:60:ARG:HB2	2.12	0.48
37:h:254:THR:HA	37:h:257:ASP:OD2	2.13	0.48
38:i:366:ALA:HA	38:i:369:LYS:CG	2.43	0.48
1:2:145:U:C2	1:2:146:U:C5	3.01	0.48
1:2:442:U:O2'	1:2:443:C:H5"	2.13	0.48
1:2:1767:G:H2'	1:2:1768:A:C4'	2.42	0.48
33:d:67:LEU:O	33:d:71:LEU:HG	2.13	0.48
36:g:543:LYS:HZ3	36:g:581:PRO:HG3	1.78	0.48
38:i:394:HIS:ND1	38: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
5:B:171:LYS:HG2	27:X:447:ARG:NH2	2.29	0.48
11:H:330:VAL:HG22	11:H:365:CYS:SG	2.53	0.48
35:f:38:ASP:HA	35:f:41:ASP:OD2	2.13	0.48
40:l:502:GLU:HA	40:l:505:ARG:HD2	1.96	0.48
5:B:96:ARG:NH2	27:X:326:ALA:HB3	2.24	0.48
5:B:490:SER:O	5:B:533:LEU:HG	2.14	0.48
35:f:96:LYS:O	35:f:96:LYS:CD	2.61	0.48
37:h:198:ASN:ND2	37: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
6:C:180:ILE:HG22	6:C:191:TRP:CE2	2.47	0.48
33:d:104:LYS:HG2	33:d:105:PRO:HD2	1.96	0.48
37:h:307:ALA:HB3	37:h:364:MET:HE2	1.94	0.48
31:b:84:GLN:HE21	31:b:84:GLN:HB3	1.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:f:187:TYR:O	35:f:191:ARG:HD2	2.14	0.48
35:f:202:LEU:HD22	35:f:313:LEU:HD23	1.96	0.48
35:f:257:TYR:CD1	35:f:258:PRO:HD2	2.48	0.48
40:l:453:ALA:HA	40:l:458:MET:HE1	1.95	0.48
7:D:308:LEU:HD22	7:D:344:ARG:CZ	2.44	0.48
9:F:38:ARG:HB3	9:F:39:PRO:HD3	1.94	0.48
22:S:60:GLN:HG3	22: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"	31:b:76:TRP:CH2	2.48	0.48
1:2:1744:C:H3'	1:2:1745:A:C4'	2.44	0.48
5:B:14:LYS:O	5:B:15:ASN:HB3	2.13	0.48
8:E:16:LYS:NZ	25:V:189:LEU:HD11	2.29	0.48
13:J:279:ARG:HH11	13:J:290:ASN:HB2	1.79	0.48
20:Q:189:GLU:HG2	22:S:50:SER:HB3	1.95	0.48
37:h:95:ASP:O	37: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
11:H:219:LYS:C	24:U:124:LEU:HD21	2.38	0.48
14:K:42:PRO:HD3	14:K:48:ALA:O	2.14	0.48
22:S:96:LYS:HA	39:k:26:MET:HE1	1.96	0.48
37:h:225:PHE:HA	37:h:228:CYS:HG	1.79	0.48
40:l:309:THR:HG22	40:l:313:LYS:HE3	1.95	0.48
1:2:1567:G:OP2	23:T:49:GLY:HA2	2.14	0.48
1:2:1721:A:H5'	1:2:1722:C:OP2	2.14	0.48
4:A:50:LEU:HD23	4:A:50:LEU:C	2.39	0.48
6:C:168:ARG:O	6:C:172:LYS:HB2	2.14	0.48
8:E:89:LEU:C	8:E:90:ARG:HG2	2.39	0.48
23:T:52:ASP:OD2	23:T:55:THR:HG23	2.14	0.48
25:V:194:THR:HG22	25:V:195:LEU:N	2.28	0.48
37:h:154:VAL:HG11	37:h:179:LEU:HD22	1.95	0.48
37:h:201:LEU:O	37:h:204:GLU:HG2	2.14	0.48
38:i:435:PHE:CD1	38:i:436:GLU:N	2.79	0.48
1:2:18:A:OP2	7:D:481:ARG:HD2	2.14	0.47
1:2:732:U:H2'	1:2:733:C:C6	2.49	0.47
1:2:793:C:OP1	13:J:312:ARG:HD2	2.14	0.47
1:2:1721:A:H2'	1:2:1721:A:N3	2.28	0.47
8:E:89:LEU:O	8:E:90:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:298:PRO:CD	17:N:301:LEU:HD12	2.44	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
8:E:16:LYS:HZ1	25:V:189:LEU:HD11	1.78	0.47
17:N:306:LYS:HD3	25:V:177:GLU:OE1	2.13	0.47
21:R:89:ILE:O	21:R:93:ASN:HB2	2.14	0.47
33:d:104:LYS:HB2	33:d:104:LYS:HE2	1.68	0.47
34:e:164:MET:O	34:e:168:LEU:HG	2.13	0.47
38:i:131:ILE:HD12	38:i:131:ILE:H	1.79	0.47
40:l:279:ARG:HD3	40:l:281:PHE:CE2	2.49	0.47
1:2:1123:A:H8	1:2:1123:A:OP2	1.97	0.47
6:C:178:LYS:O	6:C:182:LYS:HB3	2.14	0.47
6:C:221:ARG:HD3	34:e:250:GLU:OE2	2.14	0.47
7:D:186:THR:HG23	38:i:244:ARG:NH1	2.29	0.47
11:H:241:ILE:HA	38:i:295:MET:CE	2.44	0.47
37:h:221:ALA:HB2	37:h:244:PHE:CZ	2.49	0.47
38:i:129:LEU:HA	38:i:132:VAL:HG12	1.96	0.47
40:l:465:LEU:HD21	40: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
6:C:256:LEU:HD11	6:C:287:LEU:HD23	1.96	0.47
11:H:226:LYS:HB3	24:U:113:GLU:OE1	2.15	0.47
13:J:251:LYS:HE3	13:J:282:TYR:CZ	2.49	0.47
22:S:89:LYS:HB3	31:b:19:LEU:HD11	1.96	0.47
37:h:136:ARG:HG2	37:h:140:LEU:HD12	1.97	0.47
37:h:204:GLU:O	37:h:208:LEU:HD13	2.14	0.47
1:2:1700:U:H2'	1:2:1701:C:H6	1.79	0.47
7:D:150:SER:O	7:D:151:GLU:HB2	2.14	0.47
11:H:220:GLU:HG3	24:U:124:LEU:HD11	1.96	0.47
24:U:116:GLU:HA	24:U:119:LYS:HD3	1.97	0.47
37:h:173:LYS:HG3	37: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
7:D:129:LYS:O	7:D:133:LEU:HD13	2.14	0.47
24:U:81:PRO:HA	24:U:84:VAL:CG1	2.44	0.47
24:U:112:ALA:O	24:U:115:LYS:HE3	2.15	0.47
27:X:436:GLU:O	27:X:440:GLU:HG2	2.15	0.47
30:a:185:ARG:HA	30:a:185:ARG:HD3	1.64	0.47
37:h:349:ASP:O	37:h:353:VAL:HG23	2.14	0.47
1:2:158:A:H2'	1:2:158:A:N3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:6:1:U:H2'	2:6:1:U:O2	2.14	0.47
7:D:204:HIS:C	7:D:205:PHE:HD1	2.23	0.47
14:K:110:ARG:HD2	14:K:110:ARG:HA	1.74	0.47
16:M:140:PHE:HB3	16:M:142:MET:HE3	1.96	0.47
24:U:67:LYS:HG3	24:U:69:VAL:HG23	1.96	0.47
24:U:88:ARG:NH1	38:i:420:LEU:CD2	2.78	0.47
27:X:401:PRO:HG3	30:a:361:ARG:HG2	1.96	0.47
29:Z:55:GLU:HG3	29:Z:91:ARG:HG3	1.96	0.47
33:d:64:LEU:CD1	33:d:70:LEU:HD13	2.45	0.47
36:g:606:ASN:O	36:g:607:PHE:CD1	2.68	0.47
37:h:171:LEU:C	37:h:181:PRO:HB3	2.39	0.47
37:h:234:TRP:HA	37:h:237:LEU:CD1	2.19	0.47
38:i:353:ILE:HA	38:i:356:ILE:CG1	2.45	0.47
40:l:335:PRO:HD2	40:l:338:PHE:HD2	1.80	0.47
40:l:487:TYR:HB2	40:l:496:ALA:HB2	1.97	0.47
1:2:164:A:H2'	1:2:165:A:H8	1.68	0.47
5:B:204:THR:HG23	5:B:207:PHE:H	1.80	0.47
8:E:12:PRO:HD3	8:E:61:GLN:O	2.14	0.47
14:K:89:ASP:O	14:K:91:PRO:HD3	2.14	0.47
18:O:105:PRO:O	34:e:319:LYS:O	2.33	0.47
24:U:112:ALA:CA	24:U:115:LYS:HE3	2.44	0.47
38:i:107:ILE:HG21	38:i:169:VAL:HG13	1.95	0.47
38:i:281:LYS:HB2	38:i:281:LYS:HE3	1.56	0.47
1:2:275:U:H2'	1:2:276:U:C6	2.50	0.47
5:B:242:PHE:CD1	27:X:449:LYS:HD3	2.50	0.47
6:C:204:THR:HG22	7:D:116:GLU:HG2	1.97	0.47
7:D:439:TYR:CE2	7:D:488:LYS:HD3	2.50	0.47
38:i:126:GLY:O	38:i:129:LEU:HG	2.15	0.47
38:i:407:LEU:CD1	38:i:410:MET:HE2	2.44	0.47
38:i:408:LYS:O	38:i:412:GLN:HG3	2.14	0.47
1:2:1736:U:H5'	1:2:1737:A:O4'	2.15	0.47
2:6:2:U:H3'	2:6:3:U:C6	2.50	0.47
6:C:210:LEU:HD12	7:D:87:VAL:CG2	2.40	0.47
11:H:419:ALA:HB3	11:H:423:LYS:HD3	1.97	0.47
29:Z:68:HIS:CE1	29:Z:128:SER:HA	2.50	0.47
37:h:202:MET:HE1	37:h:236:LEU:HD13	1.97	0.47
40:l:379:ILE:HG21	40:l:409:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:763:A:H2'	1:2:764:A:H8	1.80	0.46
1:2:1385:A:H3'	1:2:1386:A:C8	2.49	0.46
6:C:257:LEU:CD1	7:D:194:MET:HE1	2.42	0.46
13:J:251:LYS:HD3	13:J:251:LYS:C	2.39	0.46
35:f:351:PHE:O	35:f:355:ILE:HG13	2.15	0.46
37:h:330:PHE:CG	37:h:375:VAL:HG11	2.49	0.46
38:i:99:GLU:CD	38:i:177:MET:HE3	2.40	0.46
38:i:222:GLU:HA	38:i:222:GLU:OE2	2.15	0.46
38:i:363:ASN:ND2	38:i:366:ALA:HB2	2.27	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
16:M:109:TYR:HB2	21:R:147:MET:HE2	1.96	0.46
24:U:115:LYS:HD2	24:U:116:GLU:N	2.30	0.46
34:e:304:LEU:HD12	34:e:304:LEU:HA	1.72	0.46
35:f:210:VAL:HG22	35:f:256:VAL:CG2	2.43	0.46
1:2:1110:C:H1'	1:2:1442:A:C4	2.49	0.46
6:C:254:ARG:O	6:C:258:LYS:HB2	2.14	0.46
8:E:5:ASP:OD1	8:E:68:THR:HG23	2.15	0.46
24:U:105:VAL:HA	24:U:108:MET:SD	2.56	0.46
34:e:149:HIS:CA	34:e:152:VAL:HG12	2.45	0.46
37:h:153:GLN:CA	37:h:156:LYS:HG2	2.42	0.46
37:h:342:LEU:HD21	37:h:387:ALA:CB	2.42	0.46
1:2:1091:A:OP2	4: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
6:C:236:GLY:O	6:C:240:VAL:HG23	2.15	0.46
7:D:208:ALA:HB1	7:D:210:GLU:OE2	2.15	0.46
25:V:162:LYS:HZ3	25:V:162:LYS:HB2	1.80	0.46
30:a:390:VAL:HG11	40:l:553:LEU:HA	1.97	0.46
34:e:367:VAL:O	34:e:370:MET:HB2	2.15	0.46
38:i:103:ARG:O	38:i:107:ILE:HG22	2.15	0.46
38:i:141:ARG:HA	38:i:141:ARG:CZ	2.45	0.46
40:l:529:TRP:CD1	40: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
3:8:231:LEU:HG	3:8:260:VAL:HA	1.98	0.46
7:D:138:GLU:CD	7:D:141:ARG:HD2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:412:LYS:HA	30:a:412:LYS:HD2	1.73	0.46
40:l:501:ASN:ND2	40:l:505:ARG:HH22	2.14	0.46
1:2:1733:C:H42	1:2:1737:A:N6	2.13	0.46
3:8:163:ARG:HB2	3:8:163:ARG:HH11	1.81	0.46
5:B:524:VAL:HG12	5:B:535:VAL:HB	1.98	0.46
35:f:144:MET:CE	35:f:212:MET:HE1	2.46	0.46
37:h:289:SER:HA	37:h:292:PHE:HB3	1.98	0.46
1:2:549:U:H2'	1:2:550:U:H6	1.81	0.46
6:C:175:LEU:HD22	6:C:199:PHE:HE1	1.81	0.46
17:N:379:VAL:HG12	17:N:383:LYS:HZ2	1.80	0.46
21:R:28:TYR:HA	21:R:106:VAL:HG11	1.97	0.46
24:U:27:LEU:O	24:U:31:GLU:HG3	2.16	0.46
26:W:286:ARG:HD2	26:W:286:ARG:HA	1.61	0.46
35:f:102:ALA:HB1	35: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
5:B:171:LYS:HG2	27:X:447:ARG:CZ	2.46	0.46
14:K:56:ARG:HE	14:K:56:ARG:HB2	1.56	0.46
21:R:141:PHE:O	21:R:164:THR:HG22	2.15	0.46
27:X:491:ARG:NH2	28:Y:30:LEU:O	2.48	0.46
35:f:202:LEU:HD22	35:f:313:LEU:CD2	2.46	0.46
38:i:322:MET:HA	38:i:325:LEU:CD1	2.45	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
11:H:318:ARG:HH21	11:H:366:THR:HG21	1.81	0.46
13:J:189:LEU:HD12	20:Q:248:GLU:HA	1.97	0.46
13:J:293:VAL:O	22:S:31:VAL:HG12	2.16	0.46
28:Y:14:VAL:HG11	30:a:327:HIS:HB3	1.98	0.46
36:g:602:MET:SD	36:g:603:THR:HB	2.56	0.46
37:h:116:CYS:C	37:h:117:ARG:HD2	2.41	0.46
37:h:252:ARG:O	37:h:255:THR:HG22	2.15	0.46
40:l:267:LYS:NZ	40:l:271:LEU:HD11	2.30	0.46
7:D:88:GLU:OE1	7:D:88:GLU:O	2.34	0.46
7:D:443:LYS:HD3	7:D:445:TYR:CE1	2.51	0.46
11:H:225:ILE:HA	11:H:228:PRO:CA	2.46	0.46
11:H:357:THR:HB	11:H:361:TRP:HE1	1.81	0.46
17:N:331:LYS:HB2	17:N:331:LYS:HZ3	1.81	0.46
37:h:152:ARG:HD2	37:h:153:GLN:NE2	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:303:LEU:HD23	6:C:303:LEU:C	2.42	0.45
10:G:104:THR:O	10:G:122:GLY:HA3	2.15	0.45
13:J:249:ARG:HG3	13:J:249:ARG:NH1	2.31	0.45
26:W:394:MET:HE3	26:W:394:MET:HB3	1.83	0.45
37:h:202:MET:O	37:h:206:MET:HE2	2.17	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
7:D:115:GLU:O	7:D:115:GLU:HG3	2.17	0.45
11:H:238:LYS:HE3	11:H:238:LYS:HB2	1.63	0.45
30:a:99:PRO:HA	30:a:102:ILE:HG22	1.99	0.45
34:e:245:LEU:HD23	34:e:252:PHE:CE2	2.51	0.45
38:i:310:GLU:OE2	38:i:310:GLU:N	2.39	0.45
40:l:510:PRO:HB2	40: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
37:h:361:ILE:CG2	37:h:362:PRO:CD	2.92	0.45
5:B:62:ILE:CD1	5:B:71:ILE:HG12	2.45	0.45
11:H:241:ILE:CA	38:i:295:MET:CE	2.94	0.45
27:X:343:LYS:HE3	27:X:343:LYS:HB3	1.84	0.45
35:f:174:GLU:O	35:f:177:ILE:HG22	2.16	0.45
35:f:290:VAL:O	35:f:294:GLY:HA2	2.15	0.45
35:f:300:LYS:NZ	35:f:300:LYS:HB2	2.32	0.45
40:l:268:THR:O	40:l:272:THR:HG22	2.16	0.45
40:l:503:MET:HB2	40: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
3:8:228:GLY:HA2	3:8:263:MET:HB3	1.99	0.45
4:A:95:ASN:OD1	4:A:122:LYS:HG2	2.16	0.45
13:J:249:ARG:HG3	13:J:249:ARG:HH11	1.82	0.45
36:g:553:LYS:HD3	36:g:553:LYS:HA	1.71	0.45
38:i:104:PHE:CE1	38:i:169:VAL:HG12	2.52	0.45
38:i:290:PRO:CA	38:i:293:VAL:HG22	2.40	0.45
38:i:322:MET:CA	38: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
3:8:234:SER:O	3:8:245:VAL:HG23	2.16	0.45
7:D:441:LYS:HA	7:D:441:LYS:HD2	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:10:PHE:HB2	8:E:63:GLN:HB2	1.99	0.45
8:E:48:LEU:HD12	8:E:59:HIS:O	2.17	0.45
29:Z:63:TRP:CD1	37:h:137:LEU:HD12	2.52	0.45
30:a:211:LYS:HD3	30:a:211:LYS:HA	1.79	0.45
35:f:286:MET:HE2	35:f:302:LEU:HG	1.99	0.45
38:i:147:VAL:HG12	38:i:147:VAL:O	2.17	0.45
40:l:556:ALA:O	40: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
1:2:1170: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
5:B:333:PHE:CE2	5:B:336:PHE:HE2	2.34	0.45
6:C:252:MET:CE	34:e:150:SER:HA	2.47	0.45
11:H:215:GLU:O	11:H:219:LYS:HB2	2.17	0.45
25:V:135:PHE:CE2	25:V:139:LEU:HD11	2.52	0.45
38:i:133:GLU:HA	38:i:136:VAL:HG12	1.98	0.45
38:i:207:ILE:HG23	38:i:211:LEU:HD23	1.99	0.45
40:l:269:TYR:HB3	40: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
19:P:15:LYS:HA	19:P:44:ASP:O	2.17	0.45
19:P:64:SER:OG	19:P:67:LYS:HB2	2.16	0.45
35:f:165:THR:HA	35:f:222:CYS:O	2.17	0.45
35:f:338:ILE:HG23	35:f:384:TYR:HD2	1.82	0.45
37:h:271:SER:O	37:h:275:VAL:HG22	2.17	0.45
40:l:269:TYR:O	40:l:273:LEU:HG	2.17	0.45
40:l:529:TRP:HE1	40:l:557:VAL:HB	1.82	0.45
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	36:g:579:ILE:HD12	1.82	0.45
1:2:1724:U:O2	1:2:1724:U:H2'	2.15	0.45
5:B:262:ALA:H	30:a:196:THR:HG21	1.81	0.45
6:C:183:LEU:HB3	7:D:71:ILE:HD12	1.99	0.45
11:H:230:ARG:HG3	11:H:230:ARG:NH1	2.24	0.45
30:a:124:SER:HB2	30:a:128:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:h:223:LEU:HD12	37: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
30:a:405:GLN:OE1	30:a:405:GLN:C	2.60	0.45
31:b:50:LYS:HE2	31:b:50:LYS:HA	1.99	0.45
37:h:190:LEU:HG	37: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
13:J:285:SER:HB2	31:b:46:LEU:HB2	1.99	0.44
