Full wwPDB EM Validation Report ⓘ

Sep 7, 2026 – 08:57 pm BST

PDB ID	:	5NCO / pdb_00005nco
EMDB ID	:	EMD-3617
Title	:	Quaternary complex between SRP, SR, and SecYEG bound to the translating ribosome
Authors	:	Jomaa, A.; Hwang Fu, Y.; Boerhinger, D.; Leibundgut, M.; Shan, S.O.; Ban, N.
Deposited on	:	2017-03-06
Resolution	:	4.80 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:

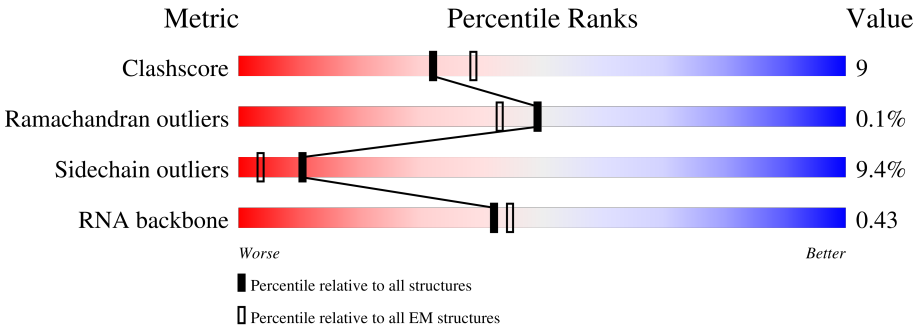
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

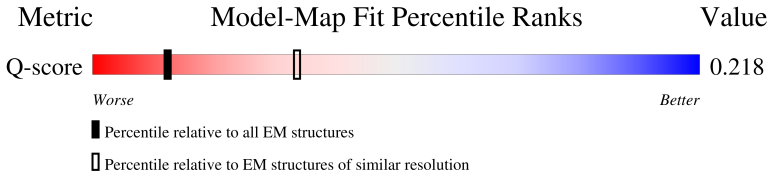
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.80 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	1575 (4.30 - 5.30)

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	1	104	12% 65% 29% 6%
2	2	3	33% 67%
3	A	2903	57% 35% 7%

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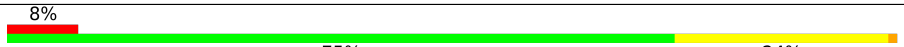
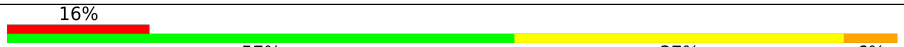
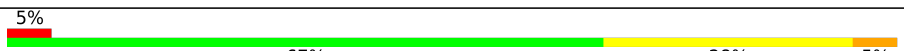
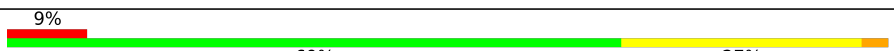
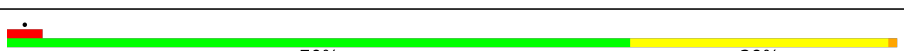
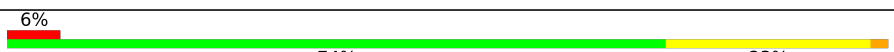
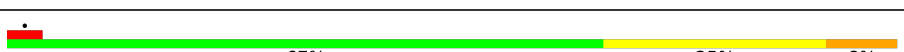
Mol	Chain	Length	Quality of chain
4	B	120	
5	C	271	
6	D	209	
7	E	201	
8	F	177	
9	G	176	
10	H	149	
11	I	125	
12	J	134	
13	K	142	
14	L	123	
15	M	144	
16	N	136	
17	O	125	
18	P	117	
19	Q	114	
20	R	117	
21	S	103	
22	T	110	
23	U	95	
24	V	102	
25	W	94	
26	X	76	
27	Y	77	
28	Z	62	

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Mol	Chain	Length	Quality of chain
29	a	58	71% 28%
30	b	56	5% 61% 29% 11%
31	c	51	10% 76% 22%
32	d	46	7% 70% 26%
33	e	64	11% 59% 39%
34	f	38	5% 71% 21% 8%
35	g	416	63% 98%
36	h	56	82% 100%
37	i	450	42% 72% 28%
38	j	71	66% 100%
39	k	23	30% 100%
40	l	271	28% 83% 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
42	ALF	i	1001	-	-	X	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 101694 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 4.5S SRP RNA (Ffs).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	104	2224	991	401	728	104	0	0

- Molecule 2 is a RNA chain called P-site tRNA-CCA end.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	3	62	28	11	20	3	0	0

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A	2883	61902	27613	11397	20009	2883	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	B	120	2569	1144	468	837	120	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	271	2083	1288	423	365	7	0	0

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	209	1565	979	288	294	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	598	169	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	V	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	g	416	Total	C	N	O	0	0
			1664	832	416	416		

- Molecule 36 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	h	56	Total	C	N	O	0	0
			224	112	56	56		

- Molecule 37 is a protein called Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	450	Total	C	N	O	S	0	0
			3384	2129	609	628	18		

- Molecule 38 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	j	71	Total	C	N	O	0	0
			284	142	71	71		

- Molecule 39 is a protein called Signal sequence (1A9L).

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	23	Total	C	N	O	0	0
			159	107	25	27		

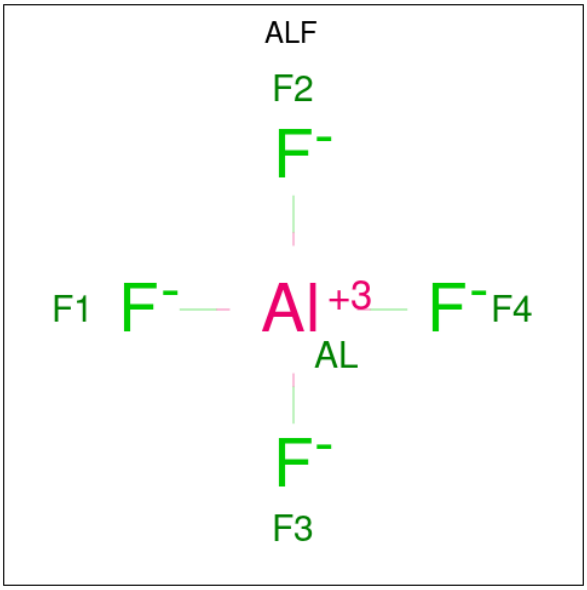
- Molecule 40 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	271	Total	C	N	O	S	0	0
			2067	1306	356	399	6		

- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
41	f	1	Total	Zn	0
			1	1	

- Molecule 42 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).

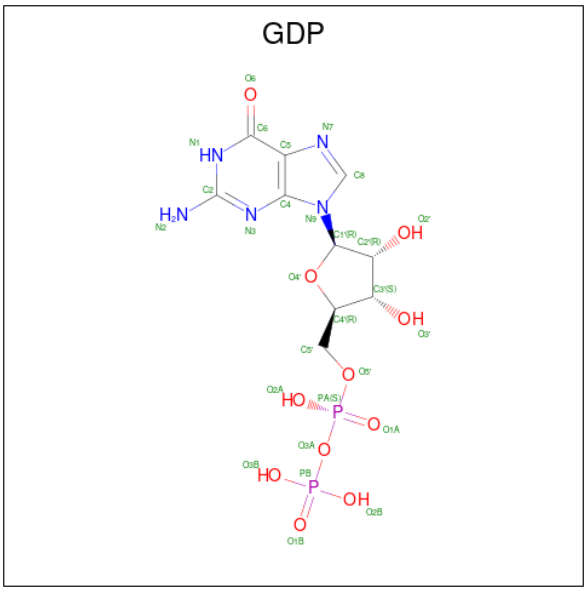


Mol	Chain	Residues	Atoms	AltConf
42	i	1	Total Al F 5 1 4	0
42	l	1	Total Al F 5 1 4	0

- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
43	i	1	Total Mg 1 1	0
43	l	1	Total Mg 1 1	0

- Molecule 44 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
44	i	1	Total	C	N	O	P	0
			28	10	5	11	2	
44	l	1	Total	C	N	O	P	0
			28	10	5	11	2	

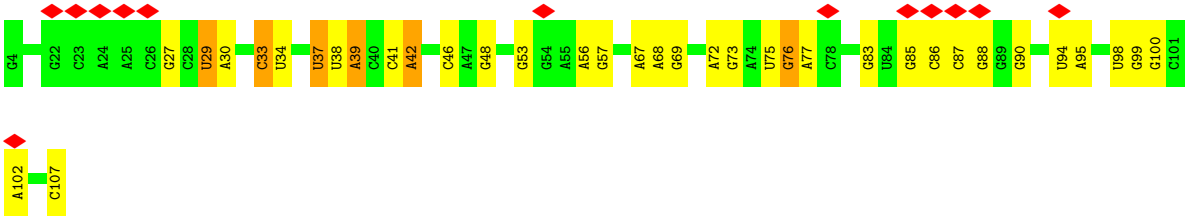
3 Residue-property plots (i)

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: 4.5S SRP RNA (Ffs)

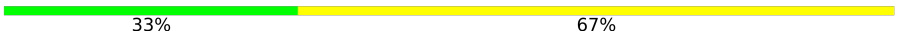
Chain 1:





- Molecule 2: P-site tRNA-CCA end

Chain 2:

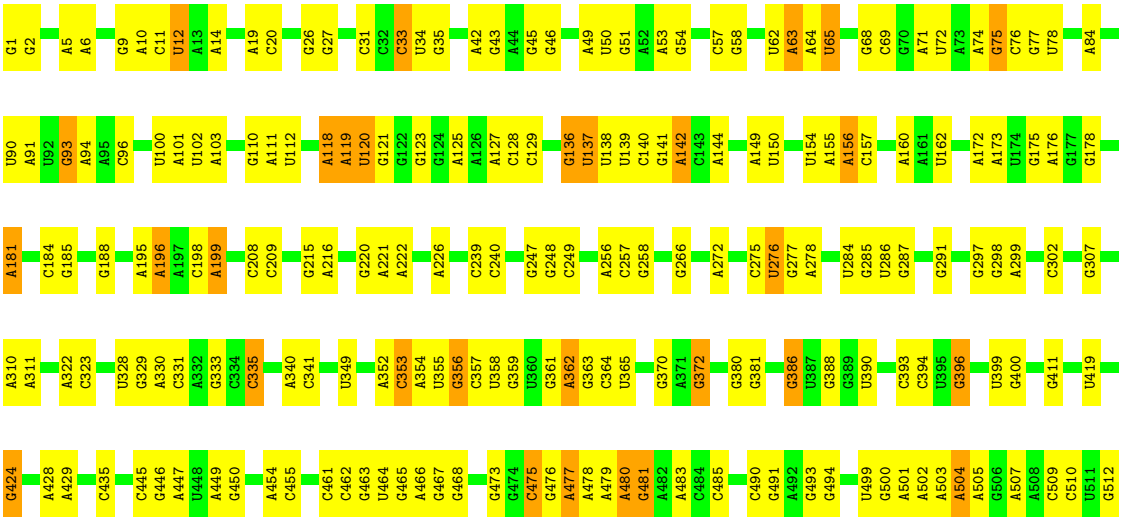


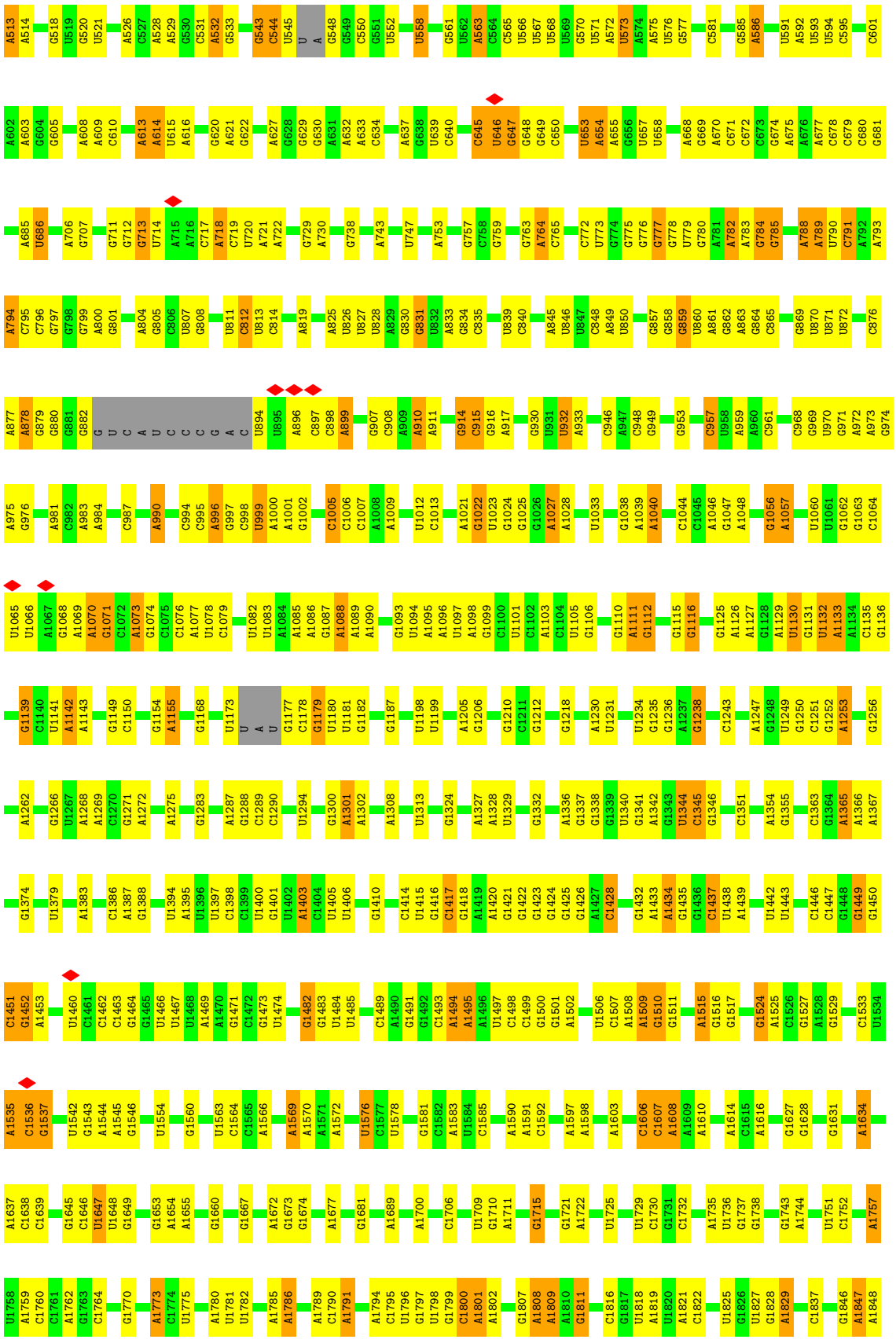


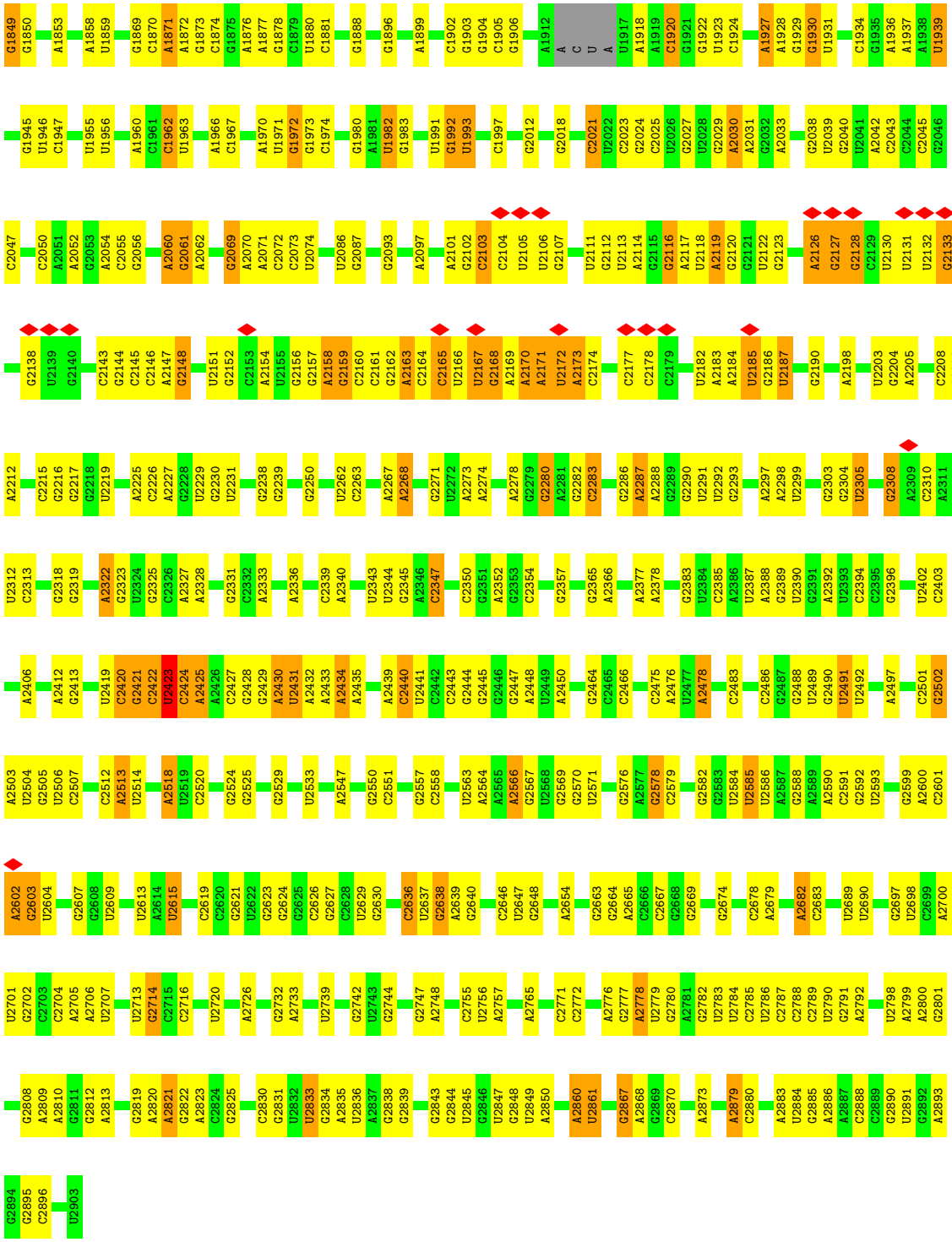
- Molecule 3: 23S rRNA

Chain A:





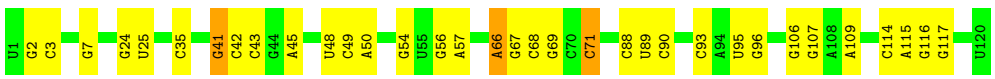




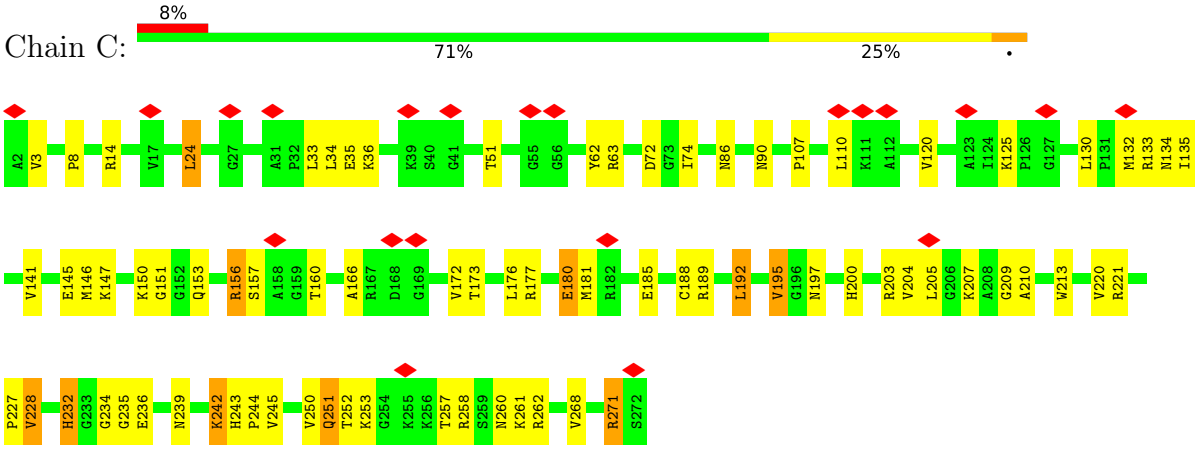
• Molecule 4: 5S rRNA

Chain B:

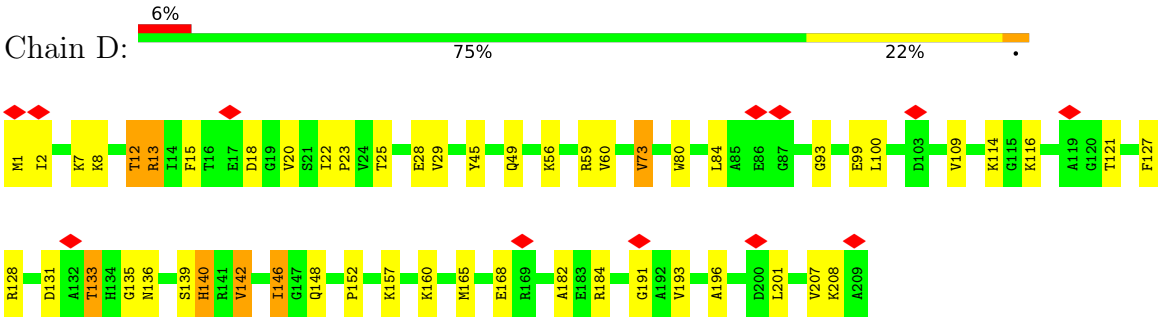




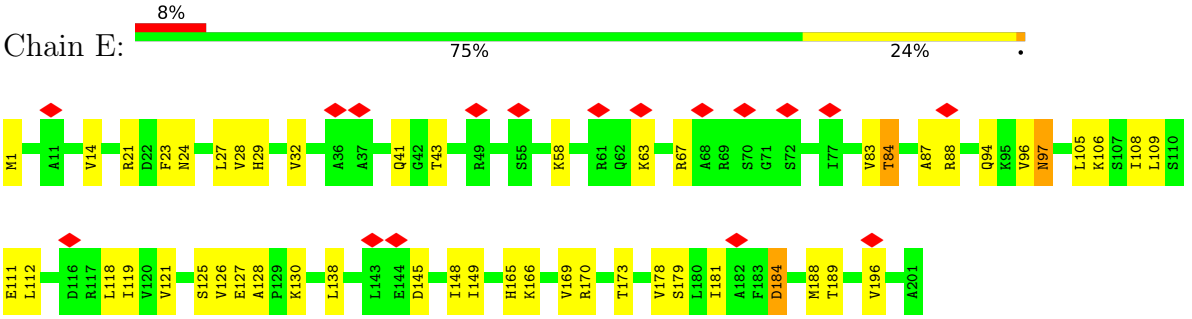
• Molecule 5: 50S ribosomal protein L2



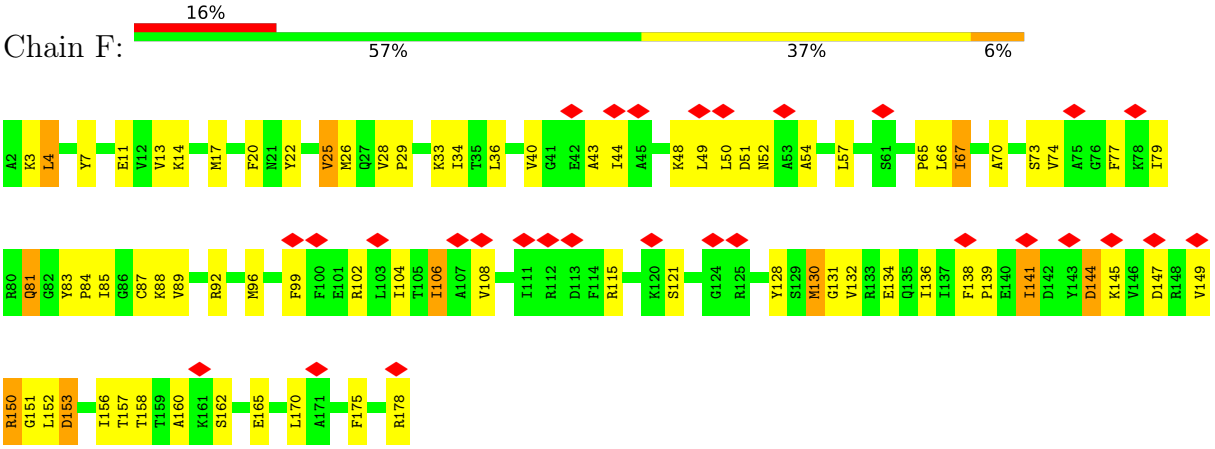
• Molecule 6: 50S ribosomal protein L3



• Molecule 7: 50S ribosomal protein L4

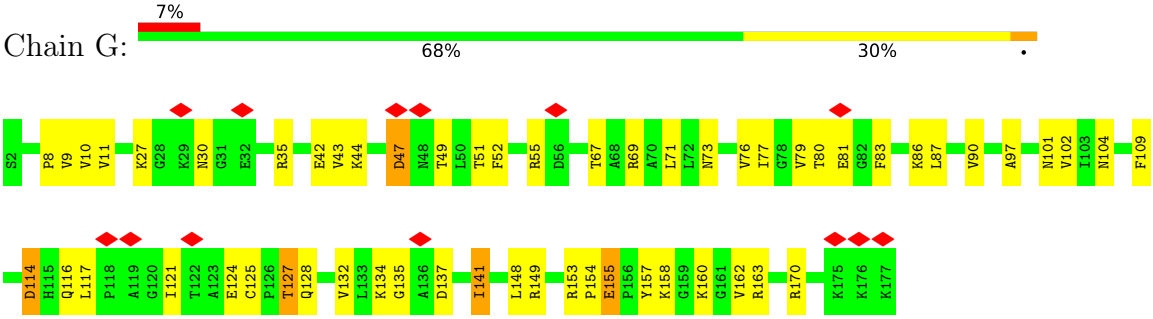


• Molecule 8: 50S ribosomal protein L5



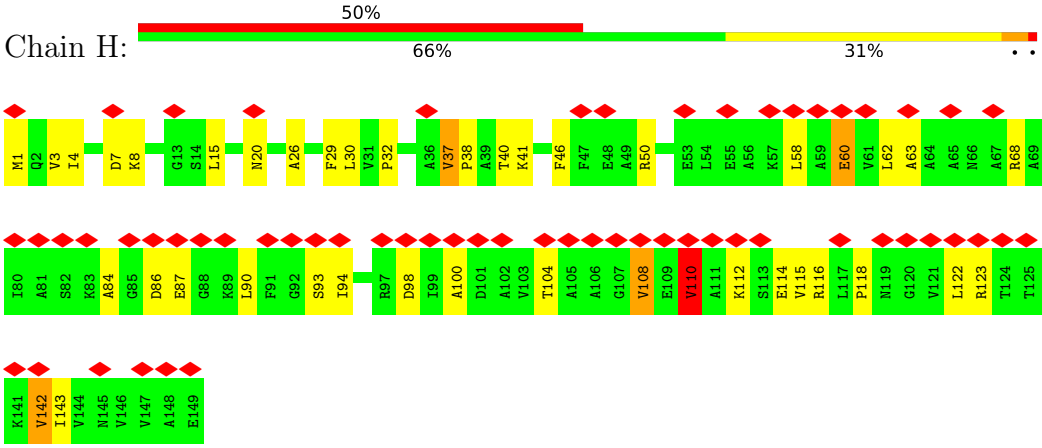
• Molecule 9: 50S ribosomal protein L6

Chain G:



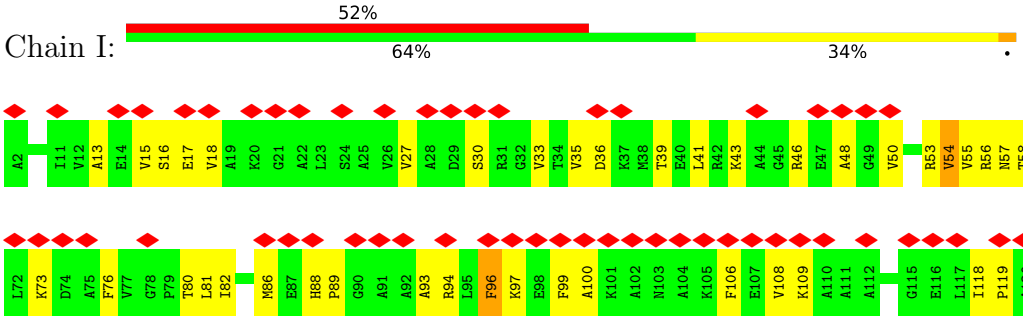
• Molecule 10: 50S ribosomal protein L9

Chain H:



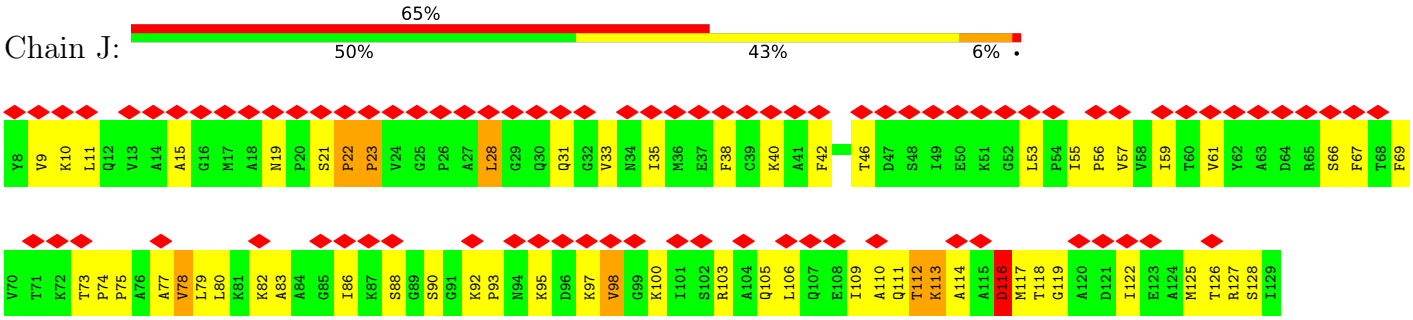
• Molecule 11: 50S ribosomal protein L10

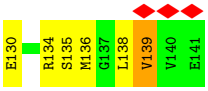
Chain I:



• Molecule 12: 50S ribosomal protein L11

Chain J:

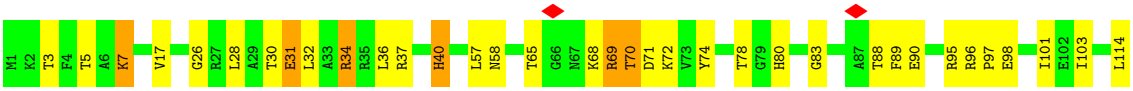


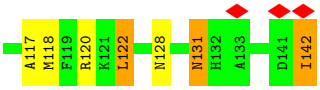


• Molecule 13: 50S ribosomal protein L13

Chain K:



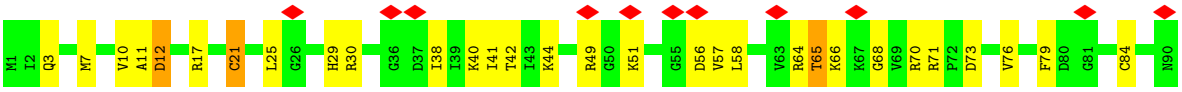




• Molecule 14: 50S ribosomal protein L14

Chain L:



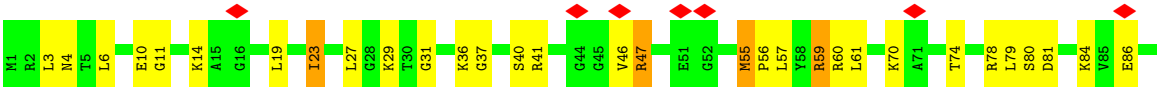




• Molecule 15: 50S ribosomal protein L15

Chain M:



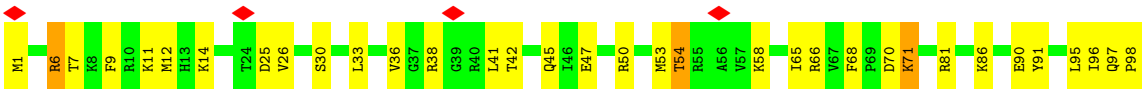


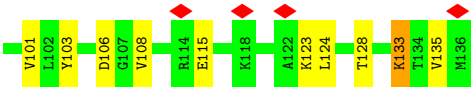


• Molecule 16: 50S ribosomal protein L16

Chain N:

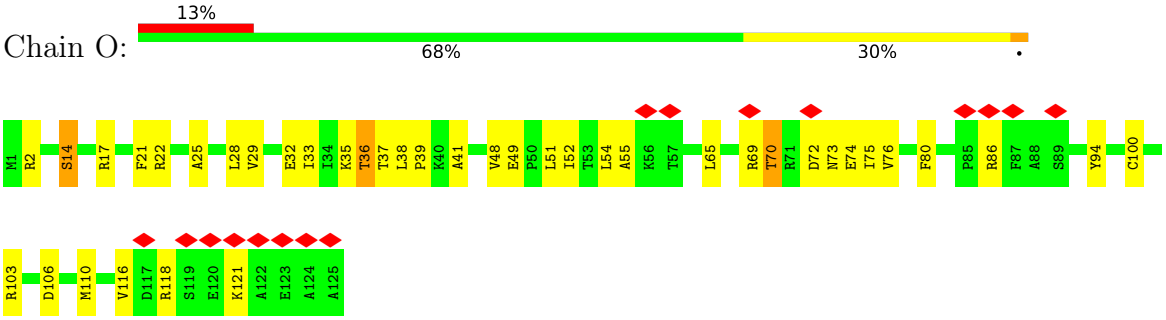






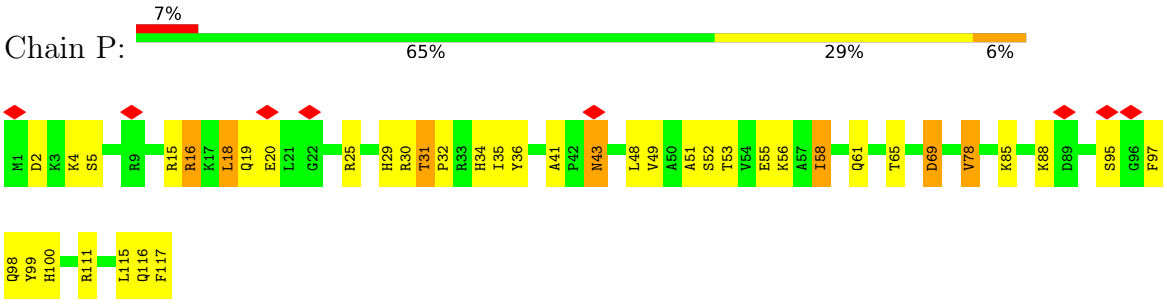
• Molecule 17: 50S ribosomal protein L17

Chain O:



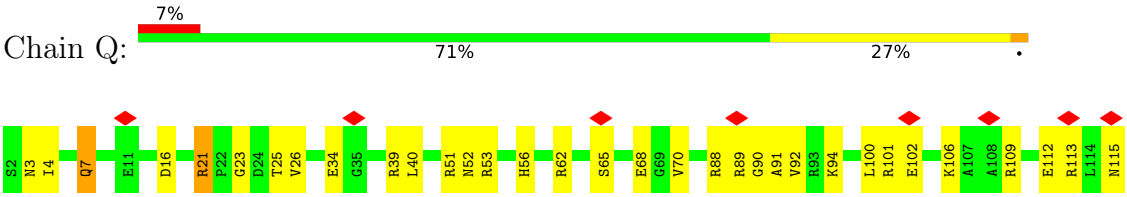
• Molecule 18: 50S ribosomal protein L18

Chain P:



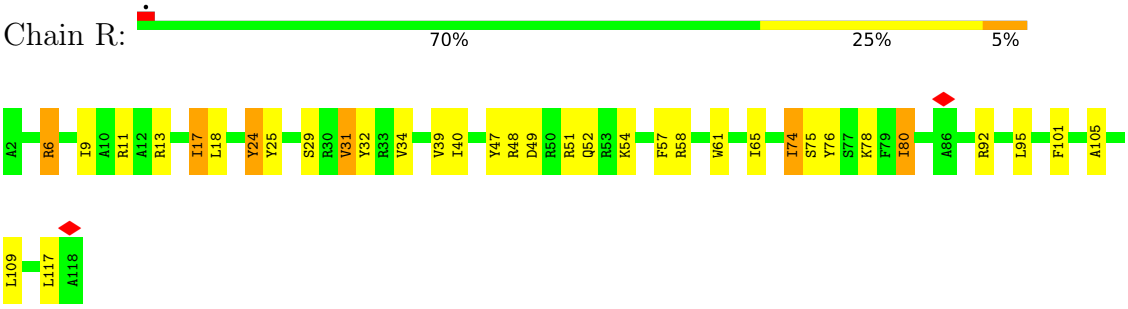
• Molecule 19: 50S ribosomal protein L19

Chain Q:



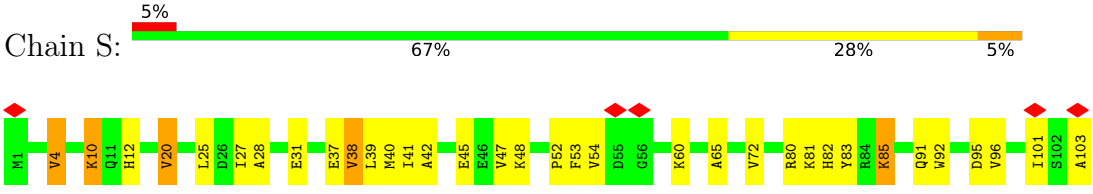
• Molecule 20: 50S ribosomal protein L20

Chain R:



• Molecule 21: 50S ribosomal protein L21

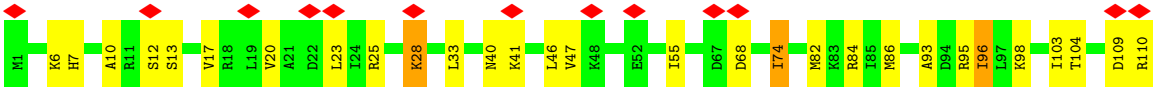
Chain S:



• Molecule 22: 50S ribosomal protein L22

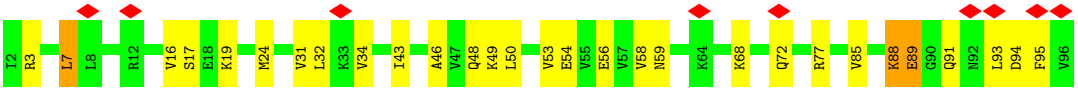
Chain T:





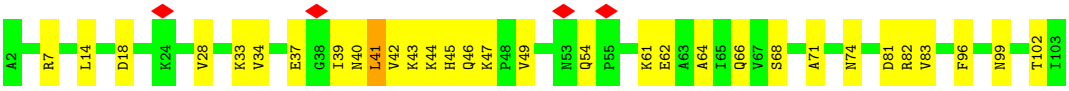
• Molecule 23: 50S ribosomal protein L23



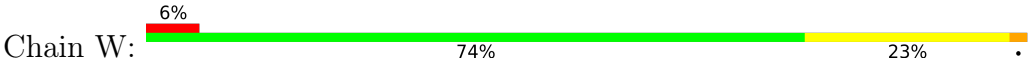


• Molecule 24: 50S ribosomal protein L24





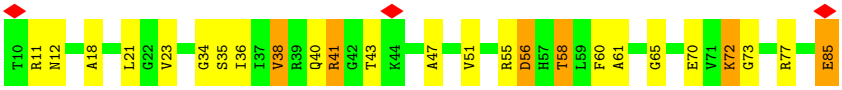
• Molecule 25: 50S ribosomal protein L25





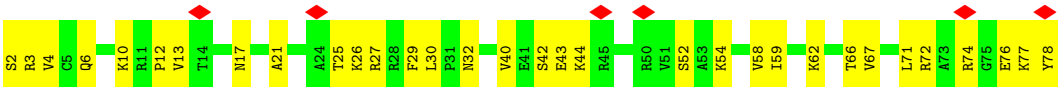
• Molecule 26: 50S ribosomal protein L27





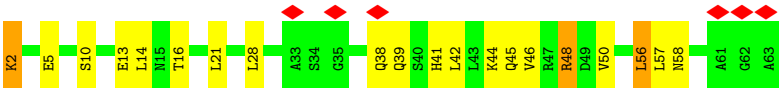
• Molecule 27: 50S ribosomal protein L28





• Molecule 28: 50S ribosomal protein L29

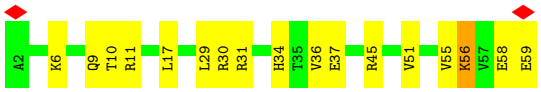




• Molecule 29: 50S ribosomal protein L30

Chain a:

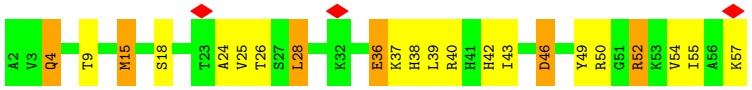




• Molecule 30: 50S ribosomal protein L32

Chain b:

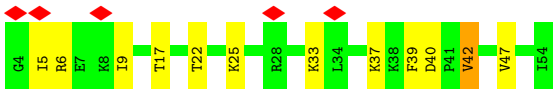




• Molecule 31: 50S ribosomal protein L33

Chain c:

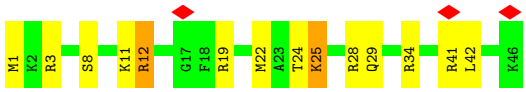




• Molecule 32: 50S ribosomal protein L34

Chain d:

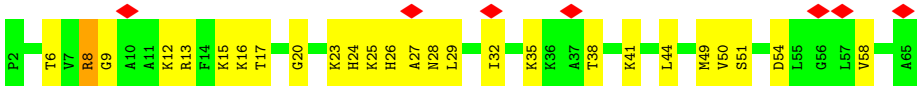




• Molecule 33: 50S ribosomal protein L35

Chain e:

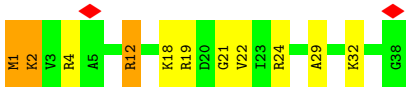




• Molecule 34: 50S ribosomal protein L36

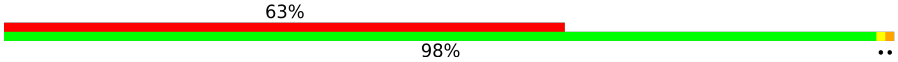
Chain f:

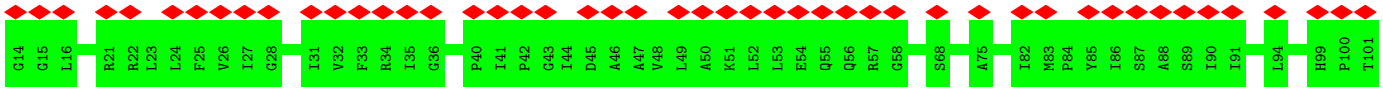


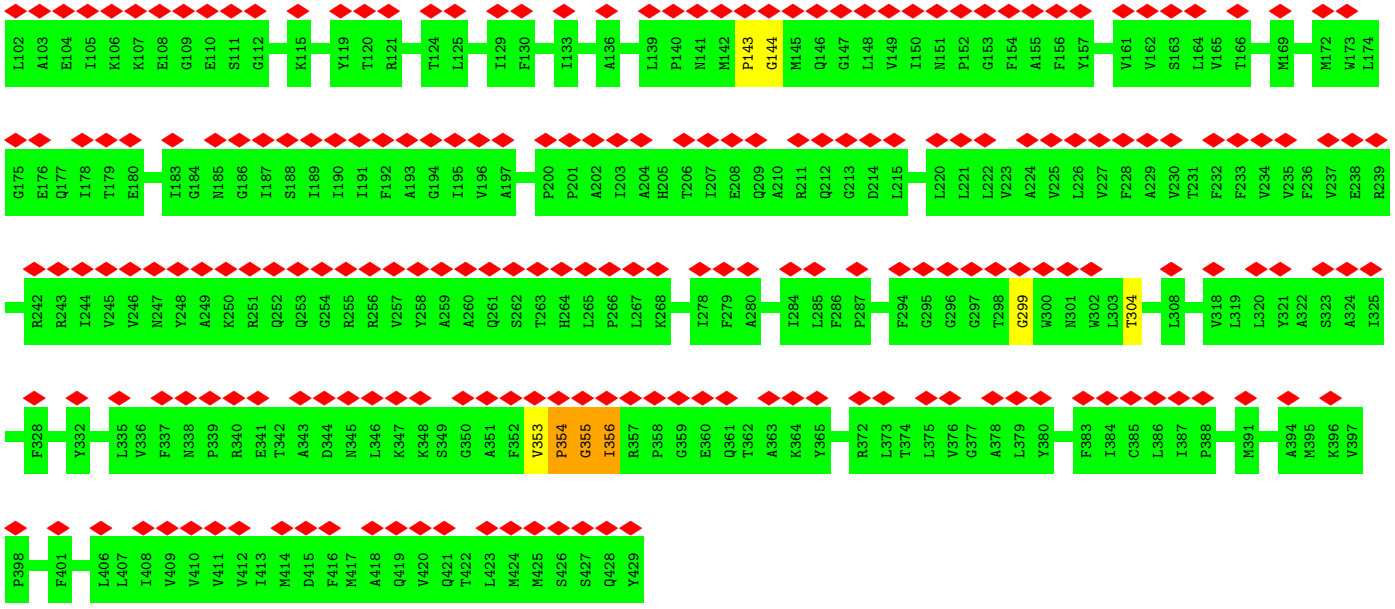


• Molecule 35: Protein translocase subunit SecY

Chain g:



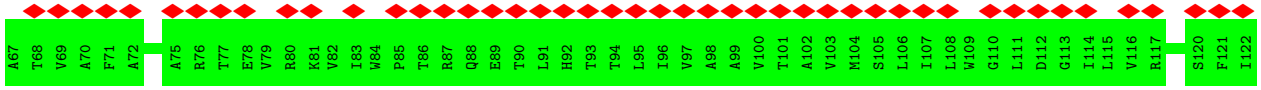




• Molecule 36: Protein translocase subunit SecE

Chain h:

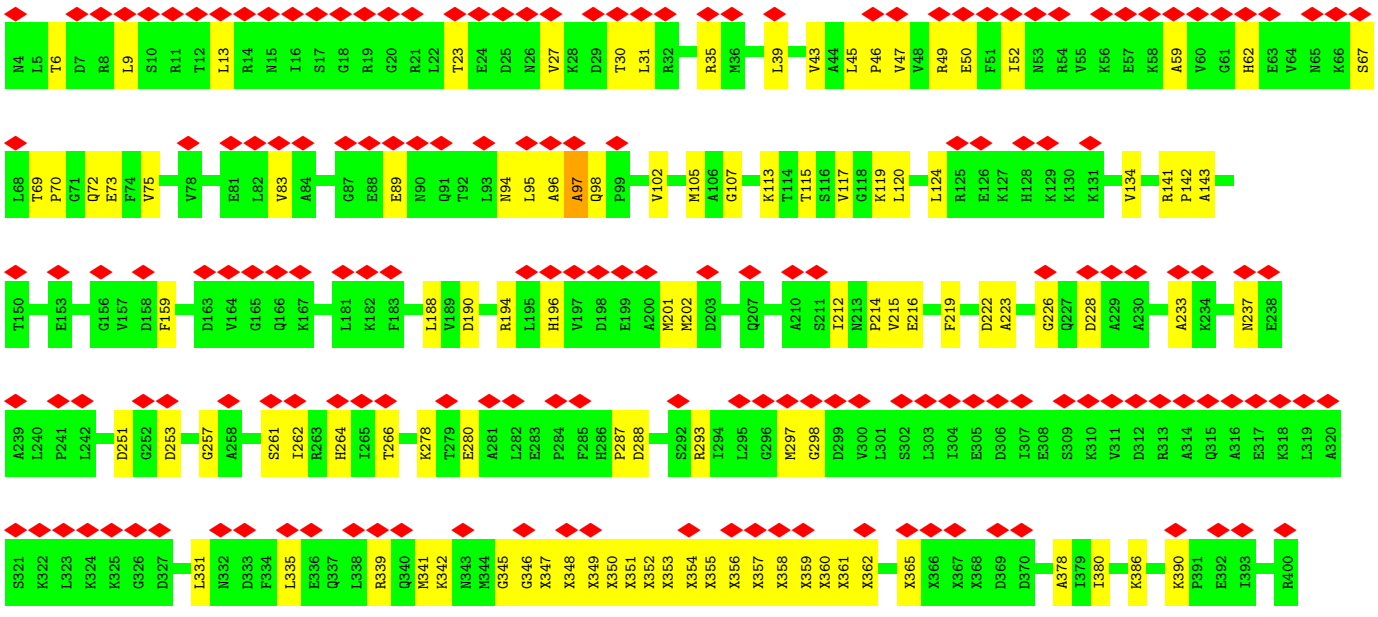


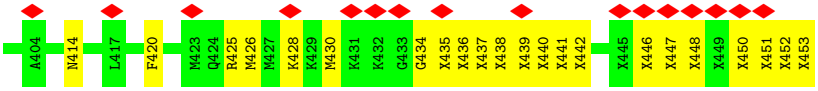


• Molecule 37: Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein

Chain i:



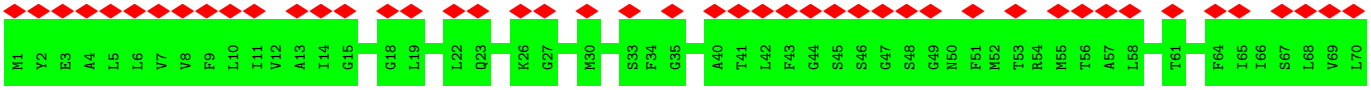




• Molecule 38: Protein-export membrane protein SecG

Chain j:

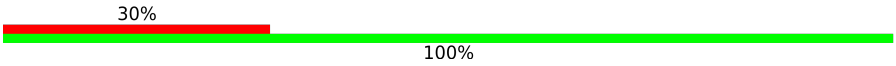


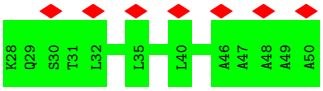




• Molecule 39: Signal sequence (1A9L)

Chain k:

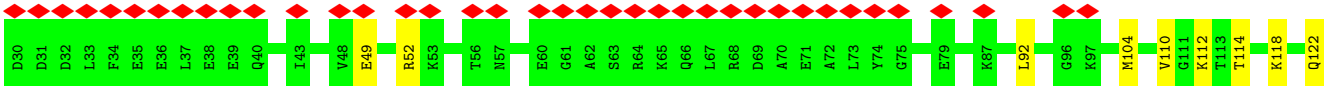


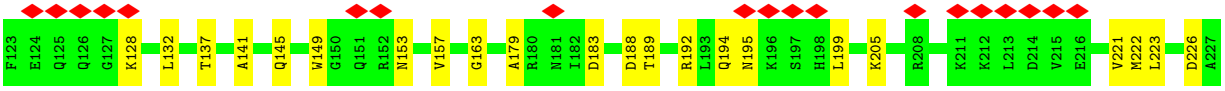


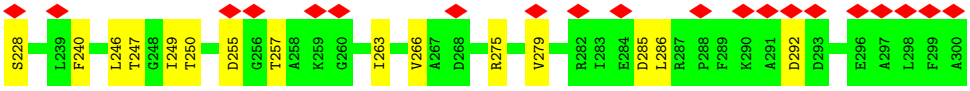
• Molecule 40: Signal recognition particle receptor FtsY

Chain l:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; After 3D reconstruction 3D maps were sharpened	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.07	0/2486	0.14	0/3874
2	2	0.35	0/68	0.51	0/103
3	A	0.35	0/69329	0.48	1/108152 (0.0%)
4	B	0.28	0/2872	0.40	0/4478
5	C	0.61	0/2122	0.96	0/2852
6	D	0.60	0/1586	0.95	5/2134 (0.2%)
7	E	0.57	0/1571	0.91	0/2113
8	F	0.52	1/1435 (0.1%)	0.93	5/1926 (0.3%)
9	G	0.51	0/1343	0.97	3/1816 (0.2%)
10	H	0.59	0/1121	0.90	1/1515 (0.1%)
11	I	0.72	0/958	0.95	0/1290
12	J	0.94	1/993 (0.1%)	1.13	8/1341 (0.6%)
13	K	0.58	0/1152	0.88	2/1551 (0.1%)
14	L	0.57	0/955	0.97	2/1279 (0.2%)
15	M	0.57	0/1062	0.97	3/1413 (0.2%)
16	N	0.59	0/1093	0.96	6/1460 (0.4%)
17	O	0.61	0/1006	0.95	1/1345 (0.1%)
18	P	0.50	0/910	0.93	0/1219
19	Q	0.54	0/929	0.94	2/1242 (0.2%)
20	R	0.73	0/960	0.91	1/1278 (0.1%)
21	S	0.57	0/829	0.95	0/1107
22	T	0.66	0/864	1.05	2/1156 (0.2%)
23	U	0.63	1/763 (0.1%)	0.99	2/1021 (0.2%)
24	V	0.45	0/788	0.88	2/1051 (0.2%)
25	W	0.47	0/766	0.92	0/1025
26	X	0.59	0/587	0.98	2/776 (0.3%)
27	Y	0.61	0/635	0.92	0/848
28	Z	0.51	0/502	0.90	0/667
29	a	0.53	0/453	0.87	0/605
30	b	0.55	0/450	0.89	0/599
31	c	0.55	0/421	1.01	2/561 (0.4%)
32	d	0.66	0/380	0.95	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.62	0/513	0.97	0/676
34	f	0.61	0/303	0.99	0/397
35	g	0.45	1/1663 (0.1%)	1.07	7/2077 (0.3%)
36	h	0.30	0/223	0.83	0/277
37	i	0.27	0/3170	0.73	2/4255 (0.0%)
38	j	0.30	0/283	0.81	0/352
39	k	0.35	0/159	0.76	0/218
40	l	0.26	0/2091	0.68	0/2822
All	All	0.42	4/109794 (0.0%)	0.63	59/163369 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	C	0	1
9	G	0	1
12	J	0	1
35	g	0	1
37	i	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	355	GLY	C-N	6.39	1.42	1.33
12	J	22	PRO	CA-C	5.66	1.57	1.52
8	F	108	VAL	CA-CB	5.42	1.57	1.53
23	U	94	ASP	N-CA	5.24	1.52	1.46

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	155	GLU	CA-C-N	9.35	128.98	119.82
9	G	155	GLU	C-N-CA	9.35	128.98	119.82
35	g	354	PRO	CA-C-N	-9.12	103.53	121.41
35	g	354	PRO	C-N-CA	-9.12	103.53	121.41
12	J	116	ASP	N-CA-C	8.01	123.26	113.17
35	g	356	ILE	N-CA-C	7.79	125.54	109.34
12	J	98	VAL	N-CA-C	7.60	120.36	112.83
35	g	356	ILE	CA-C-N	7.00	134.87	122.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	g	356	ILE	C-N-CA	7.00	134.87	122.48
35	g	355	GLY	CA-C-O	-6.97	108.44	120.57
12	J	22	PRO	N-CA-C	6.57	118.72	110.70
16	N	71	LYS	CA-C-N	6.45	126.68	119.90
16	N	71	LYS	C-N-CA	6.45	126.68	119.90
6	D	142	VAL	CA-C-N	6.32	126.23	119.28
6	D	142	VAL	C-N-CA	6.32	126.23	119.28
6	D	140	HIS	N-CA-C	-6.28	103.71	112.12
14	L	12	ASP	N-CA-C	6.28	117.71	108.86
16	N	108	VAL	CA-C-N	6.26	126.21	119.76
16	N	108	VAL	C-N-CA	6.26	126.21	119.76
8	F	175	PHE	CA-C-N	6.15	126.51	119.93
8	F	175	PHE	C-N-CA	6.15	126.51	119.93
13	K	7	LYS	CA-C-N	6.09	126.54	119.47
13	K	7	LYS	C-N-CA	6.09	126.54	119.47
17	O	70	THR	N-CA-C	6.04	120.81	113.38
35	g	355	GLY	N-CA-C	-5.95	99.08	113.18
15	M	23	ILE	N-CA-C	5.92	117.37	110.62
23	U	89	GLU	N-CA-C	5.89	123.35	110.80
6	D	146	ILE	N-CA-C	5.80	118.57	112.83
14	L	51	LYS	N-CA-C	-5.75	106.02	113.16
9	G	47	ASP	CB-CA-C	-5.71	110.00	116.63
15	M	61	LEU	N-CA-C	5.67	117.22	110.07
31	c	40	ASP	CA-C-N	5.55	125.07	119.19
31	c	40	ASP	C-N-CA	5.55	125.07	119.19
12	J	92	LYS	CA-C-N	5.46	125.72	119.83
12	J	92	LYS	C-N-CA	5.46	125.72	119.83
3	A	2423	U	N1-C1'-C2'	5.36	120.05	112.00
26	X	73	GLY	CA-C-N	5.33	125.00	119.56
26	X	73	GLY	C-N-CA	5.33	125.00	119.56
37	i	390	LYS	CA-C-N	5.29	124.90	119.56
37	i	390	LYS	C-N-CA	5.29	124.90	119.56
10	H	110	VAL	N-CA-C	5.27	116.21	109.30
12	J	119	GLY	N-CA-C	5.23	117.95	111.93
19	Q	21	ARG	CA-C-N	-5.17	114.91	120.03
19	Q	21	ARG	C-N-CA	-5.17	114.91	120.03
16	N	124	LEU	CA-C-N	5.17	124.78	119.56
16	N	124	LEU	C-N-CA	5.17	124.78	119.56
20	R	101	PHE	N-CA-C	5.15	116.97	111.36
15	M	59	ARG	N-CA-C	-5.14	105.85	112.68
8	F	106	ILE	CB-CA-C	-5.13	107.35	111.71
12	J	23	PRO	N-CA-C	5.13	120.27	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	U	88	LYS	N-CA-C	-5.09	102.32	109.96
24	V	49	VAL	CA-C-N	5.08	124.58	119.19
24	V	49	VAL	C-N-CA	5.08	124.58	119.19
12	J	100	LYS	N-CA-C	5.06	117.39	108.75
6	D	191	GLY	N-CA-C	5.05	118.16	111.70
8	F	83	TYR	CA-C-N	-5.04	114.13	119.98
8	F	83	TYR	C-N-CA	-5.04	114.13	119.98
22	T	86	MET	CA-C-N	5.03	125.31	119.93
22	T	86	MET	C-N-CA	5.03	125.31	119.93

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	g	354	PRO	Peptide
37	i	293	ARG	Peptide

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	1	2224	0	1124	16	0
2	2	62	0	34	1	0
3	A	61902	0	31134	740	0
4	B	2569	0	1301	20	0
5	C	2083	0	2154	51	0
6	D	1565	0	1616	34	0
7	E	1552	0	1619	30	0
8	F	1411	0	1444	45	0
9	G	1323	0	1371	34	0
10	H	1110	0	1148	24	0
11	I	946	0	976	30	0
12	J	979	0	1028	42	0
13	K	1129	0	1162	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	L	946	0	1023	22	0
15	M	1053	0	1129	29	0
16	N	1074	0	1157	26	0
17	O	993	0	1034	26	0
18	P	900	0	935	22	0
19	Q	917	0	962	20	0
20	R	947	0	1019	26	0
21	S	816	0	839	23	0
22	T	857	0	922	16	0
23	U	756	0	817	21	0
24	V	780	0	831	16	0
25	W	753	0	780	16	0
26	X	580	0	594	16	0
27	Y	625	0	652	16	0
28	Z	501	0	531	13	0
29	a	449	0	488	9	0
30	b	444	0	458	16	0
31	c	414	0	442	5	0
32	d	377	0	418	7	0
33	e	504	0	572	14	0
34	f	302	0	340	12	0
35	g	1664	0	476	13	0
36	h	224	0	58	0	0
37	i	3384	0	3512	150	0
38	j	284	0	95	0	0
39	k	159	0	189	0	0
40	l	2067	0	2114	32	0
41	f	1	0	0	0	0
42	i	5	0	0	2	0
42	l	5	0	0	1	0
43	i	1	0	0	0	0
43	l	1	0	0	0	0
44	i	28	0	12	3	0
44	l	28	0	12	1	0
All	All	101694	0	68522	1449	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 9.