29:Z:86:LEU:CD2	29:Z:90:GLY:HA2	2.48	0.44
35:f:277:ASP:HB3	38:i:121:LYS:HZ3	1.82	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
3:8:184:SER:HA	3:8:227:ILE:HD11	1.99	0.44
3:8:245:VAL:C	3:8:246:ILE:HD12	2.41	0.44
4:A:123:LEU:C	4:A:123:LEU:HD12	2.42	0.44
5:B:333:PHE:CE2	5:B:336:PHE:CE2	3.06	0.44
17:N:320:SER:OG	17:N:323:GLU:HG3	2.18	0.44
28:Y:77:LYS:HB2	28:Y:77:LYS:HE3	1.70	0.44
29:Z:87:TYR:HB2	29:Z:92:HIS:O	2.17	0.44
35:f:253:SER:HB3	38:i:283:TYR:OH	2.17	0.44
36:g:621:MET:HG2	36:g:653:MET:CE	2.45	0.44
37:h:122:ILE:HG21	37:h:158:CYS:SG	2.57	0.44
37:h:326:LEU:C	37: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
5:B:285:ILE:HA	5:B:288:ARG:HG3	2.00	0.44
6:C:252:MET:HE2	34:e:150:SER:CA	2.47	0.44
7:D:166:MET:O	7:D:170:LYS:HG3	2.17	0.44
7:D:322:LEU:HG	7:D:322:LEU:O	2.18	0.44
33:d:69:LYS:HD2	33:d:69:LYS:HA	1.85	0.44
37:h:210:LYS:HD3	37:h:243:LYS:NZ	2.31	0.44
37:h:228:CYS:HA	37:h:231:THR:HG1	1.81	0.44
38:i:317:LYS:HE2	38:i:344:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:360:ARG:HG3	38:i:367:TYR:CE2	2.53	0.44
38:i:395:ALA:HA	38:i:428:MET:SD	2.57	0.44
40:l:517:LYS:HD3	40: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
5:B:447:GLN:HB3	30:a:155:ASP:HA	2.00	0.44
7:D:109:ASP:C	7:D:111:GLU:H	2.25	0.44
7:D:464:MET:HE2	7:D:464:MET:HB3	1.82	0.44
29:Z:91:ARG:HG2	29: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
1:2:1173:U:O2	1:2:1173:U:H2'	2.16	0.44
1:2:1413:A:H2'	1:2:1414:C:C6	2.52	0.44
5:B:309:ARG:HA	5:B:309:ARG:HD3	1.74	0.44
13:J:199:LYS:HB3	13:J:199:LYS:HE3	1.49	0.44
29:Z:101:LYS:O	29:Z:102:ASP:OD1	2.34	0.44
40:l:410:PHE:HE1	40: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
9:F:132:LEU:HD12	9:F:132:LEU:O	2.18	0.44
21:R:154:LEU:HD11	21:R:169:TYR:CG	2.52	0.44
25:V:141:LYS:HE2	25:V:141:LYS:CA	2.47	0.44
30:a:380:LYS:HE3	30:a:380:LYS:HB3	1.68	0.44
33:d:110:ILE:HG23	33:d:111:LYS:N	2.33	0.44
37:h:258:VAL:HA	37:h:261:GLU:HG2	1.99	0.44
38:i:303:GLU:CB	38:i:309:ARG:HH21	2.25	0.44
40:l:547:ASN:C	40: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
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
5:B:263:PRO:HB3	30:a:200:GLU:OE1	2.17	0.44
13:J:246:ILE:O	13:J:250:VAL:HG23	2.17	0.44
20:Q:189:GLU:CG	22:S:50:SER:HB3	2.47	0.44
21:R:206:LYS:NZ	21:R:208:HIS:CE1	2.85	0.44
27:X:401:PRO:HD2	30:a:365:LEU:HD22	2.00	0.44
29:Z:65:ILE:HD11	37:h:143:HIS:CG	2.52	0.44
35:f:318:GLN:O	35:f:322:GLU:HB2	2.17	0.44
37:h:85:ALA:HB2	37:h:115:ASN:HD21	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:134:LYS:HZ2	38:i:163:TRP:HH2	1.66	0.44
1:2:389:G:O2'	1:2:390:A:H5'	2.16	0.44
1:2:439:A:H2'	1:2:441:U:C6	2.53	0.44
1:2:440:A:H2	5:B:50:ARG:HB3	1.83	0.44
1:2:1740:C:OP2	1:2:1740:C:H6	1.99	0.44
25:V:141:LYS:HD3	25:V:141:LYS:HA	1.90	0.44
35:f:280:GLU:HA	35:f:283:ILE:HG22	1.99	0.44
38:i:141:ARG:HA	38:i:141:ARG:HH11	1.81	0.44
40:l:519:ILE:CG2	40: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
3:8:166:ILE:HG23	3:8:196:ARG:O	2.18	0.44
5:B:408:GLY:O	5:B:409:ILE:HB	2.18	0.44
8:E:47:GLU:OE1	8:E:61:GLN:HG3	2.18	0.44
13:J:310:ARG:HD2	13:J:311:LYS:O	2.17	0.44
18:O:60:LYS:HG2	25:V:84:TYR:CD1	2.53	0.44
21:R:206:LYS:HE2	21:R:206:LYS:HB2	1.48	0.44
35:f:388:ALA:HB3	35:f:397:GLU:OE1	2.17	0.44
38:i:214:GLU:O	38:i:218:LYS:HG2	2.18	0.44
38:i:349:ARG:O	38:i:349:ARG:HD3	2.18	0.44
40:l:340:ALA:HB1	40:l:374:PRO:HG3	2.00	0.44
40:l:519:ILE:HG23	40: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
7:D:517:LEU:HD21	34:e:271:LYS:HD3	1.99	0.43
13:J:285:SER:H	31:b:46:LEU:HD23	1.82	0.43
21:R:24:GLY:HA2	21:R:27:ARG:HE	1.82	0.43
37:h:171:LEU:HD12	37:h:208:LEU:HD23	1.99	0.43
38:i:109:ARG:C	38:i:109:ARG:CD	2.91	0.43
39:k:41:GLY:O	39:k:44:SER:N	2.50	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
1:2:1802:A:H1'	1:2:1803:G:P	2.58	0.43
4:A:200:GLN:HG3	4:A:205:ILE:HD12	2.00	0.43
5:B:494:LYS:HD3	5:B:494:LYS:HA	1.82	0.43
7:D:223:VAL:O	7:D:223:VAL:CG1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:59:PHE:HA	24:U:62:LYS:HG2	2.00	0.43
24:U:92:LEU:HB3	24:U:97:ILE:HG21	1.99	0.43
35:f:42:GLN:HG2	35:f:58:ARG:HB2	1.99	0.43
36:g:548:ASN:O	36:g:554:ILE:HD12	2.18	0.43
37:h:94:LEU:O	37:h:98:ASN:HB2	2.18	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
4:A:16:SER:HB2	4:A:178:ALA:HB1	2.00	0.43
4:A:61:ALA:HB2	4:A:196:PHE:CE1	2.53	0.43
5:B:383:PHE:HD1	5:B:389:ILE:HG12	1.83	0.43
13:J:245:ASN:OD1	13:J:245:ASN:C	2.61	0.43
21:R:32:LYS:HE2	21:R:76:PHE:HB3	2.00	0.43
35:f:175:VAL:HG23	35:f:312:SER:HB3	2.00	0.43
37:h:234:TRP:CG	37:h:237:LEU:HD12	2.53	0.43
38:i:243:ILE:HG12	38:i:247:GLU:OE2	2.19	0.43
38:i:417:PRO:HB3	38:i:421:THR:HG22	1.97	0.43
40:l:241:PHE:CD2	40:l:246:LYS:HB2	2.53	0.43
40:l:423:LEU:HD21	40: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"	10:G:30:SER:HB3	2.01	0.43
1:2:1722:C:O2	1:2:1722:C:H2'	2.18	0.43
5:B:171:LYS:HE3	27:X:447:ARG:NH2	2.33	0.43
8:E:33:LYS:HA	8:E:33:LYS:HD3	1.63	0.43
9:F:98:LYS:O	9:F:101:ILE:HG22	2.19	0.43
28:Y:29:MET:HE2	28:Y:29:MET:HB2	1.83	0.43
33:d:107:ALA:C	33:d:109:ALA:H	2.25	0.43
37:h:312:GLN:O	37: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
3:8:231:LEU:HD22	3:8:255:PRO:HB3	1.99	0.43
5:B:290:ALA:O	5:B:294:GLU:HG2	2.19	0.43
6:C:239:LYS:HD2	7:D:211:TYR:CE2	2.54	0.43
10:G:87:GLU:OE1	10:G:87:GLU:HA	2.19	0.43
25:V:183:LYS:O	25:V:187:GLU:HG3	2.17	0.43
26:W:189:ARG:HB3	26:W:189:ARG:HH11	1.84	0.43
30:a:110:LEU:HA	30:a:110:LEU:HD23	1.73	0.43
35:f:185:ALA:O	35:f:189:LEU:HB2	2.17	0.43
38:i:123:MET:O	38:i:127:MET:SD	2.77	0.43
38:i:360:ARG:HA	38:i:367:TYR:HB2	2.00	0.43
38:i:380:PHE:CD2	38:i:382:ALA:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:991:A:H2'	1:2:992:U:H6	1.79	0.43
1:2:1090:U:OP2	4:A:120:HIS:CD2	2.71	0.43
6:C:161:ILE:HD12	6:C:161:ILE:HA	1.81	0.43
11:H:242:THR:O	11:H:246:LEU:HB2	2.18	0.43
30:a:130:PHE:CE1	30:a:132:ASP:HB3	2.53	0.43
37:h:142:ILE:HG23	37:h:142:ILE:O	2.17	0.43
37:h:339:VAL:HA	37: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
3:8:188:LEU:HD23	3:8:227:ILE:HG12	2.01	0.43
3:8:255:PRO:O	3:8:256:LYS:HB3	2.18	0.43
5:B:314:ILE:H	5:B:314:ILE:HD12	1.84	0.43
5:B:465:ARG:HB2	5:B:469:SER:OG	2.17	0.43
19:P:13:MET:HB2	19:P:16:SER:HB2	2.00	0.43
29:Z:62:ASN:OD1	37:h:144:ASP:HA	2.19	0.43
29:Z:122:LYS:HE2	29:Z:124:ILE:CD1	2.48	0.43
35:f:327:THR:OG1	35:f:330:GLN:HG3	2.18	0.43
37:h:195:GLU:OE2	37:h:195:GLU:C	2.62	0.43
38:i:104:PHE:CE2	38:i:135:VAL:HG21	2.54	0.43
40:l:229:LEU:H	40:l:229:LEU:HD12	1.84	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
5:B:303:LEU:HD23	5:B:303:LEU:HA	1.92	0.43
13:J:191:THR:HG22	20:Q:246:GLU:OE1	2.18	0.43
14:K:8:ILE:HD11	19:P:32:ARG:HB2	2.00	0.43
30:a:150:ASP:OD1	30:a:152:GLU:HG2	2.19	0.43
35:f:389:THR:HG22	35:f:397:GLU:HG3	2.00	0.43
38:i:390:LEU:HB3	38: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
5:B:145:GLU:H	5:B:145:GLU:CD	2.26	0.43
7:D:338:ARG:O	7:D:342:GLU:HG2	2.18	0.43
14:K:39:THR:HA	14:K:50:ARG:O	2.19	0.43
19:P:82:SER:HB3	19:P:85:ALA:CB	2.48	0.43
24:U:53:ASP:N	24:U:54:PRO:HD2	2.34	0.43
25:V:127:GLU:OE1	25:V:127:GLU:O	2.37	0.43
35:f:160:MET:HG2	35:f:161:PHE:CE2	2.54	0.43
35:f:314:LYS:HD2	35:f:376:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:h:122:ILE:HD11	37:h:161:VAL:CG2	2.46	0.43
40:l:317:ALA:HB2	40: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
5:B:287:SER:N	5:B:321:ARG:HH12	2.17	0.43
5:B:383:PHE:CD1	5:B:389:ILE:HG12	2.54	0.43
6:C:55:ARG:HA	6:C:55:ARG:HD2	1.74	0.43
7:D:258:GLY:O	7:D:355:LEU:HD22	2.19	0.43
20:Q:227:MET:CE	22:S:52:MET:HG2	2.32	0.43
34:e:312:LEU:HA	34:e:315:LYS:HB2	2.01	0.43
38:i:116:TYR:HB3	38:i:119:CYS:SG	2.59	0.43
38:i:127:MET:O	38: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	6: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
6:C:254:ARG:NH2	38:i:226:ASP:HA	2.34	0.42
10:G:105:THR:HB	10:G:120:VAL:HG22	2.00	0.42
11:H:224:VAL:C	11:H:225:ILE:HG13	2.43	0.42
11:H:224:VAL:O	11:H:225:ILE:CB	2.66	0.42
12:I:177:GLU:HG2	12:I:179:PHE:CE1	2.54	0.42
24:U:59:PHE:CD1	24:U:85:TYR:CD2	3.06	0.42
1:2:479:G:OP1	33: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
4:A:157:VAL:HG22	4:A:174:TYR:HB2	2.01	0.42
6:C:182:LYS:HE3	6:C:220:LEU:HD22	2.00	0.42
13:J:279:ARG:NH1	13:J:290:ASN:HB2	2.34	0.42
19:P:13:MET:CB	19:P:16:SER:HB2	2.48	0.42
20:Q:181:ARG:NH2	20:Q:234:PHE:HE2	2.16	0.42
33:d:42:ILE:N	33:d:43:PRO:HD2	2.33	0.42
37:h:82:PRO:HB2	37:h:87:LYS:CG	2.49	0.42
37:h:199:SER:HB2	37:h:231:THR:HB	2.01	0.42
40:l:202:ALA:HA	40:l:240:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:334:PRO:O	12:I:202:PHE:CZ	2.73	0.42
7:D:180:THR:HG21	7:D:193:TRP:CE2	2.54	0.42
9:F:91:TRP:HH2	9:F:132:LEU:HD23	1.85	0.42
14:K:31:LEU:HD11	14:K:102:LYS:HD2	2.00	0.42
29:Z:87:TYR:CE2	29: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
3:8:178:LYS:O	3:8:181:LYS:HB3	2.19	0.42
4:A:73:ASN:HB3	4:A:76:PHE:CD2	2.54	0.42
5:B:478:ILE:HD13	5:B:478:ILE:HA	1.87	0.42
6:C:285:SER:HA	6:C:288:SER:OG	2.20	0.42
11:H:321:ILE:HG22	11:H:363:ILE:HG12	2.01	0.42
21:R:132:MET:HE3	21:R:134:ARG:HB2	2.00	0.42
35:f:160:MET:HE2	35:f:160:MET:HB2	1.91	0.42
37:h:316:GLN:OE1	37:h:316:GLN:CA	2.67	0.42
38:i:120:ASP:O	38:i:124:ILE:HG13	2.20	0.42
38:i:127:MET:C	38:i:131:ILE:HD12	2.43	0.42
38:i:179:LYS:CE	38:i:183:LYS:HE3	2.47	0.42
38:i:407:LEU:O	38:i:410:MET:HE3	2.18	0.42
40:l:455:GLY:O	40:l:457:MET:HE2	2.19	0.42
40:l:501:ASN:ND2	40:l:505:ARG:HH12	2.18	0.42
1:2:611:G:O2'	1:2:612:U:H5'	2.18	0.42
7:D:445:TYR:CE1	7:D:478:ILE:HD12	2.54	0.42
10:G:12:THR:HG22	10:G:24:VAL:HG21	2.02	0.42
14:K:79:GLN:O	14:K:103:ASP:HB2	2.19	0.42
22:S:86:PHE:C	22:S:88:ARG:N	2.75	0.42
25:V:128:ARG:NE	25:V:132:GLN:HG3	2.35	0.42
37:h:109:LEU:HD12	37:h:109:LEU:O	2.19	0.42
37:h:113:ILE:HD11	37:h:153:GLN:C	2.44	0.42
38:i:387:TYR:CE2	38:i:410:MET:HA	2.53	0.42
40:l:279:ARG:HD3	40: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
5:B:487:ILE:HG12	5:B:537:VAL:HG22	2.00	0.42
6:C:21:THR:HG21	6:C:77:LEU:CD1	2.34	0.42
25:V:160:LYS:HE3	25:V:160:LYS:HB3	1.79	0.42
29:Z:53:LEU:HB3	29:Z:116:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:e:319:LYS:C	34:e:321:HIS:H	2.28	0.42
35:f:67:ALA:HB3	35:f:68:PRO:HD3	2.02	0.42
37:h:221:ALA:HB2	37:h:244:PHE:CE1	2.55	0.42
38:i:376:ASP:OD1	38:i:376:ASP:N	2.45	0.42
4:A:4:HIS:O	4:A:8:ILE:HG12	2.20	0.42
4:A:166:LEU:O	4:A:170:GLU:HG2	2.20	0.42
22:S:96:LYS:HG3	39:k:26:MET:CE	2.49	0.42
25:V:172:SER:HA	25:V:175:TRP:CD2	2.55	0.42
27:X:323:GLU:HG2	27:X:324:GLU:N	2.34	0.42
40:l:305:GLY:O	40:l:308:ILE:HG22	2.19	0.42
40:l:308:ILE:CG2	40:l:338:PHE:HB3	2.48	0.42
40:l:492:GLU:CD	40:l:495:GLU:H	2.28	0.42
1:2:154:G:H1'	37:h:174:HIS:HB2	2.01	0.42
1:2:1782:G:H2'	1:2:1783:G:O5'	2.20	0.42
7:D:362:VAL:HG12	7:D:386:MET:HE3	2.01	0.42
10:G:106:PRO:HD2	10:G:120:VAL:CG2	2.49	0.42
25:V:126:GLU:HA	25:V:126:GLU:OE2	2.19	0.42
26:W:416:LEU:HB2	26:W:419:VAL:HG11	2.02	0.42
27:X:505:ASP:HA	27:X:508:TYR:CE2	2.55	0.42
37:h:296:LYS:HA	37:h:337:TRP:CZ2	2.55	0.42
38:i:436:GLU:O	38:i:440:GLU:HG3	2.19	0.42
1:2:1380:U:H5'	21:R:70:ARG:HH22	1.85	0.42
1:2:1785:G:H2'	1:2:1786:U:C6	2.54	0.42
6:C:325:THR:N	6:C:326:PRO:HA	2.33	0.42
26:W:192:ASP:OD1	26:W:192:ASP:O	2.38	0.42
29:Z:58:GLN:HA	29:Z:63:TRP:CZ3	2.55	0.42
33:d:46:LEU:HD11	33:d:60:LEU:HD12	2.01	0.42
36:g:616:VAL:O	36:g:620:MET:HG2	2.20	0.42
1:2:1685:G:N3	1:2:1685:G:H2'	2.34	0.42
3:8:262:LEU:HD12	3:8:264:LYS:H	1.85	0.42
7:D:517:LEU:CD2	34:e:271:LYS:HD3	2.50	0.42
10:G:9:ALA:HB1	10:G:26:LEU:HD13	2.01	0.42
17:N:298:PRO:CG	17:N:301:LEU:HD12	2.49	0.42
25:V:178:PRO:HG2	25:V:179:LYS:CE	2.47	0.42
37:h:171:LEU:CA	37:h:181:PRO:HB3	2.47	0.42
37:h:229:HIS:HD2	37:h:258:VAL:HG13	1.79	0.42
37:h:338:PRO:O	37:h:341:VAL:HG22	2.20	0.42
38:i:161:ASP:N	38:i:161:ASP:OD1	2.52	0.42
38:i:366:ALA:HA	38: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:6:1:U:H3'	2:6:2:U:C5	2.55	0.41
6:C:248:GLU:HG3	6:C:251:ARG:HH21	1.85	0.41
24:U:67:LYS:CG	24:U:69:VAL:HG23	2.50	0.41
35:f:286:MET:CE	35:f:302:LEU:HG	2.50	0.41
37:h:258:VAL:O	37:h:262:PHE:HB2	2.20	0.41
37:h:275:VAL:HG23	37:h:276:ASP:N	2.35	0.41
37:h:279:ARG:HH12	37:h:290:ALA:HB2	1.85	0.41
38:i:375:LEU:CD1	38:i:387:TYR:HE1	2.24	0.41
40:l:547:ASN:HD22	40:l:547:ASN:N	2.18	0.41
1:2:153:A:H3'	1:2:153:A:N3	2.35	0.41
1:2:440:A:H62	1:2:442:U:C1'	2.33	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
11:H:246:LEU:HD12	11:H:246:LEU:HA	1.91	0.41
11:H:427:TRP:CZ3	11:H:429:LYS:HA	2.55	0.41
22:S:64:ILE:HD12	22:S:64:ILE:N	2.35	0.41
24:U:88:ARG:HD3	24:U:91:GLU:OE1	2.20	0.41
25:V:62:ALA:HB1	33:d:102:LEU:HD23	2.02	0.41
29:Z:84:ILE:HD11	37:h:137:LEU:HD13	2.02	0.41
35:f:57:ASP:O	35:f:59:PRO:HD3	2.19	0.41
37:h:299:LEU:HG	37:h:360:ASP:OD2	2.20	0.41
38:i:205:ILE:HD13	38:i:205:ILE:HA	1.84	0.41
38:i:345:LEU:O	38:i:346:GLU:HB2	2.19	0.41
38:i:375:LEU:HD23	38: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	31:b:14:ARG:HH21	2.43	0.41
1:2:1686:U:H2'	1:2:1687:U:O4'	2.21	0.41
12:I:170:HIS:ND1	12:I:171:VAL:HG22	2.36	0.41
17:N:298:PRO:HG2	17:N:301:LEU:HG	2.01	0.41
20:Q:234:PHE:CZ	25:V:195:LEU:HD13	2.54	0.41
22:S:80:LYS:HB3	22:S:80:LYS:HE2	1.62	0.41
27:X:472:ARG:HG2	27:X:472:ARG:HH11	1.84	0.41
38:i:179:LYS:HE2	38: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:188:LEU:HD23	3:8:227:ILE:HG23	2.02	0.41
3:8:232:VAL:HA	3:8:247:VAL:HG12	2.02	0.41
6:C:174:ILE:HA	6:C:178:LYS:HG2	2.02	0.41
6:C:313:GLU:OE2	34:e:253:VAL:HB	2.21	0.41
10:G:29:ILE:HA	10:G:33:MET:CE	2.50	0.41
15:L:67:LEU:HD22	15:L:84:ASP:HB3	2.02	0.41
21:R:63:MET:HB3	21:R:72:ARG:HD3	2.02	0.41
31:b:60:LEU:HA	31:b:63:VAL:HG12	2.02	0.41
35:f:78:GLU:O	35:f:82:GLU:HG2	2.20	0.41
37:h:130:GLN:HG3	37:h:131:ASN:N	2.35	0.41
37:h:151:CYS:HA	37:h:154:VAL:CG1	2.51	0.41
37:h:361:ILE:HG21	37:h:382:LEU:HD21	2.02	0.41
38:i:127:MET:SD	38: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'	40: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
5:B:152:LYS:HD3	5:B:152:LYS:HA	1.88	0.41
13:J:261:LYS:HE2	13:J:296:GLU:OE1	2.20	0.41
17:N:314:PHE:CE2	25:V:165:LYS:HE3	2.55	0.41
24:U:78:ILE:O	24:U:78:ILE:HG13	2.20	0.41
26:W:472:MET:HE3	26:W:472:MET:HB2	1.84	0.41
29:Z:119:ARG:HG2	29:Z:119:ARG:HH11	1.85	0.41
33:d:45:PHE:O	33:d:49:ILE:HG13	2.19	0.41
33:d:104:LYS:CG	33:d:105:PRO:HD2	2.49	0.41
37:h:82:PRO:HB2	37:h:87:LYS:HG2	2.01	0.41
38:i:125:ASP:O	38:i:129:LEU:HD23	2.21	0.41
38:i:309:ARG:HA	38:i:309:ARG:HD3	1.80	0.41
40:l:369:ARG:O	40:l:403:PRO:HB3	2.21	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
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
9:F:108:GLU:H	9:F:108:GLU:CD	2.25	0.41
21:R:132:MET:CE	21:R:134:ARG:HB2	2.51	0.41
35:f:230:VAL:HG22	35:f:252:TYR:HB3	2.02	0.41
38:i:290:PRO:C	38:i:293:VAL:HG22	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:442:VAL:H	40:l:442:VAL:HG22	1.64	0.41
1:2:144:U:C2	1:2:145:U:C5	3.09	0.41
1:2:1067:U:OP1	4:A:151:LYS:HE2	2.21	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
4:A:138:ASP:OD2	4:A:141:ARG:HA	2.20	0.41
5:B:199:ASP:HA	5:B:202:LYS:HE3	2.02	0.41
5:B:463:LYS:HA	5:B:463:LYS:HD3	1.83	0.41
6:C:160:ILE:HG13	6:C:161:ILE:N	2.35	0.41
7:D:498:GLU:HG2	7:D:503:VAL:CG2	2.50	0.41
15:L:77:LEU:HD22	15:L:81:GLU:HB3	2.03	0.41
20:Q:234:PHE:CE2	25:V:195:LEU:HD13	2.55	0.41
29:Z:60:LEU:HD23	29:Z:60:LEU:HA	1.91	0.41
30:a:394:LEU:HD23	30:a:394:LEU:HA	1.87	0.41
35:f:83:ASN:HB3	35:f:86:ILE:HD12	2.02	0.41
36:g:537:PRO:HG2	36:g:542:TYR:CZ	2.55	0.41
37:h:149:ASN:O	37:h:152:ARG:HB3	2.21	0.41
37:h:224:VAL:CG1	37:h:225:PHE:N	2.83	0.41
38:i:182:LYS:HA	38:i:182:LYS:HD2	1.71	0.41
38:i:317:LYS:CE	38:i:344:LEU:HD11	2.50	0.41
40:l:398:MET:SD	40: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
3:8:194:GLY:HA2	3:8:252:PHE:CZ	2.55	0.41
4:A:50:LEU:HD23	4:A:50:LEU:O	2.21	0.41
6:C:250:LYS:HD2	6:C:250:LYS:HA	1.71	0.41
17:N:314:PHE:CZ	25:V:168:LEU:HD23	2.56	0.41
19:P:77:LYS:HE3	19:P:77:LYS:HB3	1.66	0.41
21:R:207:LYS:H	21:R:207:LYS:HG2	1.78	0.41
24:U:45:LEU:HD12	24:U:45:LEU:HA	1.83	0.41
30:a:153:LEU:HD23	30:a:153:LEU:HA	1.85	0.41
35:f:185:ALA:HA	35:f:188:TYR:CZ	2.55	0.41
37:h:85:ALA:HB3	37:h:115:ASN:ND2	2.26	0.41
37:h:122:ILE:HD13	37:h:158:CYS:SG	2.60	0.41
37:h:251:LEU:HB2	37:h:256:PHE:CE2	2.55	0.41
38:i:384:ILE:HG22	38:i:415:ILE:HG21	2.02	0.41
40:l:208:MET:N	40:l:208:MET:SD	2.94	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:2:1344: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
3:8:196:ARG:CD	3:8:248:ARG:HH22	2.34	0.41
4:A:186:TYR:CG	11:H:264:LEU:HD13	2.56	0.41
5:B:145:GLU:HG2	5:B:146:ILE:N	2.36	0.41
7:D:172:GLN:O	7:D:175:LYS:HB2	2.21	0.41
9:F:143:ALA:C	9:F:145:PHE:H	2.29	0.41
11:H:241:ILE:N	38:i:295:MET:CE	2.83	0.41
20:Q:226:THR:O	20:Q:226:THR:CG2	2.68	0.41
20:Q:248:GLU:OE2	20:Q:250:ILE:HB	2.20	0.41
27:X:326:ALA:HA	27:X:329:GLU:HB2	2.02	0.41
29:Z:118:LYS:O	29:Z:121:TRP:HD1	2.03	0.41
34:e:149:HIS:O	34:e:152:VAL:HG12	2.20	0.41
34:e:273:MET:HA	34:e:273:MET:HE3	2.02	0.41
34:e:319:LYS:O	34:e:320:CYS:HB2	2.21	0.41
34:e:384:LEU:C	34:e:384:LEU:HD12	2.46	0.41
38:i:134:LYS:HZ3	38:i:138:GLU:HB2	1.86	0.41
40:l:240:LEU:HD12	40:l:240:LEU:HA	1.92	0.41
40:l:307:ILE:HD13	40:l:310:TRP:CZ3	2.56	0.41
40:l:374:PRO:O	40: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
1:2:1844:A:P	1:2:1845:A:H5"	2.61	0.41
6:C:63:LEU:HD11	7:D:363:HIS:NE2	2.36	0.41
6:C:256:LEU:HD23	6:C:257:LEU:HD22	2.03	0.41
17:N:376:ILE:HD13	17:N:376:ILE:HA	1.85	0.41
18:O:101:ARG:HA	18:O:102:PRO:HD3	1.98	0.41
34:e:149:HIS:C	34:e:152:VAL:HG12	2.46	0.41
37:h:164:ILE:H	37:h:164:ILE:HG12	1.65	0.41
40:l:410:PHE:HZ	40: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	14: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
7:D:181:LEU:HD13	7:D:193:TRP:HB3	2.01	0.40
11:H:327:LYS:HE2	11:H:327:LYS:HB3	1.80	0.40
30:a:153:LEU:O	30:a:154:GLU:HB2	2.21	0.40
31:b:48:ASN:OD1	31:b:50:LYS:HG2	2.21	0.40
35:f:157:ILE:N	35:f:158:PRO:CD	2.84	0.40
35:f:189:LEU:O	35:f:192:LEU:HD12	2.21	0.40
36:g:567:LEU:HB2	36:g:568:PRO:HD3	2.03	0.40
37:h:201:LEU:HD23	37:h:201:LEU:C	2.45	0.40
37:h:288:LEU:HB2	37:h:318:TYR:CE2	2.51	0.40
37:h:299:LEU:HB3	37:h:337:TRP:CH2	2.49	0.40
38:i:290:PRO:O	38:i:293:VAL:HG22	2.20	0.40
38:i:375:LEU:HG	38: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	31:b:76:TRP:CH2	3.13	0.40
1:2:1675:C:H2'	1:2:1676:U:O4'	2.21	0.40
2:6:3:U:H2'	2:6:4:U:C5'	2.51	0.40
5:B:191:ILE:HG12	30:a:192:ILE:HD13	2.03	0.40
6:C:182:LYS:C	6:C:184:LEU:H	2.29	0.40
7:D:78:ARG:HB3	7:D:78:ARG:CZ	2.51	0.40
13:J:195:ILE:HD12	13:J:211:ASP:O	2.20	0.40
37:h:206:MET:HA	37:h:209:LEU:HB3	2.03	0.40
37:h:272:LEU:O	37:h:275:VAL:HG22	2.22	0.40
38:i:134:LYS:NZ	38:i:163:TRP:HH2	2.20	0.40
40:l:392:LYS:HD2	40:l:396:LEU:HG	2.04	0.40
1:2:440:A:H62	1:2:442:U:H1'	1.86	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	37:h:110:TRP:HH2	2.05	0.40
7:D:109:ASP:O	7:D:110:ASP:CG	2.64	0.40
18:O:83:LEU:HD23	18:O:83:LEU:HA	1.92	0.40
25:V:184:LYS:HB3	25:V:184:LYS:HE2	1.79	0.40
30:a:385:ILE:C	30:a:385:ILE:HD12	2.45	0.40
35:f:147:VAL:HG13	35:f:149:MET:HE3	2.03	0.40
35:f:164:ALA:O	35:f:221:PHE:HA	2.21	0.40
35:f:273:TYR:O	35:f:276:LEU:HG	2.21	0.40
1:2:65:G:H2'	1:2:66:C:H6	1.85	0.40
1:2:1172:U:H2'	1:2:1173:U:O4'	2.21	0.40
1:2:1312:A:H2'	1:2:1313:A:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:163:ARG:HD3	3:8:252:PHE:CE2	2.55	0.40
5:B:307:LYS:HD3	5:B:307:LYS:HA	1.88	0.40
6:C:312:ILE:HD13	6:C:312:ILE:HA	1.91	0.40
7:D:134:LYS:HD2	7:D:134:LYS:HA	1.94	0.40
7:D:364:VAL:HG22	7:D:386:MET:SD	2.61	0.40
21:R:25:SER:HA	21:R:28:TYR:OH	2.21	0.40
22:S:86:PHE:O	22:S:87:ALA:C	2.63	0.40
22:S:93:ILE:HD11	31:b:19:LEU:HD12	1.98	0.40
35:f:170:LEU:HD22	35:f:212:MET:HE3	2.03	0.40
38:i:363:ASN:HB3	38:i:366:ALA:CB	2.36	0.40
40:l:563:GLU:HA	40: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
1:2:1052:U:O2'	12: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
5:B:282:GLN:CD	5:B:282:GLN:H	2.30	0.40
7:D:170:LYS:HD3	7:D:204:HIS:ND1	2.37	0.40
26:W:204:LYS:HD3	26:W:205:PRO:HD2	2.04	0.40
37:h:264:ALA:O	37:h:341:VAL:HG12	2.21	0.40
38:i:352:TRP:O	38:i:356:ILE:HG13	2.22	0.40
40:l:256:LYS:HA	40:l:259:GLU:HB2	2.03	0.40
40:l:360:LEU:HD12	40:l:361:GLY:N	2.36	0.40
40:l:470:LYS:HB2	40: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
3	8	107/520 (21%)	83 (78%)	21 (20%)	3 (3%)	4 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	202/212 (95%)	191 (95%)	11 (5%)	0	100	100
5	B	457/554 (82%)	427 (93%)	28 (6%)	2 (0%)	30	39
6	C	329/362 (91%)	323 (98%)	6 (2%)	0	100	100
7	D	409/501 (82%)	392 (96%)	17 (4%)	0	100	100
8	E	99/138 (72%)	97 (98%)	2 (2%)	0	100	100
9	F	146/157 (93%)	141 (97%)	5 (3%)	0	100	100
10	G	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
11	H	208/383 (54%)	200 (96%)	7 (3%)	1 (0%)	24	34
12	I	111/228 (49%)	107 (96%)	4 (4%)	0	100	100
13	J	125/304 (41%)	118 (94%)	7 (6%)	0	100	100
14	K	122/125 (98%)	116 (95%)	6 (5%)	0	100	100
15	L	108/154 (70%)	105 (97%)	3 (3%)	0	100	100
16	M	99/155 (64%)	98 (99%)	1 (1%)	0	100	100
17	N	114/414 (28%)	114 (100%)	0	0	100	100
18	O	108/136 (79%)	108 (100%)	0	0	100	100
19	P	89/110 (81%)	89 (100%)	0	0	100	100
20	Q	88/237 (37%)	88 (100%)	0	0	100	100
21	R	162/212 (76%)	153 (94%)	9 (6%)	0	100	100
22	S	73/100 (73%)	71 (97%)	2 (3%)	0	100	100
23	T	48/94 (51%)	45 (94%)	3 (6%)	0	100	100
24	U	125/192 (65%)	122 (98%)	3 (2%)	0	100	100
25	V	162/193 (84%)	158 (98%)	3 (2%)	1 (1%)	21	29
26	W	376/483 (78%)	374 (100%)	2 (0%)	0	100	100
27	X	202/496 (41%)	200 (99%)	1 (0%)	1 (0%)	24	34
28	Y	96/102 (94%)	96 (100%)	0	0	100	100
29	Z	78/153 (51%)	74 (95%)	4 (5%)	0	100	100
30	a	311/424 (73%)	303 (97%)	8 (3%)	0	100	100
31	b	75/80 (94%)	63 (84%)	12 (16%)	0	100	100
32	c	24/128 (19%)	23 (96%)	1 (4%)	0	100	100
33	d	76/110 (69%)	74 (97%)	1 (1%)	1 (1%)	9	12
34	e	244/383 (64%)	240 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	f	375/410 (92%)	362 (96%)	13 (4%)	0	100 100
36	g	121/668 (18%)	113 (93%)	8 (7%)	0	100 100
37	h	308/384 (80%)	299 (97%)	9 (3%)	0	100 100
38	i	334/725 (46%)	324 (97%)	10 (3%)	0	100 100
39	k	43/153 (28%)	32 (74%)	8 (19%)	3 (7%)	1 0
40	l	376/576 (65%)	369 (98%)	7 (2%)	0	100 100
All	All	6656/10885 (61%)	6413 (96%)	231 (4%)	12 (0%)	44 56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	H	225	ILE
3	8	228	GLY
33	d	108	ASP
39	k	40	VAL
5	B	409	ILE
39	k	43	LEU
3	8	232	VAL
3	8	266	ILE
25	V	44	LEU
27	X	428	ILE
39	k	41	GLY
5	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
3	8	95/461 (21%)	87 (92%)	8 (8%)	10 14
4	A	177/182 (97%)	176 (99%)	1 (1%)	78 87
5	B	421/492 (86%)	413 (98%)	8 (2%)	50 69
6	C	312/343 (91%)	307 (98%)	5 (2%)	55 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	366/444 (82%)	361 (99%)	5 (1%)	59	75
8	E	90/126 (71%)	88 (98%)	2 (2%)	45	64
9	F	124/124 (100%)	117 (94%)	7 (6%)	19	29
10	G	112/113 (99%)	110 (98%)	2 (2%)	51	70
11	H	175/320 (55%)	170 (97%)	5 (3%)	37	55
12	I	104/197 (53%)	103 (99%)	1 (1%)	68	80
13	J	108/256 (42%)	105 (97%)	3 (3%)	38	57
14	K	106/107 (99%)	104 (98%)	2 (2%)	50	69
15	L	93/128 (73%)	88 (95%)	5 (5%)	20	30
16	M	90/137 (66%)	88 (98%)	2 (2%)	45	64
17	N	107/362 (30%)	107 (100%)	0	100	100
18	O	93/117 (80%)	92 (99%)	1 (1%)	65	79
19	P	78/95 (82%)	76 (97%)	2 (3%)	40	59
20	Q	75/203 (37%)	74 (99%)	1 (1%)	61	76
21	R	141/180 (78%)	140 (99%)	1 (1%)	76	85
22	S	68/90 (76%)	66 (97%)	2 (3%)	37	55
23	T	44/79 (56%)	43 (98%)	1 (2%)	44	62
24	U	109/170 (64%)	107 (98%)	2 (2%)	51	70
25	V	147/173 (85%)	143 (97%)	4 (3%)	39	58
26	W	328/410 (80%)	321 (98%)	7 (2%)	47	66
27	X	174/395 (44%)	170 (98%)	4 (2%)	44	62
28	Y	84/86 (98%)	82 (98%)	2 (2%)	43	61
29	Z	65/119 (55%)	61 (94%)	4 (6%)	16	24
30	a	252/375 (67%)	247 (98%)	5 (2%)	48	67
31	b	68/71 (96%)	65 (96%)	3 (4%)	25	38
32	c	25/116 (22%)	25 (100%)	0	100	100
33	d	65/93 (70%)	65 (100%)	0	100	100
34	e	226/339 (67%)	220 (97%)	6 (3%)	39	58
35	f	321/351 (92%)	317 (99%)	4 (1%)	63	78
36	g	112/597 (19%)	110 (98%)	2 (2%)	51	70
37	h	271/337 (80%)	264 (97%)	7 (3%)	40	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	i	299/629 (48%)	293 (98%)	6 (2%)	48 67
39	k	23/109 (21%)	23 (100%)	0	100 100
40	l	319/492 (65%)	313 (98%)	6 (2%)	50 69
All	All	5867/9418 (62%)	5741 (98%)	126 (2%)	46 66