All (1449) 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)
3:A:1283:G:OP1	37:i:428:LYS:NZ	1.79	1.14
37:i:357:UNK:O	37:i:361:UNK:HG3	1.56	1.05
37:i:349:UNK:O	37:i:352:UNK:HG3	1.60	1.00
37:i:434:GLY:O	37:i:438:UNK:HG3	1.62	0.98
3:A:490:C:H41	37:i:425:ARG:CZ	1.80	0.95
3:A:1460:U:OP1	35:g:355:GLY:C	2.10	0.95
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
3:A:1535:A:C8	37:i:435:UNK:HG2	2.01	0.95
3:A:1283:G:P	37:i:428:LYS:NZ	2.42	0.92
23:U:24:MET:SD	23:U:93:LEU:CD1	2.60	0.90
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
3:A:1283:G:P	37:i:428:LYS:HZ3	1.97	0.88
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86
3:A:276:U:O2	3:A:278:A:N6	2.07	0.86
37:i:362:UNK:O	37:i:365:UNK:HG3	1.75	0.86
1:1:42:A:H61	1:1:67:A:H62	1.23	0.86
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.08	0.86
3:A:287:G:O6	3:A:352:A:N6	2.10	0.85
3:A:2135:A:HO2'	3:A:2159:G:HO2'	1.24	0.85
3:A:2135:A:N6	3:A:2156:G:O2'	2.10	0.84
3:A:2107:G:H1	3:A:2182:U:H3	1.22	0.83
37:i:348:UNK:O	37:i:351:UNK:HG3	1.78	0.83
5:C:107:PRO:HD2	5:C:110:LEU:HD22	1.59	0.83
37:i:349:UNK:O	37:i:352:UNK:CG	2.28	0.81
3:A:2478:A:H5'	34:f:32:LYS:HD3	1.62	0.81
3:A:807:U:OP2	15:M:41:ARG:NH1	2.14	0.81
37:i:436:UNK:O	37:i:440:UNK:HG3	1.80	0.81
15:M:109:LYS:HG2	15:M:126:ARG:HB2	1.64	0.80
3:A:1283:G:OP1	37:i:428:LYS:CE	2.29	0.80
37:i:95:LEU:HD11	37:i:124:LEU:HD22	1.63	0.80
3:A:994:C:O2	21:S:10:LYS:NZ	2.16	0.79
3:A:2128:G:N3	3:A:2173:A:O2'	2.14	0.78
11:I:18:VAL:HG13	11:I:86:MET:SD	2.23	0.78
3:A:1460:U:OP1	35:g:355:GLY:O	2.00	0.78
18:P:15:ARG:NH2	18:P:95:SER:OG	2.18	0.77
11:I:41:LEU:HD21	11:I:96:PHE:HE1	1.50	0.76
30:b:43:ILE:HG22	30:b:49:TYR:HB2	1.66	0.76
3:A:614:A:O2'	3:A:616:A:N7	2.18	0.76
37:i:435:UNK:O	37:i:439:UNK:HG3	1.84	0.76
5:C:245:VAL:HG12	5:C:251:GLN:HA	1.67	0.76
29:a:6:LYS:HG2	29:a:37:GLU:HG2	1.68	0.75
37:i:439:UNK:O	37:i:442:UNK:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2599:G:N7	5:C:236:GLU:HB2	2.02	0.75
37:i:448:UNK:CG	37:i:450:UNK:HG3	2.17	0.74
3:A:1535:A:H8	37:i:436:UNK:N	1.85	0.74
5:C:181:MET:HB2	5:C:268:VAL:HB	1.69	0.74
34:f:18:LYS:HE2	34:f:21:GLY:HA2	1.70	0.73
37:i:346:GLY:O	37:i:350:UNK:N	2.22	0.73
3:A:2848:G:O2'	3:A:2867:G:N2	2.19	0.73
23:U:24:MET:SD	23:U:93:LEU:HD12	2.27	0.73
37:i:438:UNK:HA	37:i:441:UNK:HG3	1.70	0.73
3:A:720:U:H2'	3:A:721:A:C8	2.24	0.72
3:A:331:C:H41	3:A:1210:G:H22	1.37	0.72
3:A:1460:U:OP1	35:g:356:ILE:CA	2.37	0.72
3:A:1460:U:C5	35:g:355:GLY:C	2.68	0.72
3:A:2119:A:N6	3:A:2167:U:O2	2.22	0.72
13:K:70:THR:OG1	13:K:71:ASP:OD1	2.08	0.72
37:i:436:UNK:HA	37:i:439:UNK:HG3	1.71	0.72
3:A:490:C:N4	37:i:425:ARG:CZ	2.39	0.71
7:E:1:MET:HG3	7:E:14:VAL:HG23	1.71	0.71
13:K:131:ASN:OD1	13:K:131:ASN:N	2.22	0.71
37:i:448:UNK:HG2	37:i:450:UNK:HG3	1.73	0.71
3:A:2423:U:H2'	3:A:2424:C:O4'	1.89	0.71
3:A:331:C:H41	3:A:1210:G:N2	1.88	0.71
3:A:2310:C:H2'	8:F:77:PHE:HE2	1.54	0.71
3:A:1535:A:O3'	37:i:434:GLY:HA2	1.91	0.70
3:A:1069:A:H4'	3:A:1070:A:H5"	1.71	0.70
14:L:70:ARG:HD3	14:L:76:VAL:HG22	1.72	0.70
3:A:2163:A:OP1	3:A:2170:A:O2'	2.08	0.70
3:A:258:G:H1'	15:M:104:GLN:HE22	1.56	0.70
37:i:348:UNK:O	37:i:351:UNK:CG	2.38	0.70
3:A:545:U:O2	3:A:548:G:N1	2.19	0.69
37:i:31:LEU:HD22	37:i:52:ILE:HG23	1.73	0.69
3:A:971:G:H2'	3:A:972:A:O4'	1.92	0.69
3:A:1801:A:OP2	5:C:150:LYS:NZ	2.18	0.69
21:S:40:MET:HE2	21:S:42:ALA:HB2	1.74	0.69
11:I:43:LYS:HG2	11:I:46:ARG:HH22	1.56	0.69
3:A:513:A:O2'	20:R:11:ARG:NH1	2.26	0.69
37:i:360:UNK:HG2	37:i:361:UNK:N	2.08	0.69
37:i:356:UNK:O	37:i:359:UNK:HG3	1.93	0.69
3:A:1536:C:H4'	3:A:1537:G:H5"	1.75	0.69
3:A:1340:U:OP1	23:U:19:LYS:NZ	2.26	0.68
3:A:2830:C:H5"	6:D:56:LYS:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:35:ARG:HD3	9:G:71:LEU:HD13	1.73	0.68
37:i:451:UNK:O	37:i:452:UNK:HG3	1.93	0.68
3:A:249:C:O2	33:e:12:LYS:NZ	2.25	0.68
14:L:79:PHE:HD1	19:Q:70:VAL:HG22	1.58	0.68
3:A:63:A:C8	37:i:450:UNK:HB1	2.27	0.68
3:A:362:A:H3'	3:A:363:G:H8	1.59	0.68
12:J:79:LEU:HB3	12:J:109:ILE:HG12	1.76	0.68
37:i:355:UNK:O	37:i:358:UNK:HG3	1.92	0.68
3:A:878:A:H3'	3:A:879:G:H8	1.60	0.67
14:L:21:CYS:HA	14:L:41:ILE:HG22	1.76	0.67
3:A:1535:A:C1'	37:i:435:UNK:HG2	2.24	0.67
4:B:54:G:H21	8:F:26:MET:HE3	1.58	0.67
18:P:31:THR:HG22	18:P:34:HIS:H	1.59	0.67
3:A:358:U:H2'	3:A:359:G:H8	1.60	0.67
3:A:1105:U:H2'	3:A:1106:G:C8	2.29	0.67
3:A:2103:C:O2	3:A:2186:G:N1	2.27	0.67
3:A:196:A:OP2	15:M:47:ARG:NH1	2.28	0.67
27:Y:32:ASN:O	27:Y:52:SER:HA	1.95	0.67
3:A:2122:U:OP1	3:A:2168:G:N2	2.26	0.67
3:A:2713:U:H3'	3:A:2714:G:H5"	1.77	0.67
37:i:141:ARG:NH1	44:i:1003:GDP:O2A	2.28	0.67
3:A:286:U:H2'	3:A:287:G:H8	1.60	0.66
13:K:31:GLU:HG3	13:K:142:ILE:HG13	1.77	0.66
3:A:2216:G:H2'	3:A:2217:G:H8	1.60	0.66
37:i:349:UNK:C	37:i:352:UNK:HG3	2.26	0.66
3:A:1460:U:C6	35:g:355:GLY:O	2.48	0.66
3:A:2135:A:O2'	3:A:2159:G:O2'	2.06	0.66
3:A:2590:A:H2'	3:A:2591:C:H6	1.61	0.66
3:A:286:U:H2'	3:A:287:G:C8	2.31	0.66
3:A:2209:G:H1	3:A:2215:C:H42	1.44	0.66
3:A:2303:G:O2'	8:F:121:SER:O	2.13	0.66
10:H:84:ALA:HA	10:H:90:LEU:HA	1.78	0.66
3:A:2305:U:C2	8:F:151:GLY:HA3	2.31	0.65
4:B:43:C:O2	8:F:92:ARG:NH2	2.28	0.65
3:A:1597:A:H5"	3:A:1598:A:H5'	1.78	0.65
37:i:438:UNK:O	37:i:441:UNK:HG3	1.95	0.65
37:i:113:LYS:N	44:i:1003:GDP:O1B	2.29	0.65
7:E:87:ALA:O	7:E:88:ARG:NH2	2.30	0.65
8:F:158:THR:HG22	8:F:160:ALA:H	1.61	0.65
16:N:50:ARG:O	16:N:54:THR:OG1	2.13	0.65
3:A:572:A:OP2	21:S:80:ARG:NH2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1344:U:O2'	3:A:1345:C:OP1	2.14	0.65
28:Z:10:SER:N	28:Z:13:GLU:OE1	2.26	0.65
9:G:9:VAL:HG22	9:G:69:ARG:HE	1.61	0.65
25:W:2:PHE:HB3	25:W:50:MET:HE3	1.77	0.65
3:A:860:U:H1'	3:A:2268:A:H5'	1.78	0.65
3:A:1283:G:P	37:i:428:LYS:HZ1	2.20	0.65
37:i:350:UNK:O	37:i:354:UNK:HG3	1.97	0.65
3:A:2788:C:O2'	3:A:2809:A:N3	2.28	0.65
3:A:1869:G:N2	3:A:1871:A:O2'	2.30	0.64
3:A:1007:C:OP1	13:K:37:ARG:NH2	2.29	0.64
37:i:350:UNK:O	37:i:353:UNK:HG3	1.96	0.64
3:A:370:G:O2'	3:A:424:G:OP1	2.11	0.64
3:A:1460:U:H5	35:g:355:GLY:C	2.03	0.64
3:A:1535:A:N9	37:i:435:UNK:HG2	2.13	0.64
3:A:1794:A:H2'	3:A:1795:C:H6	1.61	0.64
3:A:490:C:N4	37:i:425:ARG:NH1	2.45	0.64
3:A:968:C:H2'	3:A:969:G:H8	1.62	0.64
3:A:284:U:H3	3:A:356:G:H1	1.44	0.64
3:A:322:A:H5'	3:A:340:A:H1'	1.78	0.64
30:b:28:LEU:HD13	30:b:37:LYS:HB3	1.78	0.64
40:l:132:LEU:HB2	40:l:157:VAL:HG22	1.78	0.64
3:A:1094:U:N3	3:A:1097:U:OP2	2.30	0.64
3:A:1105:U:H2'	3:A:1106:G:H8	1.63	0.64
3:A:1336:A:H4'	37:i:446:UNK:O	1.98	0.64
3:A:1510:G:H2'	3:A:1511:G:C8	2.32	0.64
3:A:2674:G:H4'	14:L:30:ARG:HG3	1.78	0.64
26:X:65:GLY:HA2	26:X:85:GLU:HG2	1.78	0.64
3:A:1980:G:O2'	3:A:1982:U:OP2	2.16	0.63
3:A:2102:G:N2	3:A:2187:U:O2	2.31	0.63
9:G:170:ARG:NH1	34:f:29:ALA:O	2.24	0.63
25:W:21:ARG:NH2	25:W:87:GLN:O	2.29	0.63
3:A:1535:A:C8	37:i:436:UNK:N	2.66	0.63
8:F:144:ASP:N	8:F:144:ASP:OD1	2.30	0.63
16:N:14:LYS:O	16:N:71:LYS:NZ	2.32	0.63
20:R:74:ILE:HD11	20:R:78:LYS:HB3	1.80	0.63
3:A:2424:C:H5"	3:A:2425:A:H5'	1.79	0.63
3:A:1614:A:N1	22:T:93:ALA:HB2	2.13	0.63
40:l:92:LEU:HB2	40:l:275:ARG:HD2	1.79	0.63
37:i:348:UNK:C	37:i:351:UNK:HG3	2.28	0.63
3:A:2151:U:H2'	3:A:2152:G:C8	2.34	0.63
22:T:82:MET:HB3	22:T:84:ARG:HH22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:117:ALA:HA	13:K:120:ARG:HH21	1.63	0.63
37:i:452:UNK:O	37:i:453:UNK:HG2	1.99	0.63
1:1:29:U:O4	1:1:77:A:N6	2.31	0.63
19:Q:91:ALA:HB2	19:Q:113:ARG:HA	1.80	0.63
37:i:350:UNK:HA	37:i:353:UNK:HG3	1.81	0.63
37:i:438:UNK:HA	37:i:441:UNK:CG	2.29	0.63
3:A:825:A:H2'	3:A:826:U:O4'	1.98	0.63
20:R:58:ARG:HA	20:R:61:TRP:CE3	2.34	0.63
37:i:435:UNK:HA	37:i:438:UNK:HG3	1.79	0.63
3:A:1535:A:H1'	37:i:435:UNK:HG2	1.81	0.62
8:F:74:VAL:HG22	8:F:79:ILE:HD11	1.79	0.62
3:A:2742:G:OP2	34:f:24:ARG:NH1	2.32	0.62
3:A:2809:A:H2'	3:A:2810:A:C8	2.34	0.62
21:S:41:ILE:HB	21:S:48:LYS:HD2	1.79	0.62
3:A:1433:A:N1	3:A:1434:A:N6	2.48	0.62
3:A:514:A:N3	3:A:581:C:O2'	2.32	0.62
19:Q:4:ILE:HD12	19:Q:4:ILE:H	1.65	0.62
3:A:784:G:C6	5:C:228:VAL:HG11	2.35	0.62
17:O:49:GLU:HA	17:O:52:ILE:HD12	1.79	0.62
37:i:50:GLU:OE1	37:i:264:HIS:NE2	2.32	0.62
10:H:68:ARG:HA	10:H:71:LYS:HD2	1.81	0.62
3:A:2590:A:H2'	3:A:2591:C:C6	2.35	0.62
16:N:50:ARG:HA	16:N:53:MET:HE3	1.82	0.62
11:I:57:ASN:ND2	11:I:76:PHE:O	2.33	0.61
37:i:438:UNK:C	37:i:441:UNK:HG3	2.30	0.61
3:A:2822:G:O6	17:O:2:ARG:NH1	2.32	0.61
12:J:53:LEU:HD11	12:J:82:LYS:HD2	1.83	0.61
26:X:56:ASP:OD1	26:X:56:ASP:N	2.28	0.61
3:A:2636:C:HO2'	6:D:45:TYR:HH	1.46	0.61
3:A:2639:A:H2'	3:A:2640:G:O4'	2.01	0.61
11:I:41:LEU:HD21	11:I:96:PHE:CE1	2.34	0.61
15:M:57:LEU:HD13	15:M:60:ARG:HH11	1.65	0.61
30:b:38:HIS:ND1	30:b:39:LEU:O	2.30	0.61
3:A:1079:C:O2'	12:J:134:ARG:NH1	2.33	0.61
37:i:434:GLY:O	37:i:438:UNK:CG	2.43	0.61
40:l:122:GLN:HG3	40:l:286:LEU:HD23	1.83	0.61
3:A:503:A:H4'	3:A:504:A:H5'	1.82	0.61
3:A:1001:A:H2'	3:A:1002:G:O4'	2.01	0.61
22:T:6:LYS:HG2	22:T:104:THR:HG23	1.82	0.60
30:b:52:ARG:HB2	30:b:52:ARG:NH2	2.16	0.60
3:A:1076:C:H2'	3:A:1077:A:C8	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:37:U:O4	1:1:68:A:N6	2.34	0.60
3:A:585:G:N7	20:R:6:ARG:NH1	2.48	0.60
3:A:1460:U:C5	35:g:355:GLY:O	2.54	0.60
3:A:2310:C:H2'	8:F:77:PHE:CE2	2.35	0.60
5:C:235:GLY:HA3	5:C:239:ASN:HB2	1.83	0.60
9:G:137:ASP:O	9:G:141:ILE:HG22	2.01	0.60
11:I:27:VAL:HG22	11:I:82:ILE:HG22	1.83	0.60
6:D:12:THR:OG1	6:D:13:ARG:N	2.34	0.60
7:E:97:ASN:N	7:E:97:ASN:OD1	2.34	0.60
15:M:81:ASP:HA	15:M:84:LYS:HD2	1.82	0.60
37:i:253:ASP:OD1	40:l:194:GLN:NE2	2.34	0.60
3:A:570:G:H2'	3:A:2030:A:N7	2.16	0.60
3:A:1794:A:H2'	3:A:1795:C:C6	2.37	0.60
17:O:54:LEU:HD21	17:O:65:LEU:HD23	1.82	0.60
30:b:52:ARG:HB2	30:b:52:ARG:HH21	1.66	0.60
3:A:1251:C:OP2	20:R:6:ARG:NH2	2.35	0.60
3:A:2831:G:OP1	6:D:56:LYS:NZ	2.35	0.60
13:K:36:LEU:HD11	13:K:122:LEU:HB2	1.83	0.60
37:i:435:UNK:HA	37:i:438:UNK:CG	2.32	0.60
3:A:355:U:H2'	3:A:356:G:C8	2.37	0.59
3:A:2615:U:C2	30:b:4:GLN:HA	2.37	0.59
11:I:64:VAL:HG22	11:I:69:PHE:HB2	1.84	0.59
8:F:44:ILE:HG21	8:F:79:ILE:HG22	1.83	0.59
3:A:1363:C:O2'	3:A:1809:A:N3	2.33	0.59
6:D:2:ILE:HG13	6:D:100:LEU:HD21	1.83	0.59
3:A:776:G:O2'	3:A:777:G:OP1	2.19	0.59
3:A:1796:U:H2'	3:A:1797:G:H8	1.67	0.59
3:A:2819:G:H2'	3:A:2821:A:N7	2.17	0.59
6:D:116:LYS:HG3	6:D:165:MET:HE2	1.84	0.59
18:P:99:TYR:OH	18:P:111:ARG:NH1	2.36	0.59
3:A:2584:U:H3'	3:A:2585:U:H5"	1.84	0.59
37:i:335:LEU:HD13	37:i:380:ILE:HG21	1.85	0.59
3:A:878:A:H3'	3:A:879:G:C8	2.38	0.59
9:G:27:LYS:NZ	9:G:27:LYS:HB3	2.17	0.59
25:W:4:ILE:HG12	25:W:50:MET:HE1	1.85	0.59
30:b:50:ARG:HB2	30:b:52:ARG:HH12	1.65	0.59
3:A:2127:G:O2'	3:A:2128:G:O4'	2.20	0.59
3:A:2833:U:O2	37:i:98:GLN:HB2	2.03	0.59
12:J:106:LEU:HB3	12:J:126:THR:HG23	1.85	0.59
37:i:347:UNK:HA	37:i:350:UNK:HG3	1.85	0.59
3:A:1808:A:H3'	3:A:1809:A:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2021:C:OP1	20:R:25:TYR:OH	2.21	0.58
37:i:448:UNK:HG2	37:i:450:UNK:CG	2.33	0.58
3:A:396:G:OP2	27:Y:10:LYS:NZ	2.36	0.58
21:S:37:GLU:HB3	21:S:53:PHE:CE1	2.39	0.58
24:V:81:ASP:OD1	24:V:82:ARG:N	2.35	0.58
1:1:39:A:OP2	37:i:386:LYS:NZ	2.36	0.58
3:A:2205:A:H61	3:A:2219:U:H3	1.50	0.58
17:O:73:ASN:HA	17:O:76:VAL:HG22	1.86	0.58
25:W:76:ASP:OD1	25:W:77:VAL:N	2.37	0.58
42:i:1001:ALF:F3	44:i:1003:GDP:O3B	2.11	0.58
3:A:1130:U:O2'	3:A:1131:G:H8	1.87	0.58
3:A:2127:G:O2'	3:A:2128:G:O5'	2.19	0.58
3:A:2412:A:H2'	3:A:2413:G:O4'	2.04	0.58
33:e:15:LYS:HB2	33:e:23:LYS:HE3	1.84	0.58
37:i:89:GLU:HG2	37:i:287:PRO:HD2	1.84	0.58
6:D:13:ARG:HD2	6:D:15:PHE:CZ	2.38	0.58
3:A:833:A:H2'	3:A:834:G:C8	2.39	0.58
40:l:137:THR:HB	40:l:163:GLY:H	1.69	0.58
37:i:355:UNK:HG2	37:i:356:UNK:N	2.18	0.58
18:P:41:ALA:HB2	18:P:48:LEU:HD21	1.86	0.58
3:A:1342:A:O2'	3:A:1344:U:OP2	2.16	0.57
3:A:1645:G:H5"	3:A:1646:C:H5'	1.86	0.57
17:O:118:ARG:NH2	30:b:54:VAL:O	2.37	0.57
5:C:227:PRO:HG3	5:C:234:GLY:H	1.69	0.57
17:O:94:TYR:O	17:O:116:VAL:HG23	2.05	0.57
37:i:447:UNK:HG3	37:i:453:UNK:O	2.03	0.57
40:l:149:TRP:O	40:l:153:ASN:ND2	2.31	0.57
3:A:2447:G:N2	3:A:2450:A:OP2	2.37	0.57
37:i:194:ARG:NH1	37:i:201:MET:O	2.36	0.57
40:l:222:MET:SD	40:l:250:THR:OG1	2.61	0.57
3:A:1403:A:HO2'	3:A:1471:G:HO2'	1.40	0.57
3:A:849:A:H2'	3:A:850:U:C6	2.39	0.57
6:D:157:LYS:HD2	13:K:80:HIS:CE1	2.40	0.57
7:E:21:ARG:HD3	7:E:106:LYS:HB3	1.85	0.57
12:J:59:ILE:HD13	12:J:69:PHE:HB3	1.86	0.57
3:A:2291:U:H2'	3:A:2292:U:C6	2.38	0.57
37:i:438:UNK:CA	37:i:441:UNK:HG3	2.34	0.57
6:D:148:GLN:HB2	6:D:152:PRO:HD2	1.85	0.57
3:A:340:A:H2'	3:A:341:C:O4'	2.05	0.57
3:A:839:U:H2'	3:A:840:C:C6	2.40	0.57
37:i:67:SER:OG	37:i:73:GLU:OE2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1063:G:H5'	12:J:77:ALA:HB1	1.87	0.56
3:A:1076:C:H2'	3:A:1077:A:H8	1.69	0.56
3:A:1905:C:H2'	3:A:1930:G:C8	2.40	0.56
3:A:2833:U:C6	37:i:97:ALA:HA	2.40	0.56
5:C:166:ALA:HB3	5:C:173:THR:HB	1.86	0.56
7:E:112:LEU:HB3	7:E:118:LEU:HB2	1.87	0.56
23:U:53:VAL:HB	23:U:91:GLN:CD	2.30	0.56
3:A:876:C:H2'	3:A:877:A:O4'	2.05	0.56
3:A:2216:G:H2'	3:A:2217:G:C8	2.40	0.56
11:I:60:LEU:O	11:I:64:VAL:HB	2.05	0.56
25:W:55:GLU:H	25:W:55:GLU:CD	2.13	0.56
3:A:26:G:C6	3:A:27:G:N1	2.73	0.56
3:A:480:A:OP2	24:V:44:LYS:NZ	2.23	0.56
3:A:721:A:H2'	3:A:722:A:C8	2.41	0.56
3:A:1715:G:O2'	3:A:1743:G:O6	2.17	0.56
3:A:2602:A:H4'	3:A:2603:G:O5'	2.04	0.56
8:F:33:LYS:HG2	8:F:157:THR:HB	1.87	0.56
3:A:1796:U:H2'	3:A:1797:G:C8	2.40	0.56
6:D:1:MET:HG2	6:D:2:ILE:H	1.70	0.56
3:A:1187:G:OP1	21:S:85:LYS:NZ	2.31	0.56
10:H:37:VAL:HG22	10:H:38:PRO:HD2	1.86	0.56
12:J:53:LEU:HD22	12:J:78:VAL:HG13	1.87	0.56
3:A:1460:U:H6	35:g:355:GLY:O	1.89	0.56
3:A:2162:G:H5"	3:A:2171:A:H2'	1.86	0.56
13:K:72:LYS:HE3	13:K:74:TYR:CE1	2.39	0.56
37:i:347:UNK:HG2	37:i:348:UNK:N	2.20	0.56
3:A:1790:C:H3'	3:A:1828:G:N2	2.21	0.56
3:A:2298:A:H2'	3:A:2299:U:O4'	2.05	0.56
3:A:2430:A:N3	3:A:2430:A:H2'	2.21	0.56
4:B:42:C:C5	8:F:66:LEU:HD22	2.41	0.56
3:A:299:A:N1	3:A:322:A:O2'	2.27	0.56
3:A:859:G:O2'	3:A:916:G:O6	2.22	0.56
3:A:2491:U:H5"	3:A:2570:G:H5"	1.88	0.56
37:i:9:LEU:HD22	37:i:30:THR:HG23	1.87	0.56
3:A:388:G:N7	3:A:390:U:H2'	2.21	0.56
3:A:849:A:H2'	3:A:850:U:H6	1.70	0.56
9:G:30:ASN:HB3	9:G:79:VAL:HA	1.88	0.56
17:O:2:ARG:NH1	17:O:2:ARG:HB3	2.21	0.56
18:P:16:ARG:HA	18:P:16:ARG:HH21	1.71	0.56
3:A:812:C:H4'	20:R:13:ARG:NH1	2.21	0.55
3:A:1442:U:H2'	3:A:1443:U:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:62:THR:HG22	25:W:71:LYS:HG2	1.88	0.55
30:b:49:TYR:O	30:b:52:ARG:NH2	2.40	0.55
12:J:73:THR:HB	12:J:112:THR:HG22	1.87	0.55
3:A:2783:U:H2'	3:A:2784:U:C6	2.42	0.55
12:J:127:ARG:HA	12:J:130:GLU:HB2	1.89	0.55
3:A:19:A:H2'	3:A:20:C:C6	2.41	0.55
3:A:882:G:H1	3:A:894:U:H3	1.54	0.55
3:A:2390:U:OP2	33:e:35:LYS:NZ	2.22	0.55
10:H:7:ASP:OD1	10:H:8:LYS:N	2.40	0.55
17:O:48:VAL:O	17:O:51:LEU:HB2	2.05	0.55
33:e:17:THR:HG21	33:e:49:MET:HE1	1.87	0.55
37:i:362:UNK:HB2	37:i:365:UNK:HB1	1.89	0.55
3:A:591:U:H2'	3:A:592:A:H8	1.72	0.55
1:1:86:C:OP2	40:l:205:LYS:NZ	2.39	0.55
3:A:639:U:H2'	3:A:640:C:C6	2.42	0.55
3:A:2133:G:H2'	3:A:2157:G:H1	1.70	0.55
32:d:25:LYS:HG3	32:d:29:GLN:HE21	1.72	0.55
3:A:645:C:O2'	3:A:646:U:OP1	2.24	0.55
3:A:2171:A:H3'	3:A:2173:A:C8	2.41	0.55
3:A:184:C:H2'	3:A:185:G:C8	2.41	0.55
8:F:132:VAL:HG22	8:F:152:LEU:HB3	1.88	0.55
8:F:134:GLU:HB3	8:F:136:ILE:HG12	1.89	0.55
3:A:1800:C:H5'	5:C:146:MET:HE1	1.89	0.55
5:C:160:THR:HG22	5:C:177:ARG:HG2	1.89	0.55
24:V:33:LYS:HB3	24:V:64:ALA:HB1	1.87	0.55
37:i:297:MET:HE3	37:i:298:GLY:H	1.71	0.55
3:A:2070:A:H2'	3:A:2071:A:C8	2.42	0.55
3:A:2584:U:H3'	3:A:2585:U:C5'	2.36	0.55
3:A:2591:C:H2'	3:A:2592:G:C8	2.41	0.55
3:A:996:A:OP2	21:S:10:LYS:HD3	2.07	0.54
6:D:8:LYS:HB2	6:D:201:LEU:HD11	1.88	0.54
33:e:29:LEU:HD22	33:e:44:LEU:HB3	1.89	0.54
3:A:586:A:H5'	7:E:84:THR:HG21	1.90	0.54
6:D:184:ARG:NH1	19:Q:7:GLN:OE1	2.40	0.54
37:i:452:UNK:C	37:i:453:UNK:HG2	2.37	0.54
3:A:833:A:H2'	3:A:834:G:H8	1.73	0.54
12:J:56:PRO:HD3	12:J:75:PRO:HD3	1.90	0.54
12:J:79:LEU:HA	12:J:82:LYS:HG2	1.88	0.54
3:A:1837:C:H2'	3:A:1899:A:H61	1.73	0.54
3:A:2262:U:H2'	3:A:2263:C:H6	1.72	0.54
13:K:34:ARG:HH22	13:K:40:HIS:HB3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:172:A:H2'	3:A:173:A:C8	2.43	0.54
3:A:609:A:H2'	3:A:610:C:O4'	2.08	0.54
3:A:2579:C:O2'	6:D:136:ASN:ND2	2.41	0.54
13:K:37:ARG:HG3	13:K:118:MET:HE1	1.89	0.54
3:A:2619:C:H5"	6:D:157:LYS:HG3	1.89	0.54
7:E:88:ARG:HA	7:E:88:ARG:HH21	1.72	0.54
21:S:20:VAL:HG13	21:S:96:VAL:HG23	1.89	0.54
37:i:436:UNK:HA	37:i:439:UNK:CG	2.35	0.54
3:A:720:U:H2'	3:A:721:A:H8	1.72	0.54
3:A:2267:A:H5"	3:A:2268:A:H5"	1.89	0.54
3:A:2424:C:H5"	3:A:2425:A:C5'	2.37	0.54
21:S:48:LYS:HE3	21:S:103:ALA:HB1	1.90	0.54
23:U:68:LYS:HG3	23:U:77:ARG:NH2	2.23	0.54
3:A:1283:G:OP1	37:i:428:LYS:HE2	2.06	0.54
3:A:1460:U:C5	35:g:356:ILE:N	2.76	0.54
33:e:54:ASP:O	33:e:58:VAL:HG23	2.08	0.54
37:i:448:UNK:CG	37:i:450:UNK:CG	2.85	0.54
3:A:1923:U:H2'	3:A:1924:C:C6	2.43	0.54
37:i:134:VAL:HG12	37:i:188:LEU:HB2	1.88	0.54
3:A:1460:U:OP1	35:g:356:ILE:N	2.40	0.53
3:A:2834:G:O6	3:A:2879:A:H2'	2.08	0.53
33:e:27:ALA:O	33:e:28:ASN:HB2	2.07	0.53
3:A:2443:C:H2'	3:A:2444:G:C8	2.43	0.53
9:G:104:ASN:ND2	9:G:114:ASP:OD1	2.41	0.53
11:I:54:VAL:HG22	11:I:81:LEU:HD13	1.90	0.53
3:A:2845:U:H5"	19:Q:52:ASN:O	2.08	0.53
14:L:38:ILE:HD11	14:L:112:PHE:HZ	1.73	0.53
14:L:40:LYS:HE3	14:L:57:VAL:HG12	1.91	0.53
37:i:451:UNK:C	37:i:452:UNK:HG3	2.38	0.53
3:A:1056:G:H5"	3:A:1057:A:H5'	1.90	0.53
3:A:1056:G:O2'	3:A:1103:A:N6	2.40	0.53
3:A:2547:A:H4'	14:L:29:HIS:CD2	2.44	0.53
3:A:9:G:O2'	3:A:2800:A:N6	2.42	0.53
3:A:608:A:H2'	3:A:609:A:C8	2.44	0.53
5:C:145:GLU:HB2	5:C:188:CYS:HB3	1.89	0.53
17:O:36:THR:HG23	17:O:41:ALA:HB2	1.90	0.53
30:b:39:LEU:HB2	30:b:42:HIS:HB2	1.90	0.53
30:b:50:ARG:CB	30:b:52:ARG:HH12	2.21	0.53
5:C:145:GLU:HG2	5:C:151:GLY:C	2.34	0.53
32:d:25:LYS:HB2	32:d:25:LYS:NZ	2.22	0.53
3:A:2171:A:H3'	3:A:2173:A:H8	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:24:MET:CG	23:U:93:LEU:HD12	2.39	0.53
37:i:212:ILE:HG13	37:i:214:PRO:HD3	1.90	0.53
3:A:1535:A:C8	37:i:436:UNK:HB1	2.44	0.53
10:H:116:ARG:HH21	10:H:133:GLN:HB3	1.74	0.53
11:I:88:HIS:ND1	11:I:89:PRO:O	2.42	0.53
3:A:671:C:H2'	3:A:672:C:H6	1.74	0.52
3:A:788:A:OP1	3:A:791:C:N4	2.41	0.52
3:A:1028:A:N3	3:A:2486:C:O2'	2.42	0.52
3:A:1069:A:C2	3:A:1096:A:H5"	2.44	0.52
3:A:2808:G:O2'	3:A:2890:G:O6	2.21	0.52
4:B:93:C:OP2	25:W:18:ARG:NH1	2.41	0.52
5:C:62:TYR:HA	5:C:86:ASN:HD21	1.73	0.52
37:i:448:UNK:HG1	37:i:450:UNK:HG3	1.91	0.52
40:l:114:THR:HG22	40:l:118:LYS:HE3	1.91	0.52
3:A:1428:C:C5	3:A:1569:A:H5"	2.45	0.52
3:A:1993:U:H4'	6:D:133:THR:OG1	2.10	0.52
3:A:2086:U:H2'	3:A:2087:G:C8	2.44	0.52
3:A:2210:U:H4'	3:A:2211:A:H5'	1.91	0.52
3:A:679:C:H2'	3:A:680:C:C6	2.44	0.52
37:i:226:GLY:N	40:l:228:SER:O	2.41	0.52
40:l:192:ARG:HH11	40:l:199:LEU:HB3	1.73	0.52
3:A:1425:G:H2'	3:A:1426:G:O4'	2.09	0.52
13:K:3:THR:HB	20:R:57:PHE:HE1	1.75	0.52
14:L:7:MET:HE1	14:L:44:LYS:HG3	1.91	0.52
3:A:68:G:H2'	3:A:69:C:O4'	2.10	0.52
3:A:120:U:H4'	3:A:121:G:H5"	1.89	0.52
3:A:284:U:O2	3:A:356:G:N2	2.37	0.52
3:A:1873:G:H2'	3:A:1874:C:H6	1.74	0.52
32:d:8:SER:HB3	32:d:11:LYS:HB2	1.92	0.52
3:A:2127:G:H2'	3:A:2128:G:C8	2.45	0.52
8:F:99:PHE:HD1	8:F:102:ARG:HH22	1.57	0.52
18:P:69:ASP:N	18:P:69:ASP:OD1	2.40	0.52
3:A:1289:C:H2'	3:A:1290:C:C6	2.45	0.52
3:A:1421:G:C2	3:A:1422:G:C8	2.98	0.52
3:A:1791:A:N6	3:A:1828:G:O2'	2.42	0.52
7:E:28:VAL:O	7:E:32:VAL:HG13	2.09	0.52
21:S:52:PRO:HG2	21:S:53:PHE:CD2	2.45	0.52
3:A:90:U:H3'	3:A:91:A:H8	1.74	0.52
3:A:2133:G:H21	3:A:2158:A:H62	1.58	0.52
3:A:2637:U:C2'	3:A:2638:G:H5'	2.39	0.52
6:D:114:LYS:HD3	6:D:196:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:263:ILE:HA	40:l:266:VAL:HG22	1.92	0.52
3:A:653:U:H1'	3:A:654:A:H5"	1.91	0.52
3:A:845:A:H61	3:A:932:U:H3	1.58	0.52
3:A:898:C:H2'	3:A:899:A:O4'	2.10	0.52
28:Z:2:LYS:HG3	28:Z:5:GLU:OE1	2.10	0.52
1:1:85:G:H5"	40:l:205:LYS:HB2	1.91	0.52
3:A:1115:G:O2'	3:A:1116:G:H5"	2.10	0.52
3:A:1410:G:H1	3:A:1592:C:H42	1.57	0.52
7:E:41:GLN:HG2	7:E:43:THR:HG23	1.92	0.52
3:A:1451:C:H1'	3:A:1452:G:C2	2.45	0.51
23:U:93:LEU:HD13	23:U:95:PHE:CZ	2.45	0.51
34:f:12:ARG:HB2	34:f:12:ARG:NH1	2.26	0.51
37:i:115:THR:HG22	37:i:119:LYS:HE3	1.92	0.51
3:A:1048:A:N1	3:A:1112:G:O2'	2.36	0.51
3:A:1681:G:H21	3:A:1762:A:H3'	1.75	0.51
3:A:1798:U:H5"	5:C:258:ARG:HB2	1.92	0.51
19:Q:16:ASP:OD1	19:Q:16:ASP:N	2.33	0.51
23:U:56:GLU:HA	23:U:88:LYS:HE3	1.92	0.51
30:b:55:ILE:HG22	30:b:57:LYS:HB2	1.92	0.51
3:A:364:C:H2'	3:A:365:U:C6	2.45	0.51
3:A:968:C:H2'	3:A:969:G:C8	2.42	0.51
8:F:128:TYR:HE2	8:F:130:MET:HG2	1.76	0.51
37:i:141:ARG:NH1	42:i:1001:ALF:F2	2.33	0.51
37:i:350:UNK:HA	37:i:353:UNK:CG	2.40	0.51
3:A:576:U:H2'	3:A:577:G:C8	2.46	0.51
3:A:1790:C:H2'	3:A:1791:A:C5	2.45	0.51
3:A:2045:C:H4'	30:b:15:MET:HG2	1.93	0.51
3:A:2502:G:H5"	3:A:2503:A:H5"	1.92	0.51
3:A:2647:U:H2'	3:A:2648:G:H8	1.76	0.51
7:E:24:ASN:ND2	7:E:27:LEU:HB2	2.25	0.51
17:O:55:ALA:HA	17:O:80:PHE:CE2	2.45	0.51
24:V:18:ASP:OD2	24:V:40:ASN:N	2.38	0.51
24:V:74:ASN:HD21	24:V:99:ASN:HD21	1.58	0.51
3:A:499:U:H2'	3:A:500:G:O4'	2.10	0.51