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	8	163	ARG
3	8	171	PHE
3	8	172	THR
3	8	176	GLU
3	8	188	LEU
3	8	189	LYS
3	8	248	ARG
3	8	249	HIS
4	A	123	LEU
5	B	10	VAL
5	B	15	ASN
5	B	18	SER
5	B	69	THR
5	B	368	TRP
5	B	478	ILE
5	B	510	THR
5	B	527	SER
6	C	52	ILE
6	C	68	GLN
6	C	122	GLN
6	C	125	GLN
6	C	221	ARG
7	D	90	GLU
7	D	161	ARG
7	D	375	LYS
7	D	386	MET
7	D	395	ILE
8	E	28	LYS
8	E	45	LYS
9	F	28	VAL
9	F	63	VAL
9	F	107	LEU
9	F	116	LEU

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Mol	Chain	Res	Type
9	F	124	SER
9	F	130	GLU
9	F	138	THR
10	G	59	ARG
10	G	86	GLU
11	H	276	SER
11	H	298	ARG
11	H	300	VAL
11	H	356	LYS
11	H	366	THR
12	I	207	TYR
13	J	205	THR
13	J	259	VAL
13	J	304	ASN
14	K	25	ASP
14	K	88	LYS
15	L	82	LEU
15	L	87	GLU
15	L	93	GLN
15	L	111	GLU
15	L	112	VAL
16	M	106	LYS
16	M	157	VAL
18	O	111	VAL
19	P	28	LYS
19	P	39	LYS
20	Q	226	THR
21	R	62	VAL
22	S	40	LEU
22	S	81	ILE
23	T	73	GLN
24	U	59	PHE
24	U	63	HIS
25	V	33	HIS
25	V	119	GLU
25	V	159	GLU
25	V	177	GLU
26	W	97	LEU
26	W	139	ILE
26	W	256	GLN
26	W	275	VAL
26	W	279	GLU