3:A:1414:C:H2'	3:A:1415:U:O4'	2.11	0.51
3:A:1437:C:H2'	3:A:1438:U:C6	2.46	0.51
3:A:2439:A:H4'	3:A:2440:C:H5"	1.91	0.51
37:i:347:UNK:HA	37:i:350:UNK:CG	2.41	0.51
3:A:141:G:H2'	3:A:142:A:O4'	2.11	0.51
3:A:948:C:H2'	3:A:949:G:C8	2.45	0.51
20:R:24:TYR:N	20:R:24:TYR:CD1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:28:ALA:HB3	21:S:31:GLU:HG3	1.93	0.51
33:e:9:GLY:O	33:e:13:ARG:NH2	2.40	0.51
35:g:353:VAL:O	35:g:356:ILE:N	2.34	0.51
3:A:2271:G:H5"	26:X:18:ALA:HB1	1.93	0.51
3:A:2720:U:OP1	19:Q:53:ARG:NH2	2.41	0.51
12:J:113:LYS:HE3	12:J:116:ASP:HB3	1.92	0.51
3:A:256:A:H2'	3:A:257:C:H6	1.74	0.51
7:E:145:ASP:HA	7:E:166:LYS:HB3	1.93	0.51
8:F:40:VAL:HG11	8:F:43:ALA:HB2	1.92	0.51
33:e:26:HIS:HB3	33:e:44:LEU:HD22	1.93	0.51
37:i:435:UNK:O	37:i:439:UNK:CG	2.56	0.51
3:A:1000:A:OP2	3:A:1154:G:N1	2.32	0.51
33:e:16:LYS:HE3	33:e:20:GLY:HA2	1.93	0.51
42:l:1001:ALF:F3	44:l:1003:GDP:O2B	2.18	0.51
3:A:621:A:OP2	15:M:99:ASN:ND2	2.40	0.51
3:A:1927:A:H2'	3:A:1928:A:C8	2.46	0.51
3:A:2755:C:C4	34:f:19:ARG:NH1	2.79	0.51
15:M:36:LYS:O	15:M:40:SER:HB3	2.11	0.51
29:a:10:THR:HG22	29:a:11:ARG:HG3	1.92	0.51
3:A:1132:U:H2'	3:A:1133:A:C8	2.46	0.50
3:A:1394:U:H4'	3:A:1603:A:H4'	1.92	0.50
3:A:2333:A:P	26:X:77:ARG:HH22	2.34	0.50
13:K:32:LEU:O	13:K:36:LEU:HB2	2.12	0.50
16:N:1:MET:HA	16:N:47:GLU:HG3	1.93	0.50
17:O:36:THR:OG1	17:O:37:THR:N	2.42	0.50
3:A:2564:A:OP1	3:A:2648:G:O2'	2.19	0.50
15:M:23:ILE:HG12	21:S:82:HIS:CD2	2.47	0.50
16:N:30:SER:H	16:N:106:ASP:HB3	1.75	0.50
22:T:23:LEU:HD22	30:b:24:ALA:HB2	1.92	0.50
40:l:128:LYS:HE3	40:l:183:ASP:HB3	1.92	0.50
3:A:2024:G:H2'	3:A:2025:C:H6	1.76	0.50
3:A:2809:A:H2'	3:A:2810:A:H8	1.75	0.50
6:D:184:ARG:HH11	19:Q:7:GLN:CD	2.19	0.50
20:R:76:TYR:CZ	20:R:80:ILE:HG13	2.46	0.50
3:A:128:C:H2'	3:A:129:C:C6	2.46	0.50
3:A:357:C:H2'	3:A:358:U:C6	2.46	0.50
3:A:1405:U:H2'	3:A:1406:U:C6	2.46	0.50
3:A:2282:G:C6	3:A:2425:A:C2	3.00	0.50
12:J:73:THR:OG1	12:J:113:LYS:NZ	2.40	0.50
14:L:64:ARG:NH1	14:L:102:PRO:O	2.44	0.50
22:T:40:ASN:O	22:T:41:LYS:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:7:LEU:HD13	23:U:46:ALA:HA	1.92	0.50
3:A:1939:U:OP1	3:A:2604:U:O2'	2.28	0.50
3:A:90:U:C2	3:A:91:A:N7	2.80	0.50
3:A:256:A:H2'	3:A:257:C:C6	2.46	0.50
8:F:17:MET:SD	8:F:22:TYR:HB2	2.52	0.50
20:R:65:ILE:HD11	20:R:95:LEU:HB2	1.93	0.50
23:U:54:GLU:H	23:U:91:GLN:NE2	2.08	0.50
37:i:215:VAL:HG13	37:i:216:GLU:HG2	1.93	0.50
37:i:347:UNK:CA	37:i:350:UNK:HG3	2.41	0.50
3:A:878:A:N6	3:A:899:A:O2'	2.45	0.50
3:A:981:A:N1	3:A:2027:G:O2'	2.42	0.50
3:A:1327:A:N6	3:A:1647:U:O2	2.45	0.50
3:A:2850:A:N7	3:A:2868:A:O2'	2.39	0.50
9:G:127:THR:HG22	9:G:128:GLN:H	1.77	0.50
3:A:738:G:H1'	3:A:759:G:N2	2.27	0.50
3:A:2576:G:O2'	3:A:2579:C:OP2	2.23	0.50
4:B:2:G:H2'	4:B:3:C:C6	2.47	0.50
12:J:83:ALA:O	12:J:105:GLN:NE2	2.45	0.50
5:C:132:MET:HG2	5:C:135:ILE:HD12	1.94	0.50
23:U:24:MET:SD	23:U:93:LEU:HD13	2.50	0.50
3:A:1638:C:H1'	3:A:2698:U:O2'	2.12	0.49
9:G:83:PHE:O	9:G:134:LYS:HA	2.12	0.49
10:H:94:ILE:HB	10:H:122:LEU:HB2	1.94	0.49
28:Z:39:GLN:HB3	28:Z:41:HIS:CE1	2.47	0.49
3:A:1021:A:H3'	3:A:1021:A:N3	2.27	0.49
3:A:2183:A:H2'	3:A:2184:A:C8	2.46	0.49
24:V:46:GLN:OE1	24:V:54:GLN:NE2	2.44	0.49
37:i:452:UNK:O	37:i:453:UNK:CG	2.60	0.49
3:A:184:C:H2'	3:A:185:G:H8	1.76	0.49
3:A:1506:U:H2'	3:A:1507:C:C6	2.48	0.49
3:A:2626:C:H2'	3:A:2627:G:O4'	2.12	0.49
15:M:4:ASN:OD1	15:M:4:ASN:N	2.39	0.49
19:Q:23:GLY:O	19:Q:90:GLY:HA3	2.11	0.49
25:W:75:GLN:HB2	25:W:92:VAL:HG12	1.94	0.49
37:i:251:ASP:O	40:l:195:ASN:ND2	2.45	0.49
37:i:339:ARG:HA	37:i:342:LYS:HG2	1.94	0.49
3:A:671:C:H2'	3:A:672:C:C6	2.48	0.49
3:A:2747:G:O2'	9:G:67:THR:HG23	2.12	0.49
9:G:8:PRO:HB3	9:G:51:THR:HG22	1.94	0.49
3:A:27:G:N2	3:A:512:G:H1'	2.28	0.49
3:A:613:A:O2'	3:A:614:A:O5'	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2073:C:H2'	3:A:2074:U:H6	1.77	0.49
3:A:2151:U:H2'	3:A:2152:G:H8	1.77	0.49
3:A:2171:A:H5'	3:A:2173:A:N7	2.26	0.49
3:A:2308:G:H3'	3:A:2310:C:OP2	2.11	0.49
37:i:95:LEU:HD11	37:i:124:LEU:CD2	2.40	0.49
3:A:1005:C:H2'	3:A:1006:C:C6	2.47	0.49
3:A:1903:G:C2	3:A:1904:G:C8	3.00	0.49
8:F:50:LEU:O	8:F:54:ALA:N	2.38	0.49
12:J:15:ALA:O	12:J:46:THR:OG1	2.30	0.49
14:L:10:VAL:HG12	14:L:12:ASP:H	1.78	0.49
17:O:14:SER:HA	17:O:17:ARG:NH1	2.27	0.49
37:i:346:GLY:O	37:i:350:UNK:HG3	2.11	0.49
3:A:563:A:C4	3:A:2018:G:C2	3.01	0.49
4:B:7:G:OP1	18:P:4:LYS:NZ	2.27	0.49
3:A:1088:A:N6	12:J:135:SER:HB3	2.26	0.49
3:A:1243:C:H1'	15:M:4:ASN:O	2.13	0.49
9:G:101:ASN:ND2	9:G:116:GLN:OE1	2.45	0.49
18:P:30:ARG:HG3	18:P:35:ILE:HD12	1.94	0.49
37:i:360:UNK:CG	37:i:361:UNK:N	2.75	0.49
37:i:451:UNK:O	37:i:452:UNK:CG	2.61	0.49
35:g:143:PRO:N	35:g:144:GLY:HA2	2.26	0.49
3:A:1606:C:H5'	3:A:1607:C:OP1	2.13	0.49
15:M:19:LEU:HD23	15:M:27:LEU:HD13	1.95	0.49
3:A:160:A:N3	3:A:2208:C:O2'	2.43	0.48
7:E:23:PHE:CD1	7:E:111:GLU:HG3	2.48	0.48
22:T:96:ILE:HD13	22:T:96:ILE:HA	1.74	0.48
27:Y:17:ASN:HB2	27:Y:25:THR:OG1	2.13	0.48
37:i:13:LEU:HD13	37:i:70:PRO:HB2	1.95	0.48
1:1:98:U:H2'	1:1:99:G:H8	1.79	0.48
3:A:467:G:H2'	3:A:468:G:O4'	2.13	0.48
3:A:719:C:H2'	3:A:720:U:H6	1.78	0.48
3:A:1093:G:C2'	3:A:1098:A:H61	2.26	0.48
3:A:2290:G:H2'	3:A:2291:U:O4'	2.12	0.48
4:B:116:G:H2'	4:B:117:G:C8	2.49	0.48
10:H:110:VAL:HG12	10:H:114:GLU:HB2	1.94	0.48
21:S:65:ALA:HB3	21:S:95:ASP:HB2	1.94	0.48
37:i:350:UNK:C	37:i:353:UNK:HG3	2.42	0.48
1:1:53:G:N2	1:1:56:A:OP2	2.45	0.48
3:A:485:C:OP1	37:i:414:ASN:ND2	2.46	0.48
3:A:2833:U:C5	37:i:96:ALA:C	2.91	0.48
7:E:184:ASP:OD1	7:E:184:ASP:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:17:ASN:OD1	27:Y:27:ARG:HD2	2.13	0.48
3:A:813:U:H2'	3:A:814:C:C6	2.49	0.48
3:A:1654:A:H2'	3:A:1655:A:H8	1.78	0.48
3:A:1773:A:N7	3:A:1829:A:H1'	2.28	0.48
3:A:1790:C:H3'	3:A:1828:G:H22	1.77	0.48
11:I:33:VAL:HG21	11:I:106:PHE:CE2	2.48	0.48
25:W:25:LYS:HB3	25:W:25:LYS:HE2	1.71	0.48
26:X:34:GLY:N	26:X:61:ALA:O	2.37	0.48
3:A:1386:C:H2'	3:A:1387:A:C8	2.49	0.48
3:A:1819:A:H5"	5:C:160:THR:HG21	1.94	0.48
3:A:2158:A:H4'	3:A:2159:G:O5'	2.14	0.48
8:F:7:TYR:CD1	8:F:11:GLU:HG3	2.48	0.48
10:H:115:VAL:HG22	10:H:132:PHE:CE2	2.48	0.48
23:U:68:LYS:HG3	23:U:77:ARG:HH21	1.79	0.48
37:i:435:UNK:CA	37:i:438:UNK:HG3	2.43	0.48
3:A:136:G:H2'	3:A:137:U:O4'	2.13	0.48
3:A:428:A:H2'	3:A:429:A:C8	2.49	0.48
3:A:784:G:H5'	3:A:785:G:OP1	2.13	0.48
3:A:2116:G:C5	3:A:2165:C:N4	2.82	0.48
3:A:2834:G:H2'	3:A:2879:A:N6	2.29	0.48
9:G:86:LYS:HG2	9:G:132:VAL:HG22	1.96	0.48
10:H:93:SER:HB3	10:H:123:ARG:HG2	1.95	0.48
26:X:41:ARG:HD3	26:X:41:ARG:HA	1.53	0.48
1:1:48:G:N2	37:i:378:ALA:O	2.38	0.48
3:A:782:A:N7	5:C:220:VAL:HG21	2.29	0.48
3:A:1268:A:H2'	3:A:1269:A:O4'	2.13	0.48
40:l:118:LYS:HD3	40:l:286:LEU:HB2	1.95	0.48
3:A:483:A:O4'	24:V:45:HIS:HB3	2.14	0.48
3:A:795:C:H2'	3:A:796:C:C6	2.49	0.48
3:A:914:G:H5'	3:A:915:C:OP2	2.13	0.48
3:A:1179:G:H2'	3:A:1180:U:C6	2.48	0.48
3:A:2428:G:H21	15:M:60:ARG:NH2	2.12	0.48
9:G:35:ARG:CD	9:G:71:LEU:HD13	2.43	0.48
12:J:113:LYS:O	12:J:117:MET:N	2.46	0.48
13:K:72:LYS:HE3	13:K:74:TYR:CZ	2.49	0.48
26:X:40:GLN:NE2	26:X:43:THR:HA	2.29	0.48
40:l:223:LEU:HB3	40:l:249:ILE:HG12	1.96	0.48
3:A:957:C:C5	3:A:959:A:C5	3.01	0.48
3:A:1527:G:N1	3:A:1544:A:OP2	2.32	0.48
16:N:41:LEU:HG	16:N:96:ILE:HG13	1.94	0.48
1:1:76:G:H2'	1:1:77:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1446:C:H2'	3:A:1447:C:C6	2.49	0.48
3:A:1535:A:C8	37:i:435:UNK:CG	2.88	0.48
3:A:2060:A:H3'	7:E:63:LYS:NZ	2.29	0.48
3:A:2209:G:H1	3:A:2215:C:N4	2.12	0.48
6:D:25:THR:HG21	6:D:193:VAL:HG22	1.95	0.48
14:L:66:LYS:HB3	14:L:66:LYS:HE2	1.64	0.48
16:N:11:LYS:HD3	16:N:86:LYS:HD3	1.96	0.48
27:Y:6:GLN:NE2	27:Y:76:GLU:OE2	2.39	0.48
28:Z:14:LEU:HB3	28:Z:57:LEU:HD21	1.96	0.48
40:l:104:MET:O	40:l:189:THR:OG1	2.23	0.48
3:A:140:C:H4'	3:A:141:G:OP1	2.13	0.47
3:A:156:A:H2'	3:A:157:C:O4'	2.13	0.47
3:A:208:C:H2'	3:A:209:C:H6	1.78	0.47
3:A:477:A:H2'	3:A:478:A:C8	2.49	0.47
3:A:1007:C:H5"	13:K:37:ARG:NH2	2.29	0.47
3:A:1846:G:H5"	3:A:1847:A:OP2	2.14	0.47
3:A:2305:U:H5"	8:F:131:GLY:HA3	1.96	0.47
3:A:2347:C:O2'	31:c:39:PHE:HB3	2.14	0.47
17:O:38:LEU:HB3	17:O:39:PRO:HD3	1.96	0.47
18:P:31:THR:HG23	18:P:32:PRO:HD2	1.96	0.47
37:i:94:ASN:OD1	37:i:96:ALA:HB3	2.14	0.47
3:A:175:G:N2	3:A:176:A:N3	2.62	0.47
3:A:1132:U:H3'	3:A:1133:A:H5"	1.95	0.47
3:A:2444:G:OP2	7:E:63:LYS:HD2	2.14	0.47
3:A:2570:G:H2'	3:A:2571:U:O4'	2.14	0.47
7:E:125:SER:OG	7:E:126:VAL:N	2.46	0.47
14:L:73:ASP:OD1	14:L:73:ASP:N	2.39	0.47
18:P:51:ALA:HB3	18:P:78:VAL:HG13	1.95	0.47
3:A:910:A:H2'	3:A:911:A:C8	2.49	0.47
3:A:911:A:H2'	16:N:9:PHE:HZ	1.78	0.47
3:A:995:C:OP2	20:R:54:LYS:NZ	2.44	0.47
3:A:1085:A:H61	11:I:35:VAL:HG22	1.78	0.47
3:A:1341:G:O2'	23:U:59:ASN:ND2	2.47	0.47
3:A:1438:U:H2'	3:A:1439:A:H8	1.79	0.47
3:A:2433:A:H2	27:Y:21:ALA:HB1	1.79	0.47
23:U:58:VAL:HG22	23:U:85:VAL:HG22	1.96	0.47
5:C:200:HIS:C	5:C:200:HIS:CD2	2.92	0.47
8:F:25:VAL:O	8:F:28:VAL:HG12	2.14	0.47
10:H:142:VAL:HG12	10:H:143:ILE:H	1.79	0.47
12:J:10:LYS:O	12:J:11:LEU:HD12	2.15	0.47
12:J:122:ILE:O	12:J:126:THR:OG1	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:78:THR:HG23	13:K:83:GLY:O	2.13	0.47
31:c:9:ILE:HD13	31:c:25:LYS:HB2	1.95	0.47
37:i:142:PRO:HB2	40:l:145:GLN:HG3	1.96	0.47
3:A:1873:G:H2'	3:A:1874:C:C6	2.49	0.47
3:A:2226:C:H2'	3:A:2227:A:O4'	2.13	0.47
6:D:56:LYS:HB2	6:D:59:ARG:HB2	1.95	0.47
6:D:121:THR:HB	6:D:127:PHE:CD2	2.50	0.47
12:J:40:LYS:N	12:J:40:LYS:HD2	2.30	0.47
15:M:55:MET:SD	15:M:56:PRO:HD2	2.55	0.47
18:P:43:ASN:ND2	18:P:43:ASN:H	2.13	0.47
24:V:14:LEU:HD11	24:V:71:ALA:HB2	1.95	0.47
3:A:112:U:H5'	28:Z:58:ASN:HD21	1.80	0.47
3:A:1027:A:C6	3:A:1126:A:C4	3.02	0.47
3:A:2592:G:C6	3:A:2593:U:N3	2.83	0.47
10:H:29:PHE:O	10:H:32:PRO:HD2	2.15	0.47
12:J:75:PRO:HD2	12:J:78:VAL:HB	1.96	0.47
24:V:41:LEU:HD22	24:V:62:GLU:HG2	1.96	0.47
3:A:127:A:H5"	3:A:128:C:O4'	2.14	0.47
3:A:713:G:H2'	3:A:714:U:C6	2.50	0.47
3:A:911:A:H2'	16:N:9:PHE:CZ	2.50	0.47
3:A:975:A:H1'	3:A:990:A:C2	2.50	0.47
3:A:1420:A:N7	3:A:2211:A:N6	2.62	0.47
3:A:2419:U:O2'	3:A:2420:C:H5'	2.15	0.47
3:A:2557:G:H2'	3:A:2558:C:C6	2.50	0.47
5:C:260:ASN:OD1	5:C:262:ARG:N	2.37	0.47
9:G:102:VAL:HG22	9:G:116:GLN:HE22	1.78	0.47
9:G:155:GLU:OE1	9:G:157:TYR:N	2.44	0.47
10:H:40:THR:HG22	10:H:41:LYS:H	1.79	0.47
13:K:98:GLU:OE1	13:K:98:GLU:N	2.41	0.47
17:O:25:ALA:O	17:O:29:VAL:HG23	2.15	0.47
18:P:30:ARG:HB3	18:P:97:PHE:CE1	2.50	0.47
3:A:323:C:C4	3:A:333:G:C8	3.03	0.47
3:A:1672:A:C6	3:A:1673:G:C6	3.03	0.47
3:A:2047:C:O2'	3:A:2823:A:N1	2.42	0.47
3:A:2431:U:H5	3:A:2433:A:H5"	1.79	0.47
12:J:28:LEU:HD11	12:J:33:VAL:HG11	1.97	0.47
20:R:18:LEU:HD11	20:R:32:TYR:HA	1.97	0.47
27:Y:40:VAL:HG12	27:Y:43:GLU:H	1.80	0.47
37:i:447:UNK:CG	37:i:453:UNK:O	2.63	0.47
3:A:1062:G:N2	12:J:93:PRO:HG2	2.29	0.47
3:A:2339:C:H2'	3:A:2340:A:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:27:VAL:HG13	11:I:80:THR:HG23	1.97	0.47
19:Q:100:LEU:HA	19:Q:100:LEU:HD23	1.67	0.47
20:R:49:ASP:HA	20:R:52:GLN:HB2	1.96	0.47
29:a:31:ARG:HG2	29:a:34:HIS:HB2	1.97	0.47
30:b:36:GLU:OE2	30:b:46:ASP:HB2	2.15	0.47
3:A:2039:U:H2'	3:A:2040:G:C8	2.50	0.47
4:B:116:G:H2'	4:B:117:G:H8	1.80	0.47
7:E:149:ILE:HB	7:E:188:MET:HG2	1.96	0.47
22:T:7:HIS:CE1	22:T:10:ALA:HB2	2.49	0.47
27:Y:62:LYS:HE3	27:Y:66:THR:HG21	1.96	0.47
37:i:436:UNK:CA	37:i:439:UNK:HG3	2.41	0.47
3:A:861:A:H2'	3:A:862:G:O4'	2.15	0.46
3:A:871:U:H2'	3:A:872:U:C6	2.50	0.46
3:A:1097:U:H2'	3:A:1098:A:O4'	2.15	0.46
3:A:2060:A:H3'	7:E:63:LYS:HZ3	1.80	0.46
3:A:2483:C:N3	16:N:123:LYS:NZ	2.60	0.46
3:A:2788:C:H2'	3:A:2789:C:C6	2.50	0.46
13:K:114:LEU:O	13:K:118:MET:HG3	2.14	0.46
31:c:17:THR:HG21	31:c:42:VAL:HB	1.97	0.46
3:A:796:C:H2'	3:A:797:G:C8	2.50	0.46
3:A:825:A:C2	3:A:833:A:C2	3.03	0.46
3:A:857:G:H2'	3:A:858:G:O4'	2.16	0.46
3:A:1510:G:H2'	3:A:1511:G:H8	1.78	0.46
3:A:1689:A:C6	3:A:1700:A:C2	3.03	0.46
3:A:1946:U:H2'	3:A:1947:C:C6	2.51	0.46
3:A:2230:G:H2'	3:A:2231:U:C6	2.51	0.46
11:I:39:THR:HG22	11:I:43:LYS:HE3	1.98	0.46
21:S:38:VAL:O	21:S:54:VAL:HG23	2.15	0.46
3:A:144:A:H1'	23:U:3:ARG:HH22	1.80	0.46
3:A:1038:G:H2'	3:A:1039:A:C8	2.50	0.46
3:A:1060:U:C2	3:A:1062:G:H5'	2.50	0.46
3:A:1508:A:O2'	3:A:1509:A:O4'	2.19	0.46
3:A:2126:A:H61	3:A:2163:A:H5'	1.80	0.46
9:G:42:GLU:CG	9:G:55:ARG:HH21	2.29	0.46
19:Q:88:ARG:NH2	19:Q:112:GLU:HB2	2.31	0.46
3:A:247:G:H4'	3:A:386:G:C5	2.50	0.46
3:A:789:A:C4	32:d:3:ARG:NH1	2.84	0.46
3:A:998:C:H2'	3:A:999:U:O4'	2.14	0.46
3:A:1022:G:O2'	3:A:1024:G:O6	2.27	0.46
5:C:252:THR:OG1	5:C:253:LYS:N	2.48	0.46
9:G:121:ILE:HD13	9:G:135:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:53:THR:HB	18:P:65:THR:HB	1.98	0.46
37:i:228:ASP:OD1	40:l:257:THR:OG1	2.30	0.46
3:A:372:G:O2'	3:A:400:G:O6	2.31	0.46
3:A:861:A:C6	3:A:917:A:C8	3.03	0.46
3:A:1387:A:H5'	3:A:1469:A:H1'	1.97	0.46
3:A:1799:G:C5	5:C:176:LEU:HD13	2.50	0.46
3:A:2392:A:H2	15:M:55:MET:HE3	1.80	0.46
3:A:75:G:H4'	28:Z:48:ARG:CZ	2.45	0.46
3:A:358:U:H2'	3:A:359:G:C8	2.44	0.46
3:A:1028:A:N6	3:A:1125:G:H2'	2.30	0.46
3:A:2821:A:H2'	3:A:2822:G:C8	2.51	0.46
4:B:95:U:H2'	4:B:96:G:H8	1.81	0.46
5:C:125:LYS:HE2	5:C:125:LYS:HB2	1.77	0.46
6:D:7:LYS:HB3	6:D:7:LYS:HE2	1.78	0.46
16:N:66:ARG:HB2	16:N:101:VAL:O	2.16	0.46
19:Q:106:LYS:O	19:Q:109:ARG:NH2	2.45	0.46
24:V:81:ASP:OD2	24:V:96:PHE:HB3	2.16	0.46
3:A:490:C:H41	37:i:425:ARG:NH1	2.06	0.46
3:A:880:G:N2	3:A:898:C:C2	2.84	0.46
3:A:1808:A:H3'	3:A:1809:A:H8	1.79	0.46
3:A:2786:U:H2'	3:A:2787:C:H6	1.79	0.46
13:K:95:ARG:HG2	13:K:96:ARG:N	2.30	0.46
14:L:79:PHE:CD1	19:Q:70:VAL:HG22	2.46	0.46
25:W:2:PHE:HB3	25:W:50:MET:CE	2.44	0.46
40:l:110:VAL:HG12	40:l:226:ASP:HB2	1.97	0.46
3:A:532:A:N3	3:A:532:A:H2'	2.31	0.46
5:C:232:HIS:NE2	5:C:244:PRO:HA	2.30	0.46
11:I:30:SER:HB3	11:I:81:LEU:HB2	1.98	0.46
30:b:52:ARG:HB3	30:b:54:VAL:HG13	1.98	0.46
37:i:278:LYS:HB3	37:i:280:GLU:OE1	2.15	0.46
37:i:350:UNK:CA	37:i:353:UNK:HG3	2.45	0.46
3:A:125:A:OP2	32:d:19:ARG:HD3	2.15	0.46
3:A:1149:G:H2'	3:A:1150:C:C6	2.50	0.46
3:A:1342:A:C6	3:A:1397:U:C5	3.04	0.46
3:A:1848:A:H3'	3:A:1849:G:H8	1.80	0.46
3:A:1869:G:N2	3:A:1873:G:C5	2.83	0.46
3:A:2069:G:N2	3:A:2443:C:C2	2.83	0.46
3:A:2229:U:H2'	3:A:2230:G:C8	2.51	0.46
5:C:243:HIS:HA	5:C:244:PRO:HD3	1.79	0.46
33:e:24:HIS:ND1	33:e:25:LYS:O	2.43	0.46
3:A:1563:U:H2'	3:A:1564:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1631:G:N2	3:A:1634:A:OP2	2.32	0.45
6:D:207:VAL:HG13	6:D:208:LYS:HG3	1.98	0.45
17:O:28:LEU:O	17:O:32:GLU:N	2.45	0.45
37:i:107:GLY:HA2	37:i:219:PHE:HE1	1.81	0.45
3:A:483:A:H5"	24:V:47:LYS:HG2	1.97	0.45
3:A:772:C:H2'	3:A:773:U:C6	2.52	0.45
3:A:878:A:H5'	3:A:879:G:OP2	2.16	0.45
3:A:1570:A:H5'	5:C:36:LYS:HB2	1.98	0.45
3:A:1706:C:O2'	3:A:1757:A:H5'	2.17	0.45
3:A:1785:A:O2'	3:A:1786:A:H2'	2.16	0.45
12:J:80:LEU:HB3	12:J:138:LEU:CD1	2.46	0.45
22:T:13:SER:O	22:T:17:VAL:HG23	2.17	0.45
22:T:25:ARG:NH2	22:T:74:ILE:O	2.49	0.45
40:l:118:LYS:HB3	40:l:286:LEU:HB2	1.98	0.45
3:A:257:C:H2'	3:A:258:G:O4'	2.16	0.45
3:A:1313:U:H2'	3:A:1610:A:C2	2.51	0.45
3:A:1653:G:H3'	17:O:2:ARG:HG3	1.98	0.45
3:A:2344:U:OP1	31:c:37:LYS:HD2	2.16	0.45
5:C:160:THR:O	5:C:195:VAL:HG23	2.17	0.45
8:F:136:ILE:HG22	8:F:141:ILE:HG21	1.98	0.45
37:i:96:ALA:O	37:i:97:ALA:O	2.33	0.45
37:i:436:UNK:HG2	37:i:437:UNK:N	2.31	0.45
3:A:558:U:OP1	13:K:114:LEU:N	2.46	0.45
3:A:1086:A:H4'	3:A:1103:A:C2	2.52	0.45
3:A:2396:G:N3	3:A:2421:G:N2	2.64	0.45
7:E:1:MET:HE3	7:E:1:MET:HB2	1.88	0.45
9:G:155:GLU:OE2	9:G:158:LYS:N	2.48	0.45
11:I:53:ARG:O	11:I:81:LEU:HD12	2.16	0.45
15:M:27:LEU:O	15:M:31:GLY:HA2	2.17	0.45
18:P:88:LYS:HG2	18:P:116:GLN:HB2	1.98	0.45
20:R:105:ALA:HB1	21:S:40:MET:HE1	1.98	0.45
24:V:37:GLU:O	24:V:39:ILE:HG12	2.17	0.45
3:A:706:A:C2	3:A:707:G:H1'	2.52	0.45
3:A:831:G:H5"	15:M:37:GLY:HA2	1.97	0.45
3:A:1466:U:H5"	3:A:1467:U:H5'	1.98	0.45
3:A:1709:U:H2'	3:A:1710:G:H8	1.80	0.45
3:A:2165:C:H2'	3:A:2166:U:O4'	2.16	0.45
6:D:99:GLU:OE2	6:D:182:ALA:HB2	2.16	0.45
8:F:20:PHE:CZ	8:F:165:GLU:HA	2.51	0.45
26:X:23:VAL:HG22	26:X:38:VAL:HB	1.99	0.45
37:i:237:ASN:HB2	37:i:266:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2052:A:OP1	6:D:146:ILE:HG12	2.17	0.45
9:G:80:THR:OG1	9:G:81:GLU:N	2.46	0.45
16:N:65:ILE:HG12	16:N:103:TYR:CD2	2.51	0.45
17:O:17:ARG:HG2	17:O:21:PHE:HE2	1.82	0.45
23:U:34:VAL:HG21	23:U:43:ILE:HD11	1.99	0.45
40:l:240:PHE:HB3	40:l:246:LEU:HD21	1.98	0.45
3:A:111:A:H2'	3:A:112:U:O4'	2.16	0.45
3:A:208:C:H2'	3:A:209:C:C6	2.52	0.45
3:A:499:U:H5"	24:V:43:LYS:HE3	1.99	0.45
3:A:1918:A:O2'	3:A:1920:C:N4	2.50	0.45
3:A:2273:A:H2'	3:A:2274:A:C8	2.52	0.45
3:A:2327:A:H2'	3:A:2328:A:C8	2.51	0.45
3:A:2433:A:H5'	3:A:2434:A:P	2.57	0.45
3:A:2667:C:H1'	9:G:109:PHE:HD1	1.82	0.45
3:A:2683:C:H4'	6:D:13:ARG:HH12	1.81	0.45
8:F:73:SER:OG	8:F:81:GLN:N	2.33	0.45
10:H:62:LEU:HD23	10:H:135:HIS:CD2	2.52	0.45
18:P:85:LYS:HE2	18:P:85:LYS:HB3	1.79	0.45
29:a:56:LYS:NZ	29:a:58:GLU:HG2	2.31	0.45
3:A:593:U:H2'	3:A:594:U:C6	2.52	0.45
3:A:594:U:H2'	3:A:595:C:C6	2.51	0.45
3:A:613:A:O2'	3:A:614:A:N3	2.44	0.45
3:A:1536:C:OP1	37:i:434:GLY:N	2.49	0.45
3:A:1545:A:H2'	3:A:1546:G:O4'	2.17	0.45
11:I:41:LEU:HB2	11:I:99:PHE:CE1	2.52	0.45
12:J:117:MET:HB2	12:J:125:MET:HG2	1.99	0.45
21:S:4:VAL:HA	21:S:12:HIS:O	2.17	0.45
3:A:77:G:H2'	3:A:78:U:O4'	2.16	0.45
3:A:629:G:H5"	3:A:650:C:O2'	2.16	0.45
3:A:908:C:O2'	16:N:70:ASP:OD2	2.30	0.45
3:A:976:G:HO2'	3:A:1155:A:HO2'	1.60	0.45
3:A:1848:A:N3	3:A:1849:G:C8	2.84	0.45
3:A:2134:A:H1'	3:A:2159:G:H21	1.82	0.45
6:D:49:GLN:HA	6:D:80:TRP:O	2.16	0.45
11:I:93:ALA:O	11:I:97:LYS:NZ	2.41	0.45
12:J:130:GLU:HB3	12:J:134:ARG:NH2	2.32	0.45
14:L:25:LEU:HD23	14:L:25:LEU:HA	1.67	0.45
21:S:40:MET:HE3	21:S:47:VAL:HG13	1.99	0.45
33:e:29:LEU:HD12	33:e:29:LEU:HA	1.57	0.45
37:i:143:ALA:HB1	40:l:141:ALA:HB1	1.98	0.45
3:A:198:C:O2'	3:A:199:A:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:239:C:H2'	3:A:240:C:O4'	2.16	0.45
3:A:657:U:H2'	3:A:658:U:C6	2.52	0.45
3:A:718:A:H2'	3:A:719:C:O4'	2.16	0.45
3:A:1535:A:N7	37:i:436:UNK:HB1	2.32	0.45
3:A:2313:C:H5"	8:F:88:LYS:HD3	1.98	0.45
3:A:2396:G:C2	3:A:2421:G:C2	3.05	0.45
3:A:2524:G:H2'	3:A:2525:G:O4'	2.16	0.45
12:J:86:ILE:CD1	12:J:138:LEU:HD21	2.46	0.45
13:K:69:ARG:O	13:K:89:PHE:HB3	2.17	0.45
17:O:2:ARG:HB3	17:O:2:ARG:CZ	2.46	0.45
3:A:141:G:C8	3:A:141:G:H3'	2.51	0.44
3:A:948:C:H1'	3:A:984:A:C8	2.52	0.44
3:A:1287:A:H3'	3:A:1288:G:N2	2.32	0.44
3:A:2667:C:H1'	9:G:109:PHE:CD1	2.52	0.44
15:M:10:GLU:OE2	15:M:11:GLY:N	2.50	0.44
25:W:83:LYS:HB3	25:W:85:LYS:HG3	1.98	0.44
26:X:55:ARG:HE	26:X:55:ARG:HB2	1.45	0.44
3:A:154:U:H2'	3:A:155:A:C8	2.53	0.44
3:A:172:A:H2'	3:A:173:A:H8	1.81	0.44
3:A:620:G:H4'	3:A:621:A:O5'	2.17	0.44
3:A:764:A:H5'	5:C:209:GLY:HA2	1.98	0.44
3:A:1420:A:N7	3:A:2211:A:C6	2.86	0.44
3:A:1450:G:C6	3:A:1451:C:N4	2.86	0.44
3:A:1972:G:H2'	3:A:1973:G:H8	1.82	0.44
3:A:2292:U:H2'	3:A:2293:G:C8	2.52	0.44
9:G:117:LEU:HD13	9:G:121:ILE:HG22	1.99	0.44
10:H:100:ALA:O	10:H:104:THR:HG23	2.17	0.44
13:K:65:THR:O	13:K:68:LYS:HB2	2.16	0.44
19:Q:89:ARG:HB3	19:Q:113:ARG:NH1	2.32	0.44
37:i:233:ALA:HB2	37:i:262:ILE:HG12	1.99	0.44
3:A:239:C:HO2'	3:A:622:G:HO2'	1.60	0.44
3:A:630:G:N2	3:A:633:A:OP2	2.43	0.44
3:A:1177:G:H2'	3:A:1178:C:C6	2.51	0.44
19:Q:62:ARG:NH2	19:Q:101:ARG:HG2	2.33	0.44
21:S:27:ILE:HG22	21:S:28:ALA:O	2.18	0.44
22:T:46:LEU:HD23	22:T:46:LEU:HA	1.82	0.44
37:i:219:PHE:HE2	37:i:233:ALA:HA	1.82	0.44
40:l:188:ASP:OD1	40:l:189:THR:N	2.50	0.44
3:A:356:G:H2'	3:A:357:C:O4'	2.17	0.44
14:L:99:ILE:HG12	14:L:118:LEU:HB2	1.98	0.44
22:T:28:LYS:HB2	22:T:28:LYS:HE2	1.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:57:C:H2'	3:A:58:G:O4'	2.18	0.44
3:A:1082:U:H4'	11:I:46:ARG:NH1	2.32	0.44
3:A:1198:U:H2'	3:A:1199:U:C6	2.52	0.44
3:A:1591:A:H2'	3:A:1592:C:C6	2.53	0.44
3:A:2318:G:C6	3:A:2319:G:N1	2.85	0.44
3:A:2489:U:C4	3:A:2490:G:C6	3.06	0.44
3:A:2569:G:C2	3:A:2570:G:C8	3.05	0.44
3:A:2742:G:P	34:f:24:ARG:HH12	2.40	0.44
5:C:141:VAL:HG12	5:C:192:LEU:HA	1.98	0.44
7:E:121:VAL:O	7:E:189:THR:HA	2.18	0.44
9:G:148:LEU:HD23	9:G:148:LEU:HA	1.71	0.44
16:N:90:GLU:HB3	16:N:91:TYR:CD1	2.53	0.44
26:X:36:ILE:HG23	26:X:58:THR:HG23	2.00	0.44
3:A:181:A:H1'	3:A:435:C:O4'	2.17	0.44
3:A:997:G:H5"	20:R:92:ARG:NH1	2.33	0.44
3:A:1230:A:H2'	3:A:1231:U:O4'	2.17	0.44
3:A:1535:A:O3'	37:i:434:GLY:CA	2.65	0.44
3:A:2387:U:H1'	26:X:41:ARG:NH1	2.33	0.44
3:A:2654:A:OP1	3:A:2654:A:H8	2.01	0.44
3:A:2776:A:C8	3:A:2782:G:C5	3.05	0.44
8:F:147:ASP:OD1	8:F:150:ARG:NH2	2.51	0.44
9:G:42:GLU:HG3	9:G:55:ARG:HH21	1.83	0.44
25:W:21:ARG:HE	25:W:87:GLN:HA	1.83	0.44
28:Z:56:LEU:HD22	28:Z:56:LEU:HA	1.82	0.44
29:a:9:GLN:HB2	29:a:29:LEU:HD13	2.00	0.44
37:i:102:VAL:HB	37:i:214:PRO:HA	1.99	0.44
3:A:2024:G:H2'	3:A:2025:C:C6	2.53	0.44
3:A:2377:A:H2'	3:A:2378:A:C8	2.53	0.44
3:A:2683:C:H4'	6:D:13:ARG:NH1	2.33	0.44
3:A:2704:C:H2'	3:A:2705:A:O4'	2.17	0.44
8:F:67:ILE:HD12	8:F:84:PRO:HB3	2.00	0.44
15:M:70:LYS:O	15:M:74:THR:OG1	2.31	0.44
17:O:86:ARG:HD3	17:O:121:LYS:HG3	1.99	0.44
27:Y:59:ILE:HG12	27:Y:67:VAL:HG21	2.00	0.44
37:i:446:UNK:O	37:i:446:UNK:HG2	2.18	0.44
3:A:149:A:C2	3:A:150:U:C2	3.06	0.44
3:A:277:G:H4'	3:A:278:A:N7	2.33	0.44
3:A:677:A:O2'	3:A:2071:A:H5'	2.17	0.44
3:A:1301:A:H2'	3:A:1301:A:N3	2.33	0.44
3:A:1535:A:H8	37:i:435:UNK:C	2.30	0.44
3:A:2230:G:H1'	27:Y:32:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:24:MET:CG	23:U:93:LEU:CD1	2.96	0.44
3:A:870:U:OP1	16:N:6:ARG:NH1	2.51	0.44
3:A:1266:G:N2	3:A:2012:G:H2'	2.33	0.44
3:A:1853:A:N6	3:A:1888:G:O2'	2.51	0.44
5:C:205:LEU:HD23	5:C:205:LEU:HA	1.68	0.44
9:G:44:LYS:HE3	9:G:44:LYS:HB2	1.80	0.44
16:N:95:LEU:HA	16:N:95:LEU:HD23	1.77	0.44
19:Q:53:ARG:HB2	19:Q:56:HIS:HB2	1.99	0.44
37:i:6:THR:HG22	37:i:75:VAL:HG21	2.00	0.44
37:i:141:ARG:HA	37:i:142:PRO:HD3	1.90	0.44
3:A:11:C:H2'	3:A:12:U:H5'	2.00	0.43
3:A:973:A:OP2	21:S:81:LYS:HE3	2.18	0.43
3:A:1082:U:O2'	11:I:39:THR:HG23	2.18	0.43
3:A:1614:A:C2	22:T:93:ALA:HB2	2.52	0.43
3:A:2678:C:H2'	3:A:2679:A:O4'	2.18	0.43
8:F:48:LYS:HE2	8:F:48:LYS:HB2	1.85	0.43
16:N:97:GLN:CD	16:N:97:GLN:N	2.76	0.43
19:Q:25:THR:HB	19:Q:88:ARG:HG2	1.99	0.43
23:U:31:VAL:O	23:U:32:LEU:HD23	2.18	0.43
25:W:21:ARG:HH21	25:W:87:GLN:C	2.22	0.43
3:A:463:G:N1	3:A:467:G:C6	2.86	0.43
3:A:566:U:H5"	15:M:29:LYS:HE3	1.99	0.43
3:A:834:G:C2	3:A:835:C:C2	3.06	0.43
3:A:1287:A:H5'	17:O:103:ARG:HD2	1.98	0.43
3:A:1735:A:H2'	3:A:1736:U:O4'	2.18	0.43
3:A:1962:C:H4'	3:A:1963:U:C5	2.52	0.43
3:A:2172:U:H4'	3:A:2173:A:H5'	2.01	0.43
8:F:138:PHE:HA	8:F:139:PRO:HD3	1.90	0.43
8:F:170:LEU:HD23	8:F:170:LEU:HA	1.75	0.43
10:H:26:ALA:HA	10:H:30:LEU:HB2	1.99	0.43
18:P:52:SER:O	18:P:58:ILE:HD12	2.18	0.43
34:f:2:LYS:HD3	34:f:4:ARG:NH2	2.33	0.43
37:i:196:HIS:HA	37:i:202:MET:HE3	2.00	0.43
37:i:354:UNK:HB2	37:i:357:UNK:HG3	2.00	0.43
40:l:110:VAL:HG23	40:l:112:LYS:HG3	2.00	0.43
3:A:380:G:H2'	3:A:381:G:O4'	2.18	0.43
3:A:1068:G:N2	3:A:1095:A:O3'	2.44	0.43
3:A:1354:A:H2'	3:A:1355:G:O4'	2.19	0.43
3:A:1627:G:C2	3:A:1628:G:C8	3.07	0.43
3:A:2443:C:H2'	3:A:2444:G:H8	1.82	0.43
8:F:128:TYR:CE2	8:F:130:MET:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:46:PHE:HD1	10:H:50:ARG:NH2	2.16	0.43
12:J:90:SER:HB2	12:J:136:MET:O	2.18	0.43
3:A:33:C:N4	3:A:446:G:O2'	2.45	0.43
3:A:1056:G:H1'	3:A:1103:A:N6	2.33	0.43
3:A:1205:A:H2'	7:E:165:HIS:HE1	1.83	0.43
3:A:1667:G:N2	3:A:1992:G:OP2	2.44	0.43
3:A:1710:G:H2'	3:A:1711:A:C8	2.53	0.43
3:A:2114:A:C2	3:A:2166:U:H2'	2.53	0.43
3:A:2847:U:H2'	3:A:2848:G:O4'	2.18	0.43
15:M:80:SER:O	15:M:84:LYS:HE3	2.19	0.43
16:N:26:VAL:HB	16:N:133:LYS:HB2	2.00	0.43
18:P:18:LEU:HA	18:P:18:LEU:HD23	1.71	0.43
22:T:47:VAL:HG22	22:T:103:ILE:HD13	2.00	0.43
3:A:475:C:N4	3:A:476:G:C6	2.86	0.43
3:A:969:G:H2'	3:A:970:U:C6	2.53	0.43
3:A:1093:G:H1'	3:A:1099:G:N1	2.32	0.43
3:A:1515:A:H3'	3:A:1516:G:H8	1.84	0.43
3:A:2280:G:O2'	3:A:2388:A:N1	2.37	0.43
3:A:2647:U:H2'	3:A:2648:G:C8	2.54	0.43
3:A:2786:U:H2'	3:A:2787:C:C6	2.53	0.43
4:B:114:C:H2'	4:B:115:A:H8	1.83	0.43
5:C:153:GLN:O	5:C:156:ARG:HG3	2.18	0.43
6:D:131:ASP:O	6:D:140:HIS:HD2	2.01	0.43
20:R:24:TYR:O	20:R:29:SER:HB3	2.19	0.43
20:R:117:LEU:HD23	20:R:117:LEU:HA	1.77	0.43
34:f:2:LYS:HE2	34:f:2:LYS:HB3	1.77	0.43
3:A:783:A:C5	3:A:785:G:H1'	2.53	0.43
3:A:1351:C:H4'	3:A:1572:A:O4'	2.18	0.43
3:A:1542:U:H2'	3:A:1543:G:O4'	2.18	0.43
3:A:1858:A:H2'	3:A:1859:U:O4'	2.17	0.43
5:C:33:LEU:HA	5:C:33:LEU:HD23	1.58	0.43
12:J:110:ALA:O	12:J:114:ALA:HB2	2.18	0.43
20:R:9:ILE:H	20:R:9:ILE:HD12	1.84	0.43
21:S:91:GLN:NE2	21:S:92:TRP:H	2.16	0.43
1:1:72:A:H2'	1:1:73:G:H8	1.82	0.43
3:A:674:G:H2'	3:A:804:A:H61	1.83	0.43
3:A:686:U:O4	32:d:12:ARG:NH1	2.52	0.43
3:A:1434:A:C2	3:A:1435:G:C5	3.07	0.43
3:A:1517:G:C2	3:A:1732:C:N3	2.86	0.43
3:A:1759:A:H2'	3:A:1760:C:C6	2.54	0.43
3:A:1922:G:H2'	3:A:1923:U:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2144:G:N2	3:A:2148:G:O6	2.52	0.43
3:A:2512:C:H5"	3:A:2513:A:OP2	2.17	0.43
8:F:145:LYS:HA	8:F:145:LYS:HD3	1.89	0.43
16:N:133:LYS:HE3	16:N:133:LYS:HB3	1.42	0.43
21:S:4:VAL:HG12	21:S:39:LEU:HB2	2.00	0.43
22:T:7:HIS:C	22:T:7:HIS:CD2	2.96	0.43
23:U:34:VAL:HG11	23:U:43:ILE:HD13	2.01	0.43
40:l:221:VAL:HB	40:l:247:THR:H	1.84	0.43
3:A:14:A:C6	3:A:526:A:C2	3.07	0.43
3:A:93:G:H2'	3:A:94:A:H8	1.84	0.43
3:A:112:U:H5'	28:Z:58:ASN:ND2	2.34	0.43
3:A:141:G:C8	3:A:142:A:O4'	2.72	0.43
3:A:1736:U:H2'	3:A:1737:G:O4'	2.18	0.43
3:A:2292:U:H2'	3:A:2293:G:H8	1.84	0.43
3:A:2588:G:O6	3:A:2607:G:C6	2.72	0.43
3:A:2646:C:OP2	3:A:2732:G:O2'	2.35	0.43
4:B:49:C:H2'	4:B:50:A:C8	2.54	0.43
5:C:90:ASN:ND2	5:C:197:ASN:HB2	2.34	0.43
7:E:108:ILE:O	7:E:112:LEU:HG	2.18	0.43
15:M:41:ARG:H	15:M:41:ARG:HG2	1.62	0.43
34:f:22:VAL:HG12	34:f:24:ARG:HG3	2.00	0.43
3:A:195:A:H5"	15:M:47:ARG:HH22	1.84	0.43
3:A:461:C:H2'	3:A:462:C:H6	1.84	0.43
3:A:1062:G:O2'	12:J:135:SER:OG	2.32	0.43
3:A:1494:A:H2'	3:A:1495:A:H8	1.84	0.43
6:D:109:VAL:HG12	6:D:201:LEU:HD22	2.01	0.43
6:D:148:GLN:OE1	6:D:148:GLN:N	2.51	0.43
7:E:29:HIS:O	7:E:32:VAL:HG22	2.19	0.43
7:E:181:ILE:H	7:E:181:ILE:HG13	1.69	0.43
14:L:3:GLN:HE21	14:L:3:GLN:HB3	1.66	0.43
17:O:72:ASP:OD1	17:O:73:ASN:N	2.51	0.43
20:R:74:ILE:HG12	20:R:75:SER:N	2.34	0.43
26:X:47:ALA:HB1	26:X:51:VAL:O	2.19	0.43
37:i:46:PRO:HA	37:i:49:ARG:HE	1.84	0.43
37:i:134:VAL:HG23	37:i:159:PHE:HD1	1.83	0.43
1:1:33:C:H6	1:1:33:C:O5'	2.02	0.43
3:A:76:C:H6	3:A:76:C:O5'	2.02	0.43
3:A:493:G:H2'	3:A:494:G:O4'	2.19	0.43
3:A:1088:A:H61	12:J:135:SER:HB3	1.83	0.43
3:A:1590:A:H2'	3:A:1591:A:C8	2.54	0.43
3:A:2038:G:H2'	3:A:2039:U:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2130:U:O2'	3:A:2133:G:O2'	2.32	0.43
3:A:2843:G:H2'	3:A:2844:G:C8	2.54	0.43
5:C:8:PRO:HB3	5:C:14:ARG:HG3	1.99	0.43
5:C:245:VAL:HA	5:C:252:THR:HG22	2.01	0.43
7:E:128:ALA:O	7:E:130:LYS:N	2.51	0.43
20:R:17:ILE:HD13	20:R:17:ILE:HA	1.62	0.43
31:c:33:LYS:HD3	31:c:33:LYS:HA	1.74	0.43
34:f:1:MET:HB2	34:f:1:MET:HE2	1.75	0.43
40:l:279:VAL:HG22	40:l:285:ASP:O	2.19	0.43
40:l:292:ASP:OD1	40:l:292:ASP:N	2.51	0.43
3:A:464:U:C2	3:A:788:A:C6	3.06	0.42
3:A:573:U:O4	3:A:2029:G:O2'	2.36	0.42
3:A:1501:G:H2'	3:A:1502:A:H8	1.84	0.42
3:A:1614:A:H8	3:A:1614:A:O5'	2.02	0.42
3:A:2138:G:C6	3:A:2154:A:C2	3.06	0.42
3:A:2518:A:H2'	3:A:2518:A:N3	2.34	0.42
4:B:66:A:H61	4:B:107:G:H2'	1.84	0.42
8:F:79:ILE:HG21	8:F:85:ILE:HD11	2.01	0.42
10:H:62:LEU:HD22	10:H:137:GLU:OE1	2.19	0.42
10:H:104:THR:HA	10:H:108:VAL:O	2.19	0.42
16:N:33:LEU:HD11	16:N:128:THR:HB	2.00	0.42
19:Q:40:LEU:HD23	19:Q:40:LEU:HA	1.75	0.42
37:i:426:MET:O	37:i:430:MET:HG2	2.19	0.42
40:l:49:GLU:OE2	40:l:52:ARG:NH2	2.42	0.42
3:A:5:A:H2'	3:A:6:A:C8	2.54	0.42
3:A:307:G:N1	3:A:310:A:OP2	2.52	0.42
3:A:653:U:C1'	3:A:654:A:H5"	2.49	0.42
3:A:1044:C:O2'	3:A:1111:A:N1	2.45	0.42
3:A:1141:U:H4'	3:A:1142:A:O4'	2.19	0.42
3:A:1387:A:H2'	3:A:1388:G:O4'	2.18	0.42
5:C:133:ARG:HD2	10:H:123:ARG:NH1	2.35	0.42
8:F:4:LEU:HD23	8:F:4:LEU:HA	1.73	0.42
13:K:26:GLY:O	13:K:30:THR:HG23	2.18	0.42
14:L:11:ALA:O	14:L:100:PHE:N	2.46	0.42
3:A:729:G:H2'	3:A:1775:U:H1'	2.01	0.42
3:A:819:A:N3	3:A:819:A:H2'	2.34	0.42
3:A:1637:A:H2'	3:A:1638:C:C6	2.54	0.42
3:A:1751:U:H2'	3:A:1752:C:C6	2.54	0.42
3:A:1798:U:OP2	5:C:271:ARG:NH2	2.52	0.42
3:A:2184:A:H2'	3:A:2185:U:C6	2.53	0.42
3:A:2304:G:H22	3:A:2312:U:H3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2533:U:OP1	3:A:2665:A:O2'	2.34	0.42
3:A:2771:C:H2'	3:A:2772:C:C6	2.54	0.42
9:G:149:ARG:HG3	9:G:162:VAL:O	2.20	0.42
11:I:15:VAL:HG11	11:I:60:LEU:CD2	2.50	0.42
11:I:118:ILE:HA	11:I:119:PRO:HD2	1.84	0.42
15:M:6:LEU:HD23	15:M:6:LEU:HA	1.82	0.42
16:N:36:VAL:HG13	25:W:82:TYR:CD2	2.55	0.42
25:W:29:ILE:O	25:W:91:PHE:HB2	2.19	0.42
3:A:543:G:H5'	3:A:544:C:OP2	2.18	0.42
3:A:729:G:C5	5:C:207:LYS:HB2	2.55	0.42
3:A:987:C:O2'	3:A:1000:A:N3	2.44	0.42
3:A:1064:C:H5"	12:J:88:SER:HB2	2.01	0.42
3:A:1327:A:H2'	3:A:1328:A:O4'	2.19	0.42
3:A:1463:C:H2'	3:A:1464:G:H8	1.84	0.42
3:A:1524:G:H2'	3:A:1525:A:O4'	2.20	0.42
3:A:2322:A:C4	3:A:2323:G:C8	3.07	0.42
3:A:2776:A:C2	3:A:2778:A:C4	3.07	0.42
3:A:2790:U:H5'	3:A:2893:A:N7	2.34	0.42
4:B:57:A:C4	8:F:26:MET:HB3	2.54	0.42
5:C:210:ALA:HA	5:C:213:TRP:CE3	2.53	0.42
12:J:33:VAL:HG13	12:J:67:PHE:CD2	2.54	0.42
12:J:113:LYS:HA	12:J:116:ASP:HB2	2.01	0.42
19:Q:106:LYS:O	19:Q:109:ARG:HD3	2.20	0.42
20:R:24:TYR:N	20:R:24:TYR:HD1	2.17	0.42
29:a:17:LEU:HD23	29:a:17:LEU:HA	1.76	0.42
3:A:675:A:OP1	7:E:58:LYS:NZ	2.52	0.42
3:A:1039:A:H2'	3:A:1040:A:O4'	2.19	0.42
3:A:1047:G:OP1	11:I:56:ARG:NH1	2.52	0.42
3:A:1324:G:C4	3:A:1328:A:N6	2.88	0.42
3:A:1473:G:H2'	3:A:1474:U:O4'	2.19	0.42
3:A:1780:A:H3'	3:A:1781:U:H2'	2.01	0.42
4:B:106:G:H2'	4:B:107:G:O4'	2.19	0.42
19:Q:34:GLU:CD	19:Q:39:ARG:HB2	2.44	0.42
24:V:61:LYS:HG2	24:V:62:GLU:H	1.85	0.42
35:g:299:GLY:O	35:g:304:THR:N	2.42	0.42
37:i:434:GLY:HA3	37:i:437:UNK:HG3	2.02	0.42
1:1:72:A:H2'	1:1:73:G:C8	2.55	0.42
3:A:794:A:H2'	3:A:795:C:C6	2.55	0.42
3:A:1400:U:H2'	3:A:1401:G:O4'	2.19	0.42
3:A:2700:A:H2'	3:A:2701:U:C6	2.54	0.42
7:E:109:LEU:HA	7:E:109:LEU:HD23	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:97:ALA:HB3	9:G:104:ASN:HB2	2.01	0.42
12:J:22:PRO:HB2	12:J:23:PRO:HD3	2.02	0.42
14:L:65:THR:HB	14:L:68:GLY:H	1.84	0.42
37:i:222:ASP:OD1	37:i:223:ALA:N	2.52	0.42
37:i:348:UNK:HG2	37:i:349:UNK:N	2.34	0.42
3:A:647:G:H2'	3:A:648:G:C8	2.55	0.42
3:A:669:G:N2	3:A:670:A:C2	2.88	0.42
3:A:1597:A:C5'	3:A:1598:A:H5'	2.47	0.42
3:A:1759:A:C2	3:A:2697:G:H1'	2.54	0.42
3:A:2433:A:H5'	3:A:2434:A:OP2	2.19	0.42
5:C:24:LEU:HA	5:C:24:LEU:HD12	1.66	0.42
7:E:63:LYS:HZ2	7:E:63:LYS:HG2	1.67	0.42
16:N:42:THR:N	16:N:45:GLN:OE1	2.47	0.42
20:R:47:TYR:C	20:R:47:TYR:CD2	2.98	0.42
25:W:2:PHE:HE1	25:W:53:LYS:HD2	1.84	0.42
29:a:51:VAL:HG23	29:a:55:VAL:HG21	2.00	0.42
37:i:39:LEU:HD21	37:i:45:LEU:HD13	2.02	0.42
37:i:47:VAL:HG22	37:i:264:HIS:CD2	2.54	0.42
37:i:59:ALA:HA	37:i:62:HIS:NE2	2.35	0.42
3:A:123:G:N2	3:A:129:C:C2	2.87	0.42
3:A:812:C:C2	3:A:1250:G:N1	2.87	0.42
3:A:910:A:C6	3:A:911:A:C6	3.08	0.42
3:A:1065:U:H2'	3:A:1066:U:O4'	2.19	0.42
3:A:2119:A:H62	3:A:2167:U:H1'	1.85	0.42
6:D:73:VAL:HG11	6:D:93:GLY:HA2	2.01	0.42
12:J:38:PHE:CD1	12:J:59:ILE:HD11	2.54	0.42
12:J:103:ARG:H	12:J:103:ARG:HD2	1.83	0.42
13:K:96:ARG:HA	13:K:97:PRO:HD2	1.92	0.42
37:i:354:UNK:HB2	37:i:357:UNK:CG	2.50	0.42
37:i:355:UNK:O	37:i:358:UNK:CG	2.66	0.42
37:i:362:UNK:O	37:i:365:UNK:CG	2.57	0.42
3:A:565:C:H4'	3:A:1253:A:C6	2.55	0.42
3:A:571:U:H3'	21:S:80:ARG:NH2	2.34	0.42
3:A:1482:G:H2'	3:A:1483:G:H8	1.84	0.42
3:A:1877:A:H2'	3:A:1878:G:O4'	2.20	0.42
8:F:34:ILE:HB	8:F:96:MET:HG3	2.02	0.42
10:H:94:ILE:HG23	10:H:98:ASP:HB2	2.01	0.42
17:O:103:ARG:HB3	17:O:106:ASP:OD1	2.20	0.42
20:R:31:VAL:HG12	20:R:34:VAL:H	1.85	0.42
3:A:1449:G:N2	3:A:1463:C:C2	2.88	0.42
3:A:1681:G:O2'	3:A:1762:A:N3	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1902:C:H4'	5:C:242:LYS:O	2.19	0.42
3:A:1946:U:H2'	3:A:1947:C:H6	1.84	0.42
3:A:2209:G:C2	3:A:2216:G:C2	3.08	0.42
3:A:2466:C:OP1	34:f:4:ARG:HB2	2.20	0.42
4:B:48:U:H4'	18:P:100:HIS:HD2	1.84	0.42
8:F:79:ILE:HD12	8:F:79:ILE:O	2.20	0.42
10:H:1:MET:O	10:H:20:ASN:HA	2.20	0.42
3:A:335:C:H5"	24:V:82:ARG:HD2	2.02	0.41
3:A:1509:A:O2'	3:A:1510:G:H8	2.03	0.41
3:A:2339:C:O3'	4:B:41:G:N2	2.52	0.41
12:J:74:PRO:HA	12:J:75:PRO:HD3	1.89	0.41
22:T:33:LEU:HD23	22:T:33:LEU:HA	1.66	0.41
27:Y:26:LYS:HD3	27:Y:26:LYS:HA	1.88	0.41
37:i:43:VAL:HG22	37:i:257:GLY:HA3	2.02	0.41
37:i:47:VAL:HG21	37:i:261:SER:HA	2.02	0.41
37:i:341:MET:O	37:i:345:GLY:N	2.53	0.41
3:A:53:A:H2'	3:A:54:G:O4'	2.20	0.41
3:A:877:A:C6	3:A:899:A:C6	3.08	0.41
3:A:1417:C:H2'	3:A:1418:G:C8	2.55	0.41
3:A:1463:C:H2'	3:A:1464:G:C8	2.55	0.41
3:A:2812:G:H2'	3:A:2813:A:O4'	2.20	0.41
8:F:57:LEU:HD12	8:F:87:CYS:SG	2.61	0.41
8:F:70:ALA:HB3	8:F:81:GLN:HA	2.02	0.41
8:F:130:MET:HB2	8:F:130:MET:HE3	1.81	0.41
3:A:118:A:N3	3:A:178:G:H1'	2.36	0.41
3:A:297:G:H2'	3:A:298:G:O4'	2.20	0.41
3:A:848:C:H42	3:A:930:G:H1	1.68	0.41
3:A:1056:G:H5'	11:I:35:VAL:HG21	2.02	0.41
3:A:1432:G:H2'	3:A:1433:A:C8	2.55	0.41
3:A:1499:C:H2'	3:A:1500:G:H8	1.85	0.41
3:A:1709:U:H2'	3:A:1710:G:C8	2.55	0.41
3:A:1821:A:H2'	3:A:1822:C:C6	2.55	0.41
3:A:1825:U:O2	5:C:253:LYS:NZ	2.31	0.41
3:A:2267:A:H5"	3:A:2268:A:C5'	2.50	0.41
3:A:2286:G:C8	3:A:2287:A:N6	2.88	0.41
3:A:2365:G:H4'	26:X:60:PHE:CE2	2.55	0.41
3:A:2706:A:C2	3:A:2707:U:C2	3.08	0.41
5:C:176:LEU:HB2	5:C:180:GLU:O	2.20	0.41
11:I:43:LYS:HE2	12:J:118:THR:HA	2.01	0.41
29:a:51:VAL:O	29:a:55:VAL:HG22	2.20	0.41
37:i:83:VAL:HG22	37:i:288:ASP:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:117:VAL:HG21	37:i:190:ASP:HB2	2.02	0.41
3:A:75:G:H4'	28:Z:48:ARG:NH2	2.35	0.41
3:A:393:C:H2'	3:A:394:C:H6	1.85	0.41
3:A:481:G:O2'	3:A:507:A:N1	2.45	0.41
3:A:799:G:C6	3:A:800:A:C6	3.08	0.41
3:A:1484:U:H2'	3:A:1485:U:C6	2.55	0.41
3:A:1880:U:H2'	3:A:1881:C:C6	2.55	0.41
9:G:83:PHE:HB2	9:G:135:GLY:O	2.21	0.41
13:K:58:ASN:ND2	13:K:128:ASN:OD1	2.42	0.41
3:A:648:G:C2	3:A:649:G:C5	3.08	0.41
3:A:1078:U:O2	3:A:1088:A:H3'	2.21	0.41
3:A:1607:C:O2'	3:A:1608:A:OP1	2.37	0.41
3:A:2102:G:C2	3:A:2187:U:O2	2.73	0.41
3:A:2838:G:H2'	3:A:2839:G:O4'	2.20	0.41
3:A:2860:A:H5"	3:A:2861:U:OP2	2.21	0.41
27:Y:3:ARG:NE	27:Y:30:LEU:HD13	2.35	0.41
3:A:328:U:H4'	24:V:66:GLN:HE21	1.86	0.41
3:A:1005:C:H2'	3:A:1006:C:H6	1.84	0.41
3:A:1057:A:N7	3:A:1086:A:H2'	2.35	0.41
3:A:1073:A:H2'	3:A:1074:G:O4'	2.21	0.41
3:A:1366:A:H2'	3:A:1367:A:O4'	2.21	0.41
3:A:1770:G:C6	3:A:1983:G:C6	3.07	0.41
3:A:1972:G:H2'	3:A:1973:G:C8	2.55	0.41
4:B:71:C:C2	4:B:106:G:C2	3.08	0.41
7:E:170:ARG:HD3	7:E:170:ARG:HA	1.91	0.41
14:L:71:ARG:HA	14:L:71:ARG:HD3	1.81	0.41
14:L:93:GLN:HA	14:L:94:PRO:HD3	1.88	0.41
16:N:65:ILE:HG12	16:N:103:TYR:HD2	1.85	0.41
32:d:22:MET:O	32:d:28:ARG:NH1	2.53	0.41
3:A:528:A:C8	3:A:2042:A:C2	3.09	0.41
3:A:2895:G:H2'	3:A:2896:C:C6	2.55	0.41
4:B:95:U:H2'	4:B:96:G:C8	2.56	0.41
9:G:73:ASN:O	9:G:77:ILE:HG13	2.20	0.41
9:G:76:VAL:O	9:G:80:THR:HG23	2.20	0.41
3:A:561:G:H4'	20:R:48:ARG:HH22	1.86	0.41
3:A:678:C:H2'	3:A:679:C:H6	1.84	0.41
3:A:681:G:C2	3:A:797:G:C2	3.09	0.41
3:A:779:U:H2'	3:A:780:G:C8	2.56	0.41
3:A:948:C:H2'	3:A:949:G:H8	1.85	0.41
3:A:1789:A:H2'	3:A:1790:C:O4'	2.21	0.41
8:F:36:LEU:HA	8:F:153:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:154:PRO:HA	9:G:160:LYS:O	2.21	0.41
10:H:128:HIS:O	10:H:143:ILE:HA	2.20	0.41
15:M:3:LEU:HD23	15:M:3:LEU:HA	1.77	0.41
15:M:78:ARG:HG2	15:M:113:ALA:HB3	2.03	0.41
37:i:355:UNK:CG	37:i:356:UNK:N	2.84	0.41
1:1:98:U:H2'	1:1:99:G:C8	2.55	0.41
1:1:100:G:H5"	40:l:179:ALA:HB2	2.02	0.41
3:A:31:C:O3'	3:A:1238:G:H5'	2.21	0.41
3:A:449:A:C4	3:A:450:G:C8	3.08	0.41
3:A:520:G:H2'	3:A:521:U:C6	2.56	0.41
3:A:601:C:O2'	3:A:605:G:H5"	2.21	0.41
3:A:776:G:HO2'	3:A:777:G:P	2.41	0.41
3:A:807:U:H2'	3:A:808:G:H8	1.85	0.41
3:A:1024:G:C6	3:A:1025:G:C6	3.09	0.41
3:A:1869:G:C2	3:A:1873:G:C6	3.09	0.41
3:A:2061:G:H2'	3:A:2501:C:O2'	2.21	0.41
3:A:2352:A:N1	26:X:34:GLY:HA3	2.35	0.41
3:A:2578:G:OP2	3:A:2578:G:H4'	2.20	0.41
3:A:2627:G:H1'	3:A:2777:G:N2	2.36	0.41
3:A:2785:C:H2'	3:A:2786:U:H6	1.85	0.41
8:F:13:VAL:O	8:F:17:MET:HB2	2.21	0.41
9:G:9:VAL:HG23	9:G:52:PHE:HE1	1.86	0.41
16:N:6:ARG:CZ	16:N:6:ARG:HB2	2.50	0.41
17:O:72:ASP:O	17:O:76:VAL:HG13	2.21	0.41
22:T:109:ASP:OD1	22:T:110:ARG:N	2.54	0.41
27:Y:54:LYS:O	27:Y:58:VAL:HG23	2.19	0.41
37:i:69:THR:HG22	37:i:72:GLN:H	1.86	0.41
3:A:64:A:C6	3:A:65:U:C4	3.09	0.41
3:A:465:G:C6	3:A:466:A:N6	2.89	0.41
3:A:811:U:C2	3:A:1251:C:C5	3.09	0.41
3:A:1130:U:HO2'	3:A:1131:G:H8	1.69	0.41
3:A:1341:G:C2	3:A:1398:C:H4'	2.56	0.41
3:A:1374:G:H8	3:A:1374:G:OP2	2.04	0.41
3:A:1423:G:N2	3:A:1576:U:O2	2.54	0.41
3:A:1672:A:N6	3:A:1673:G:C6	2.89	0.41
3:A:2343:U:H2'	3:A:2344:U:C6	2.55	0.41
3:A:2394:C:H42	3:A:2422:C:N4	2.19	0.41
3:A:2550:G:C6	3:A:2551:C:C4	3.09	0.41
3:A:2682:A:C2	6:D:23:PRO:HB3	2.56	0.41
3:A:2847:U:C5	3:A:2848:G:C5	3.09	0.41
4:B:7:G:H5"	18:P:29:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:17:ARG:HA	14:L:17:ARG:HD3	1.77	0.41
27:Y:3:ARG:O	27:Y:12:PRO:HD3	2.21	0.41
28:Z:21:LEU:HD23	28:Z:21:LEU:HA	1.82	0.41
28:Z:38:GLN:HG3	28:Z:39:GLN:H	1.85	0.41
33:e:6:THR:O	33:e:8:ARG:HG2	2.21	0.41
37:i:430:MET:HE1	37:i:438:UNK:HB2	2.02	0.41
2:2:74:C:O5'	2:2:74:C:H6	2.04	0.40
3:A:141:G:C8	3:A:141:G:C3'	3.04	0.40
3:A:277:G:H4'	3:A:278:A:C5	2.56	0.40
3:A:501:A:H2'	3:A:502:A:C8	2.56	0.40
3:A:778:G:H5"	3:A:779:U:OP2	2.21	0.40
3:A:997:G:OP1	20:R:92:ARG:HD2	2.21	0.40
3:A:1365:A:N3	3:A:1365:A:H2'	2.36	0.40
3:A:1818:U:C5	5:C:156:ARG:NH2	2.90	0.40
3:A:2663:G:H2'	3:A:2664:G:O4'	2.21	0.40
5:C:34:LEU:HD21	5:C:63:ARG:HG3	2.03	0.40
5:C:176:LEU:HA	5:C:176:LEU:HD23	1.80	0.40
7:E:67:ARG:HE	7:E:67:ARG:HB3	1.61	0.40
8:F:65:PRO:HA	8:F:89:VAL:HG22	2.02	0.40
11:I:99:PHE:HD2	11:I:106:PHE:HZ	1.69	0.40
16:N:38:ARG:HB2	16:N:98:PRO:HD3	2.03	0.40
18:P:115:LEU:HD23	18:P:117:PHE:CE2	2.56	0.40
18:P:115:LEU:HD23	18:P:117:PHE:HE2	1.86	0.40
21:S:85:LYS:HE2	21:S:85:LYS:HB3	1.80	0.40
23:U:49:LYS:HG3	23:U:50:LEU:HD23	2.03	0.40
27:Y:72:ARG:HG3	27:Y:78:TYR:HE2	1.86	0.40
28:Z:42:LEU:HA	28:Z:42:LEU:HD23	1.81	0.40
37:i:35:ARG:HB2	37:i:52:ILE:HD11	2.02	0.40
37:i:448:UNK:HG3	37:i:453:UNK:O	2.20	0.40
3:A:396:G:H1'	27:Y:29:PHE:HB3	2.02	0.40
3:A:729:G:C6	5:C:207:LYS:HB2	2.56	0.40
3:A:743:A:OP1	6:D:135:GLY:HA2	2.21	0.40
3:A:863:A:H2'	3:A:864:G:H8	1.86	0.40
3:A:2423:U:H2'	3:A:2424:C:C1'	2.51	0.40
3:A:2431:U:O2	3:A:2431:U:O4'	2.39	0.40
3:A:2600:A:H2'	3:A:2601:C:C6	2.56	0.40
8:F:28:VAL:HA	8:F:29:PRO:HD3	1.91	0.40
12:J:42:PHE:CE1	12:J:57:VAL:HB	2.56	0.40
33:e:38:THR:HA	33:e:41:LYS:HE3	2.03	0.40
37:i:105:MET:HE1	37:i:120:LEU:HD12	2.03	0.40
37:i:331:LEU:HG	37:i:420:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:68:A:H2'	1:1:69:G:C8	2.56	0.40
3:A:42:A:C6	3:A:43:G:C5	3.10	0.40
3:A:118:A:C8	3:A:119:A:C8	3.09	0.40
3:A:199:A:N6	3:A:2434:A:C5	2.89	0.40
3:A:353:C:H2'	3:A:354:A:O4'	2.22	0.40
3:A:717:C:C5	3:A:718:A:C8	3.10	0.40
3:A:719:C:H2'	3:A:720:U:C6	2.57	0.40
3:A:871:U:H4'	16:N:68:PHE:CD2	2.56	0.40
3:A:2143:C:H2'	3:A:2144:G:O4'	2.21	0.40
3:A:2229:U:H2'	3:A:2230:G:H8	1.85	0.40
3:A:2421:G:H4'	3:A:2421:G:OP1	2.21	0.40
4:B:68:C:H2'	4:B:69:G:O4'	2.22	0.40
11:I:13:ALA:O	11:I:17:GLU:HB2	2.22	0.40
11:I:48:ALA:HB3	11:I:50:VAL:HG23	2.03	0.40
11:I:61:ARG:HG2	11:I:73:LYS:HG2	2.02	0.40
14:L:103:VAL:HB	14:L:107:LEU:HD12	2.02	0.40
15:M:79:LEU:HB2	15:M:113:ALA:O	2.21	0.40
17:O:65:LEU:HA	17:O:65:LEU:HD12	1.85	0.40
26:X:70:GLU:HG3	26:X:72:LYS:HE2	2.04	0.40
29:a:45:ARG:HH12	29:a:59:GLU:CD	2.29	0.40
40:l:255:ASP:OD1	40:l:255:ASP:N	2.40	0.40
3:A:1:G:H2'	3:A:2:G:C8	2.56	0.40
3:A:445:C:H2'	3:A:446:G:O4'	2.22	0.40
3:A:1071:G:O2'	3:A:1089:A:OP2	2.36	0.40
3:A:1127:A:N7	3:A:2488:G:O2'	2.54	0.40
3:A:1275:A:OP2	3:A:1646:C:N4	2.52	0.40
3:A:1462:C:O2'	3:A:2702:G:O2'	2.35	0.40
3:A:1807:G:N2	3:A:1811:G:C5	2.89	0.40
3:A:2365:G:P	26:X:55:ARG:HG2	2.61	0.40
3:A:2388:A:H5'	3:A:2389:G:OP2	2.21	0.40
5:C:251:GLN:HE21	5:C:251:GLN:HB2	1.58	0.40
9:G:90:VAL:HG21	9:G:163:ARG:NH1	2.37	0.40
11:I:100:ALA:HB2	11:I:106:PHE:CE1	2.56	0.40
15:M:81:ASP:HB3	15:M:100:ILE:HD13	2.02	0.40
17:O:22:ARG:HG3	17:O:70:THR:HA	2.03	0.40
23:U:24:MET:HE2	23:U:24:MET:HB3	1.89	0.40
3:A:362:A:H3'	3:A:363:G:C8	2.48	0.40
3:A:447:A:C5	3:A:473:G:C5	3.10	0.40
3:A:863:A:H2'	3:A:864:G:C8	2.57	0.40
3:A:1139:G:H8	3:A:1139:G:OP2	2.05	0.40
3:A:1234:U:H2'	3:A:1235:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1945:G:C5	3:A:1946:U:C4	3.09	0.40
3:A:2283:C:C2	3:A:2389:G:C2	3.09	0.40
3:A:2392:A:C2	15:M:55:MET:HE3	2.57	0.40
3:A:2563:U:O2	3:A:2566:A:C5	2.75	0.40
3:A:2603:G:C6	3:A:2604:U:C4	3.10	0.40
5:C:157:SER:O	5:C:160:THR:OG1	2.38	0.40
6:D:13:ARG:HD2	6:D:15:PHE:CE2	2.56	0.40
10:H:60:GLU:HA	10:H:63:ALA:HB3	2.04	0.40
12:J:93:PRO:C	12:J:95:LYS:H	2.29	0.40
12:J:97:LYS:HE2	12:J:139:VAL:HG12	2.03	0.40
17:O:35:LYS:HE2	17:O:110:MET:HE3	2.03	0.40
18:P:25:ARG:O	18:P:25:ARG:HG3	2.22	0.40
28:Z:46:VAL:O	28:Z:50:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	269/271 (99%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
9	G	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	18	55
11	I	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	16	52
12	J	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
20	R	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
23	U	93/95 (98%)	89 (96%)	3 (3%)	1 (1%)	11	45
24	V	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
29	a	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	b	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
31	c	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	g	414/416 (100%)	402 (97%)	12 (3%)	0	100	100
36	h	54/56 (96%)	54 (100%)	0	0	100	100
37	i	408/450 (91%)	397 (97%)	10 (2%)	1 (0%)	43	78
38	j	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
39	k	21/23 (91%)	18 (86%)	3 (14%)	0	100	100
40	l	269/271 (99%)	265 (98%)	4 (2%)	0	100	100
All	All	4667/4779 (98%)	4520 (97%)	143 (3%)	4 (0%)	49	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	i	97	ALA
23	U	89	GLU