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Mol	Chain	Res	Type
26	W	349	VAL
26	W	456	GLU
27	X	335	VAL
27	X	432	GLU
27	X	438	ILE
27	X	440	GLU
28	Y	7	LYS
28	Y	73	GLU
29	Z	51	LYS
29	Z	81	ILE
29	Z	84	ILE
29	Z	91	ARG
30	a	87	GLU
30	a	91	ASN
30	a	101	ILE
30	a	149	THR
30	a	208	HIS
31	b	34	MET
31	b	46	LEU
31	b	84	GLN
34	e	203	GLU
34	e	224	GLU
34	e	229	GLU
34	e	286	GLU
34	e	304	LEU
34	e	315	LYS
35	f	90	LEU
35	f	148	THR
35	f	175	VAL
35	f	176	GLN
36	g	562	GLU
36	g	607	PHE
37	h	110	TRP
37	h	180	THR
37	h	202	MET
37	h	204	GLU
37	h	246	LYS
37	h	323	LYS
37	h	334	VAL
38	i	123	MET
38	i	167	TRP
38	i	231	GLU

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Mol	Chain	Res	Type
38	i	281	LYS
38	i	345	LEU
38	i	447	SER
40	l	292	MET
40	l	410	PHE
40	l	412	LEU
40	l	430	LEU
40	l	503	MET
40	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	8	249	HIS
5	B	244	ASN
5	B	351	ASN
5	B	468	HIS
6	C	88	HIS
6	C	135	ASN
6	C	158	ASN
6	C	284	ASN
7	D	252	ASN
8	E	96	HIS
9	F	34	GLN
9	F	37	HIS
10	G	50	GLN
10	G	119	ASN
10	G	123	GLN
11	H	299	GLN
12	I	139	ASN
12	I	217	GLN
13	J	267	HIS
14	K	61	HIS
15	L	36	ASN
15	L	61	HIS
16	M	74	HIS
17	N	349	GLN
20	Q	198	GLN
21	R	208	HIS
22	S	63	HIS
25	V	96	GLN
26	W	248	HIS