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Mol	Chain	Res	Type
10	H	118	PRO
11	I	108	VAL

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
5	C	216/216 (100%)	190 (88%)	26 (12%)	5 18
6	D	164/164 (100%)	148 (90%)	16 (10%)	7 24
7	E	165/165 (100%)	149 (90%)	16 (10%)	8 25
8	F	148/148 (100%)	127 (86%)	21 (14%)	3 14
9	G	137/137 (100%)	126 (92%)	11 (8%)	11 31
10	H	114/114 (100%)	100 (88%)	14 (12%)	4 18
11	I	95/95 (100%)	86 (90%)	9 (10%)	8 25
12	J	104/104 (100%)	88 (85%)	16 (15%)	2 13
13	K	116/116 (100%)	99 (85%)	17 (15%)	3 14
14	L	104/104 (100%)	96 (92%)	8 (8%)	12 32
15	M	103/103 (100%)	92 (89%)	11 (11%)	6 22
16	N	109/109 (100%)	99 (91%)	10 (9%)	8 27
17	O	102/102 (100%)	95 (93%)	7 (7%)	14 36
18	P	87/87 (100%)	70 (80%)	17 (20%)	1 8
19	Q	99/99 (100%)	88 (89%)	11 (11%)	6 20
20	R	89/89 (100%)	79 (89%)	10 (11%)	6 20
21	S	84/84 (100%)	73 (87%)	11 (13%)	4 16
22	T	93/93 (100%)	84 (90%)	9 (10%)	8 25
23	U	82/82 (100%)	77 (94%)	5 (6%)	17 39
24	V	83/83 (100%)	75 (90%)	8 (10%)	8 25
25	W	78/78 (100%)	72 (92%)	6 (8%)	12 32
26	X	57/58 (98%)	47 (82%)	10 (18%)	2 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	Y	67/67 (100%)	59 (88%)	8 (12%)	5 19
28	Z	54/54 (100%)	47 (87%)	7 (13%)	4 16
29	a	48/48 (100%)	45 (94%)	3 (6%)	16 38
30	b	47/47 (100%)	36 (77%)	11 (23%)	1 5
31	c	45/46 (98%)	40 (89%)	5 (11%)	6 20
32	d	38/38 (100%)	31 (82%)	7 (18%)	1 10
33	e	51/51 (100%)	47 (92%)	4 (8%)	11 32
34	f	34/34 (100%)	31 (91%)	3 (9%)	9 29
37	i	336/338 (99%)	334 (99%)	2 (1%)	78 81
39	k	16/16 (100%)	16 (100%)	0	100 100
40	l	217/217 (100%)	217 (100%)	0	100 100
All	All	3382/3386 (100%)	3063 (91%)	319 (9%)	10 26