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Mol	Chain	Res	Type
26	W	288	ASN
26	W	405	HIS
27	X	521	ASN
28	Y	35	GLN
29	Z	73	HIS
29	Z	92	HIS
31	b	22	ASN
31	b	84	GLN
36	g	638	ASN
37	h	115	ASN
37	h	143	HIS
37	h	229	HIS
37	h	345	GLN
38	i	381	ASN
40	l	472	HIS
40	l	501	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1606/1613 (99%)	292 (18%)	22 (1%)
2	6	5/6 (83%)	2 (40%)	1 (20%)
All	All	1611/1619 (99%)	294 (18%)	23 (1%)

All (294) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	12	A
1	2	17	G
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

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Mol	Chain	Res	Type
1	2	150	A
1	2	151	A
1	2	152	G
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

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Mol	Chain	Res	Type
1	2	363	A
1	2	364	C
1	2	365	G
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	442	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

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Mol	Chain	Res	Type
1	2	562	C
1	2	566	G
1	2	571	A
1	2	573	G
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	858	A
1	2	865	A
1	2	866	A
1	2	867	A
1	2	903	C
1	2	907	A
1	2	916	A
1	2	918	G
1	2	919	G
1	2	920	G

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Mol	Chain	Res	Type
1	2	926	G
1	2	927	C
1	2	928	A
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

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Mol	Chain	Res	Type
1	2	1170	U
1	2	1172	U
1	2	1310	A
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

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Mol	Chain	Res	Type
1	2	1625	A
1	2	1626	U
1	2	1647	G
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

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Mol	Chain	Res	Type
1	2	1765	U
1	2	1766	U
1	2	1768	A
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	1842	U
1	2	1843	G
1	2	1844	A
1	2	1845	A
1	2	1846	U
2	6	3	U
2	6	5	U

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	162	C
1	2	225	G
1	2	236	A
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

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Mol	Chain	Res	Type
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
1	2	1802	A
1	2	1814	G
1	2	1842	U
1	2	1845	A
2	6	4	U

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	2	1664	1	-	1/9/29/30	0/2/2/2
1	G7M	2	525	1	-	3/7/25/26	0/3/3/3
1	2MG	2	1825	1	-	0/9/27/28	0/3/3/3
1	MA6	2	1828	1	-	2/11/29/30	0/3/3/3
1	UR3	2	1807	1	-	2/7/25/26	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	1664	4OC	1	0
1	2	1825	2MG	1	0
1	2	1828	MA6	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	$\#\|Z\| > 2$
41	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
41	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.

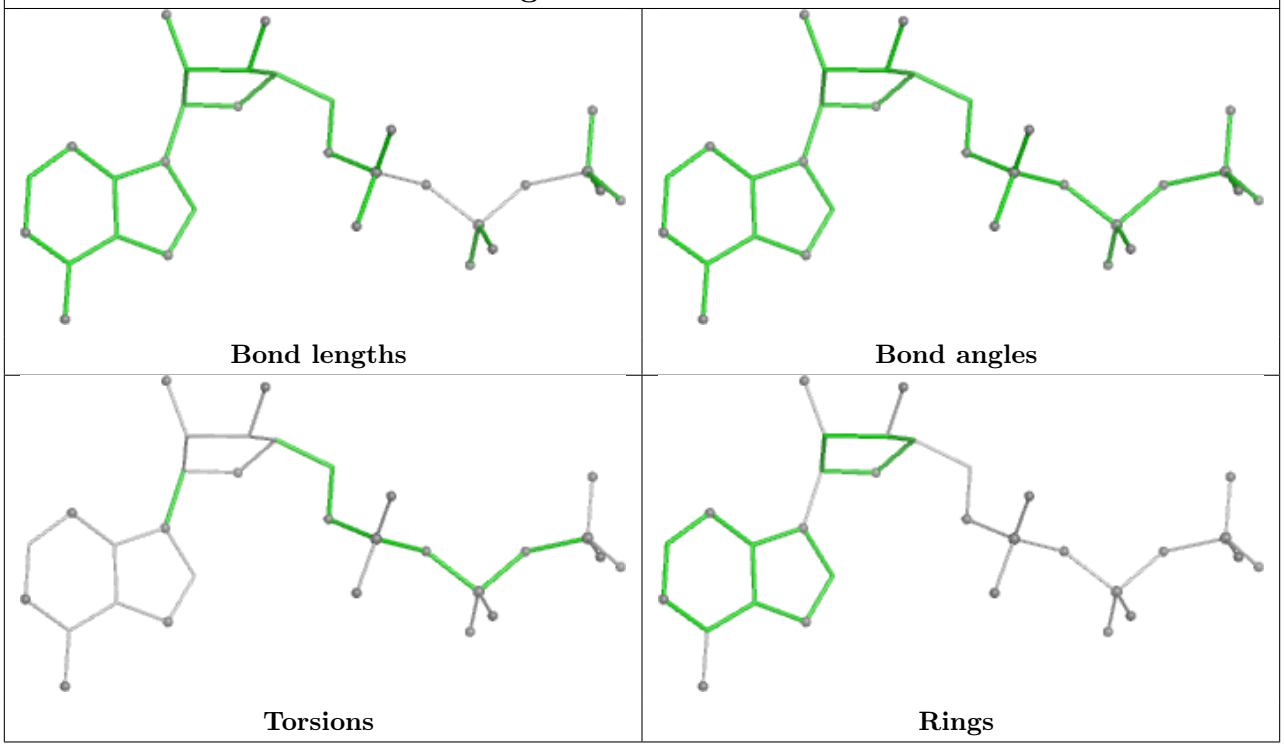
There are no ring outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1147:A	O3'	1164:U	P	22.57
1	2	1330:A	O3'	1335:U	P	18.93
1	2	1173:U	O3'	1308:A	P	18.37
1	2	83:U	O3'	129:A	P	17.63

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	137:A	O3'	142:U	P	14.70
1	2	1345:U	O3'	1376:A	P	14.09

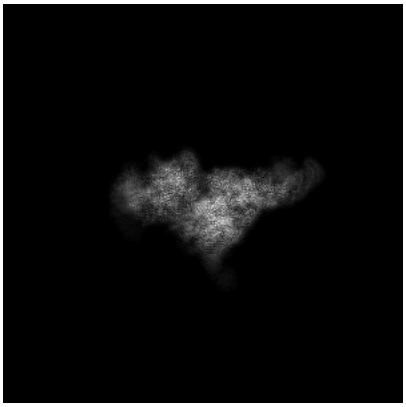
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56196. These allow visual inspection of the internal detail of the map and identification of artifacts.

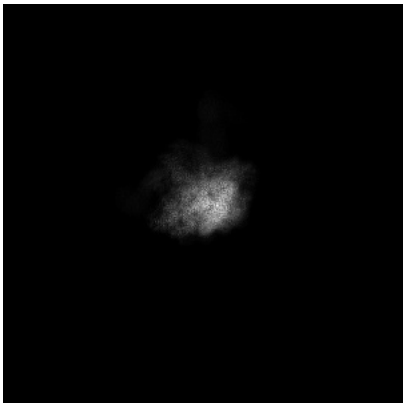
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

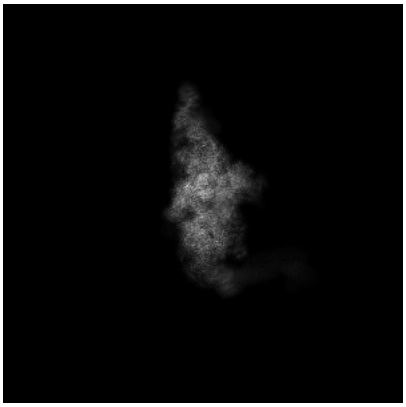
6.1.1 Primary map



X



Y

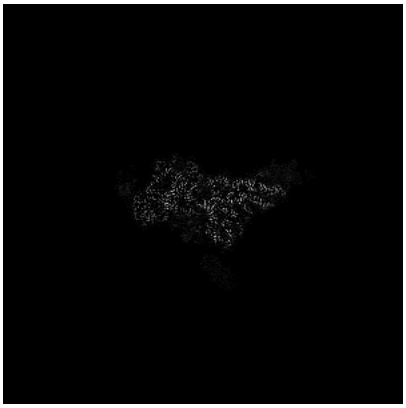


Z

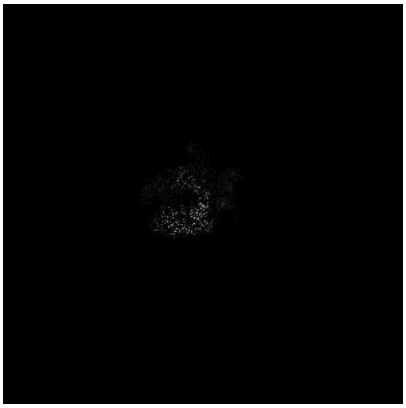
The images above show the map projected in three orthogonal directions.

6.2 Central slices

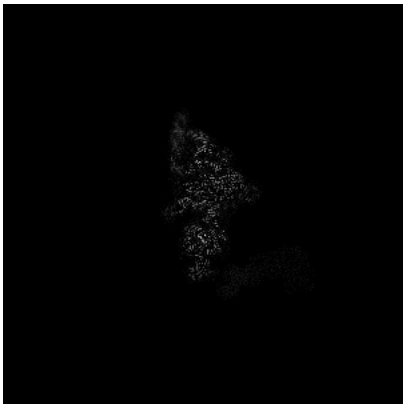
6.2.1 Primary map



X Index: 350



Y Index: 350

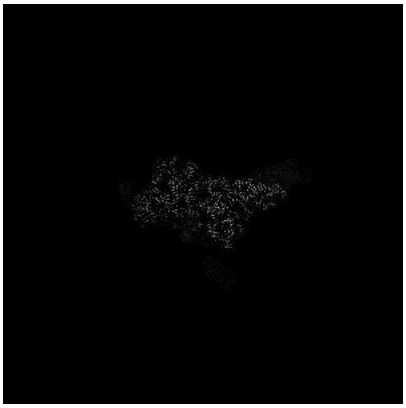


Z Index: 350

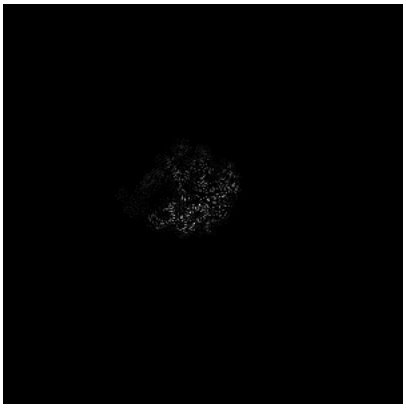
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

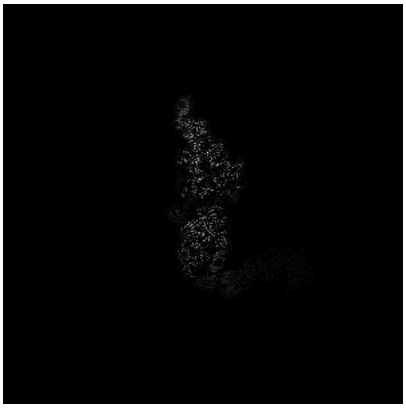
6.3.1 Primary map



X Index: 348



Y Index: 376

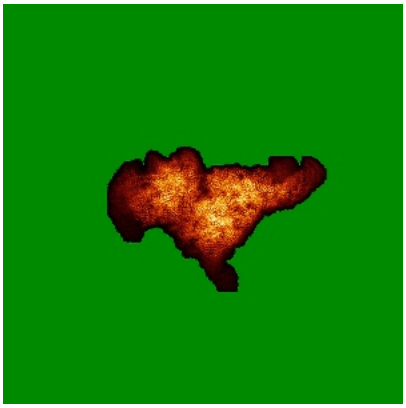


Z Index: 371

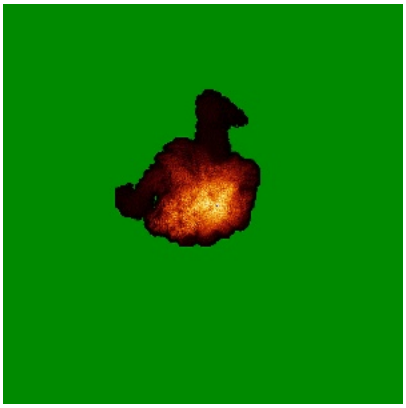
The images above show the largest variance slices of the map in three orthogonal directions.

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

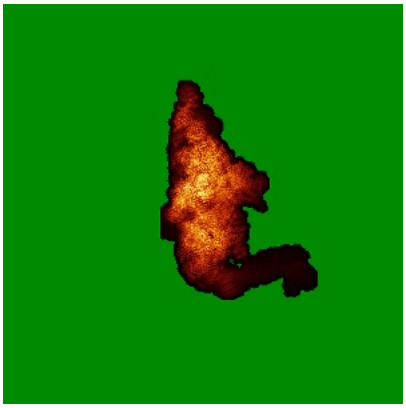
6.4.1 Primary map



X



Y

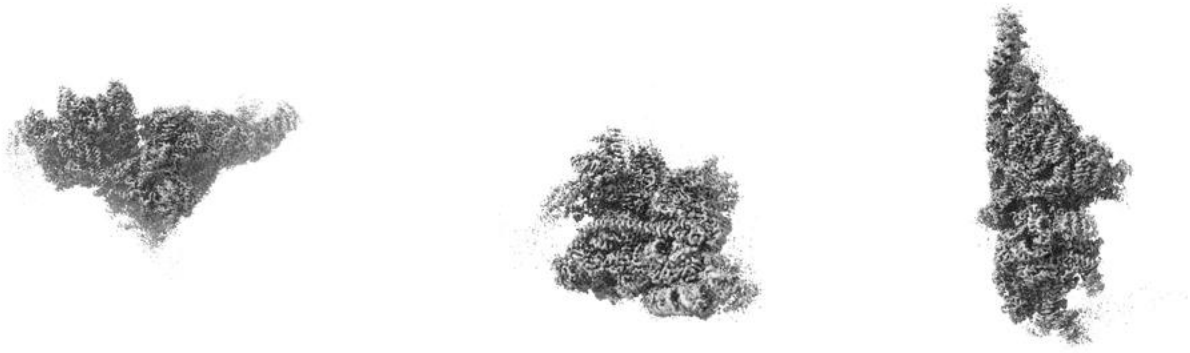


Z

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.

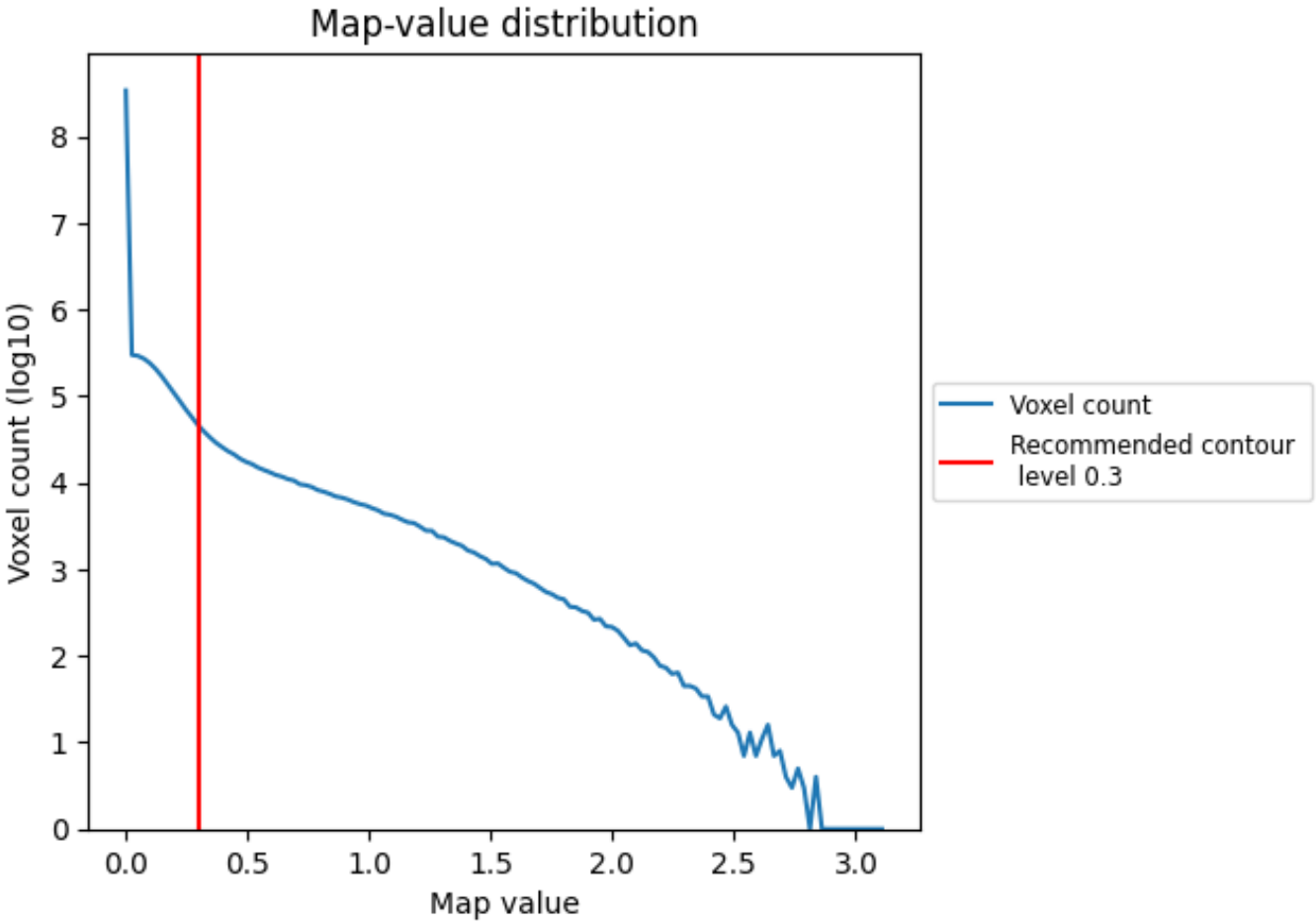
6.6 Mask visualisation (i)

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

7 Map analysis

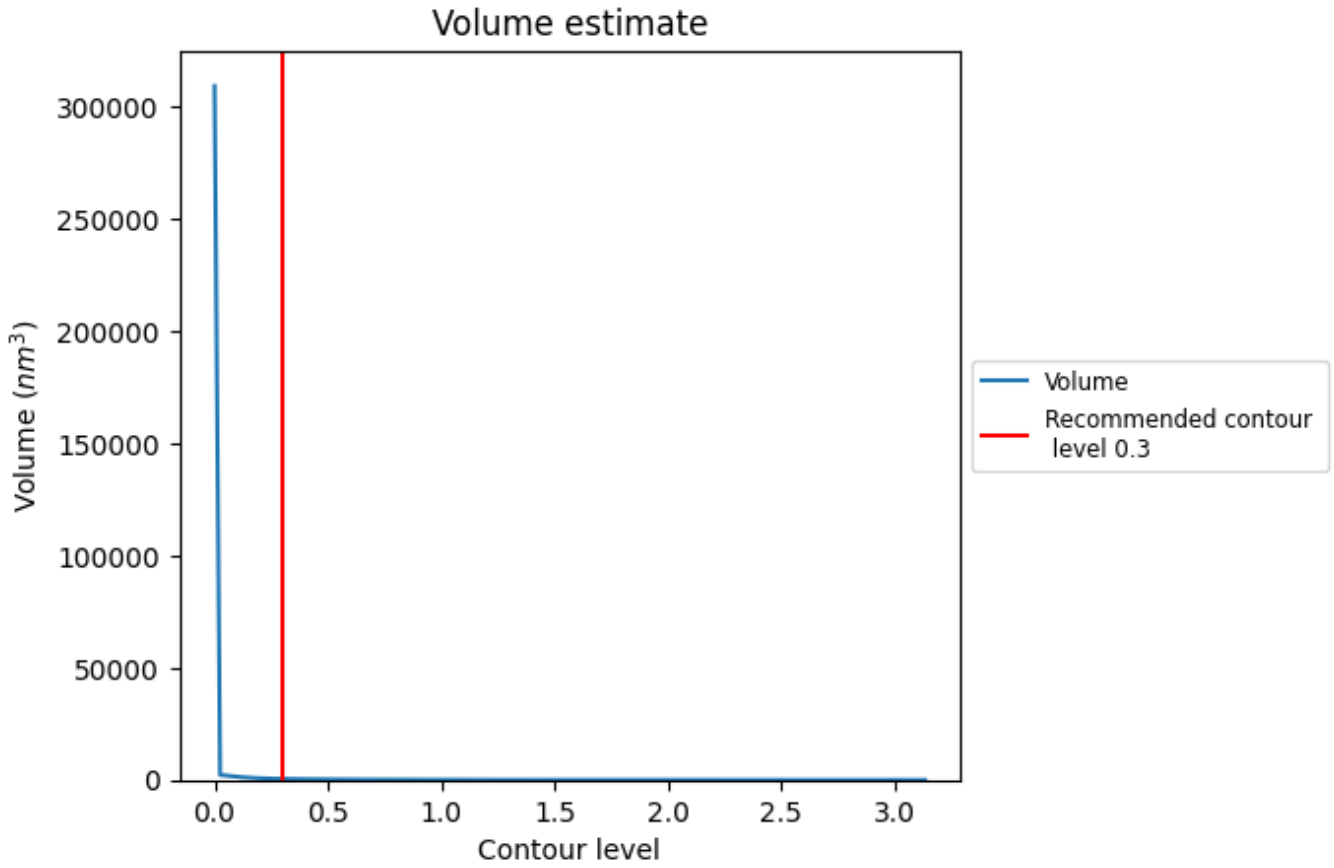
This section contains the results of statistical analysis of the map.

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.

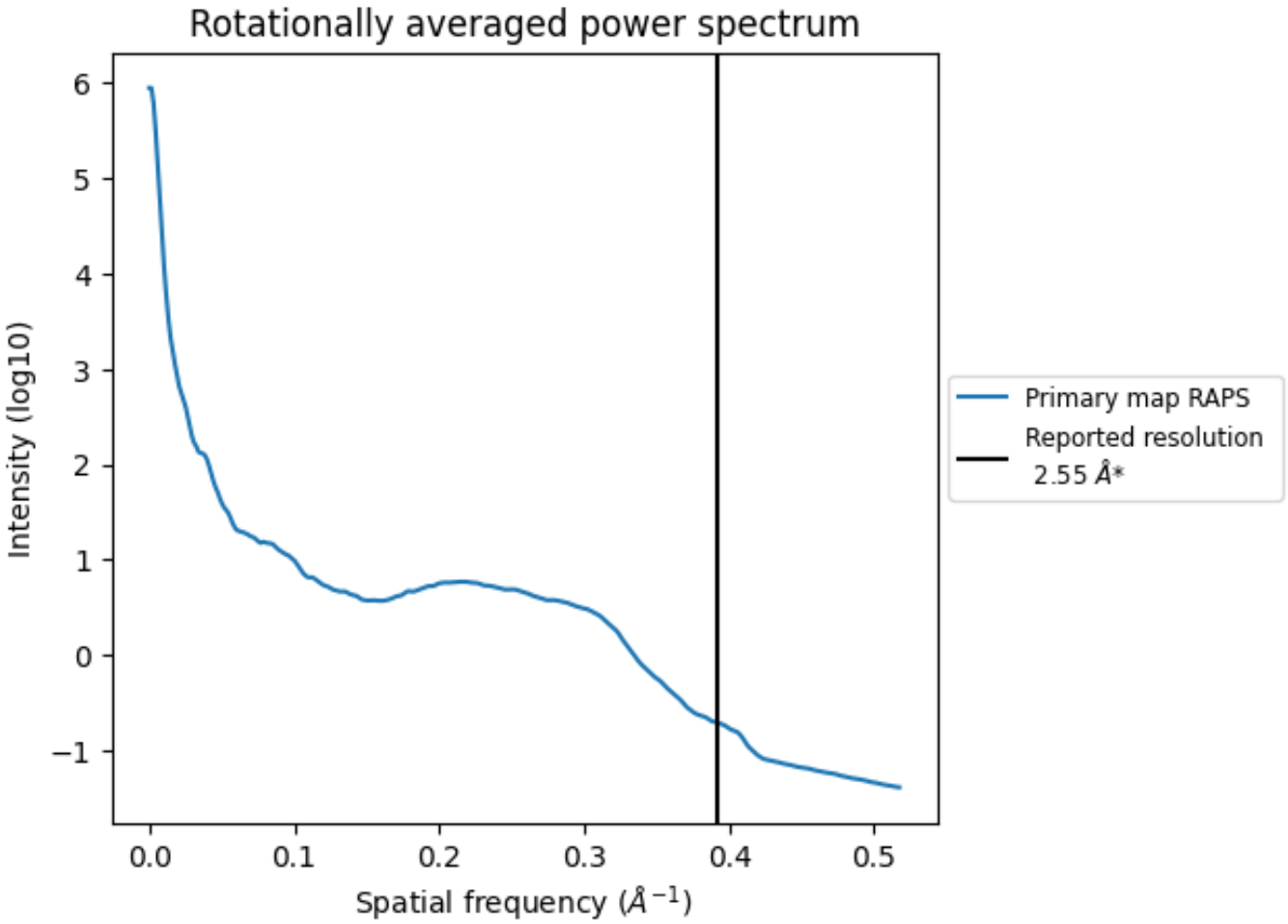
7.2 Volume estimate



The volume at the recommended contour level is 463 nm^3; this corresponds to an approximate mass of 418 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 0.392 Å^{-1}

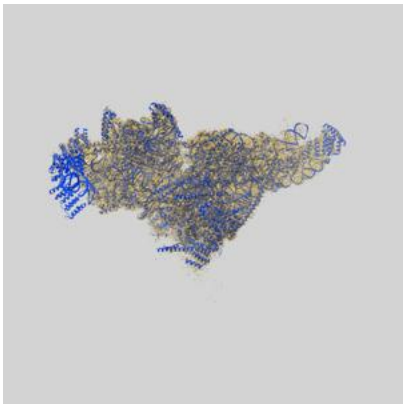
8 Fourier-Shell correlation

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

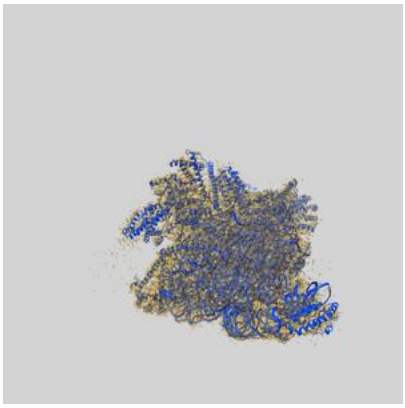
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56196 and PDB model 9TRS. Per-residue inclusion information can be found in section 3 on page 12.

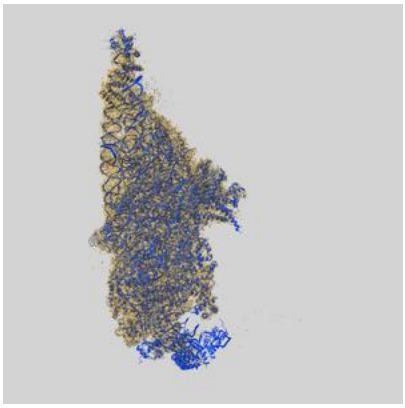
9.1 Map-model overlay



X



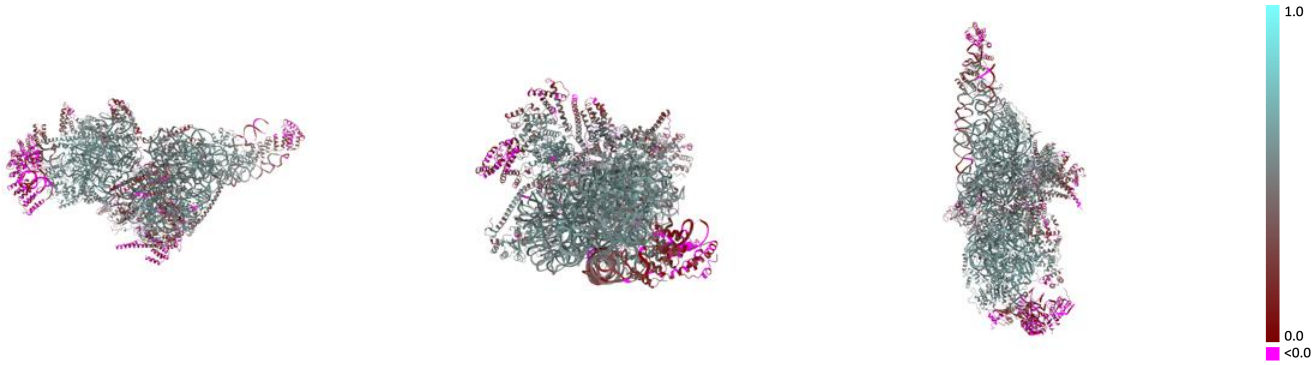
Y



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.

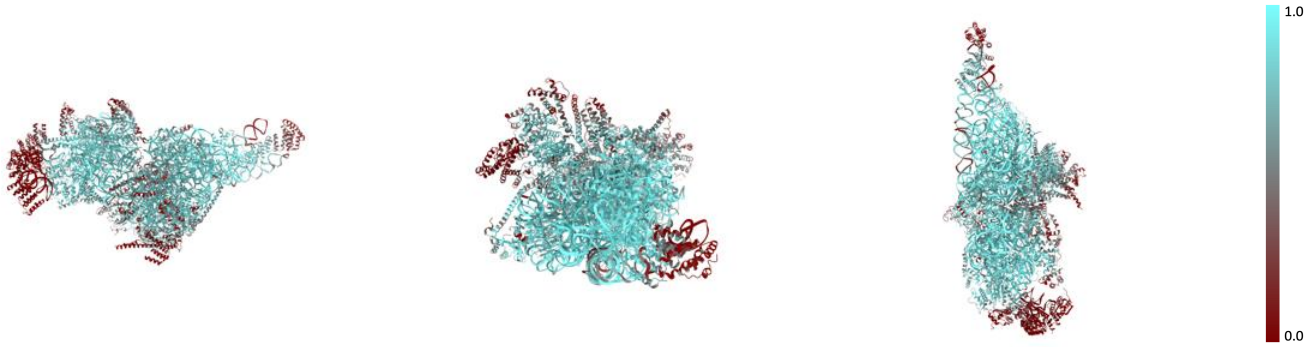
9.2 Q-score mapped to coordinate model (i)



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.

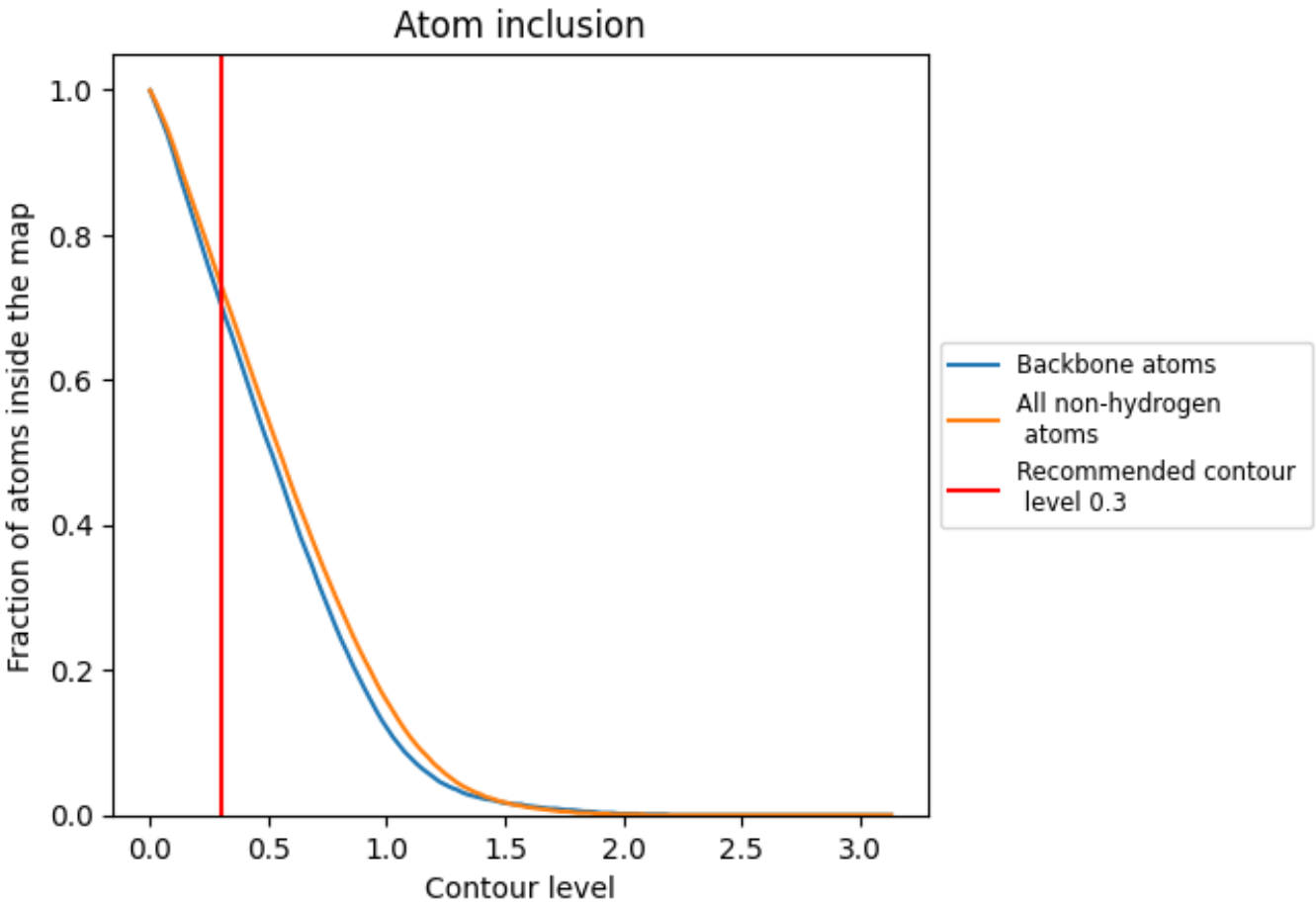
9.3 Atom inclusion mapped to coordinate model (i)



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, 70% of all backbone atoms, 73% 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	0.7310	0.4640
2	0.8710	0.5160
6	0.4000	0.1800
8	0.3620	0.2610
A	0.7930	0.5430
B	0.6920	0.4830
C	0.7820	0.4990
D	0.6830	0.4450
E	0.8300	0.5190
F	0.7020	0.4970
G	0.9150	0.5890
H	0.7050	0.4880
I	0.9110	0.6080
J	0.6460	0.4240
K	0.8700	0.5560
L	0.7100	0.5420
M	0.9370	0.6220
N	0.8230	0.5470
O	0.9410	0.5830
P	0.8500	0.5640
Q	0.7500	0.4950
R	0.3950	0.2950
S	0.6580	0.4560
T	0.9320	0.6130
U	0.3990	0.2830
V	0.7220	0.4760
W	0.8190	0.5510
X	0.7300	0.5100
Y	0.7900	0.5550
Z	0.8540	0.4960
a	0.6730	0.4870
b	0.3200	0.2440
c	0.7890	0.4870
d	0.8260	0.5020
e	0.7980	0.5150



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Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.7100	0.4990
g	0.0010	-0.0280
h	0.4690	0.2180
i	0.2600	0.1920
k	0.4010	0.3420
l	0.0650	0.0660