All (319) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	3	VAL
5	C	24	LEU
5	C	35	GLU
5	C	51	THR
5	C	72	ASP
5	C	74	ILE
5	C	120	VAL
5	C	130	LEU
5	C	134	ASN
5	C	147	LYS
5	C	156	ARG
5	C	172	VAL
5	C	180	GLU
5	C	185	GLU
5	C	189	ARG
5	C	192	LEU
5	C	195	VAL
5	C	203	ARG
5	C	204	VAL
5	C	228	VAL
5	C	242	LYS
5	C	250	VAL

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Mol	Chain	Res	Type
5	C	251	GLN
5	C	257	THR
5	C	261	LYS
5	C	271	ARG
6	D	12	THR
6	D	13	ARG
6	D	18	ASP
6	D	20	VAL
6	D	22	ILE
6	D	28	GLU
6	D	29	VAL
6	D	60	VAL
6	D	73	VAL
6	D	84	LEU
6	D	128	ARG
6	D	133	THR
6	D	139	SER
6	D	142	VAL
6	D	160	LYS
6	D	168	GLU
7	E	83	VAL
7	E	84	THR
7	E	94	GLN
7	E	96	VAL
7	E	97	ASN
7	E	105	LEU
7	E	119	ILE
7	E	127	GLU
7	E	138	LEU
7	E	148	ILE
7	E	169	VAL
7	E	173	THR
7	E	178	VAL
7	E	179	SER
7	E	184	ASP
7	E	196	VAL
8	F	3	LYS
8	F	4	LEU
8	F	14	LYS
8	F	25	VAL
8	F	49	LEU
8	F	51	ASP

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Mol	Chain	Res	Type
8	F	52	ASN
8	F	67	ILE
8	F	81	GLN
8	F	104	ILE
8	F	106	ILE
8	F	115	ARG
8	F	130	MET
8	F	141	ILE
8	F	144	ASP
8	F	149	VAL
8	F	150	ARG
8	F	153	ASP
8	F	156	ILE
8	F	162	SER
8	F	178	ARG
9	G	10	VAL
9	G	11	VAL
9	G	43	VAL
9	G	49	THR
9	G	87	LEU
9	G	114	ASP
9	G	124	GLU
9	G	125	CYS
9	G	127	THR
9	G	141	ILE
9	G	153	ARG
10	H	4	ILE
10	H	15	LEU
10	H	37	VAL
10	H	58	LEU
10	H	60	GLU
10	H	76	GLU
10	H	77	THR
10	H	78	VAL
10	H	86	ASP
10	H	87	GLU
10	H	108	VAL
10	H	110	VAL
10	H	112	LYS
10	H	142	VAL
11	I	16	SER
11	I	36	ASP

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Mol	Chain	Res	Type
11	I	54	VAL
11	I	55	VAL
11	I	58	THR
11	I	64	VAL
11	I	94	ARG
11	I	96	PHE
11	I	109	LYS
12	J	9	VAL
12	J	21	SER
12	J	28	LEU
12	J	31	GLN
12	J	35	ILE
12	J	55	ILE
12	J	61	VAL
12	J	66	SER
12	J	78	VAL
12	J	98	VAL
12	J	111	GLN
12	J	112	THR
12	J	113	LYS
12	J	116	ASP
12	J	128	SER
12	J	139	VAL
13	K	5	THR
13	K	7	LYS
13	K	17	VAL
13	K	28	LEU
13	K	31	GLU
13	K	34	ARG
13	K	40	HIS
13	K	57	LEU
13	K	69	ARG
13	K	70	THR
13	K	88	THR
13	K	90	GLU
13	K	101	ILE
13	K	103	ILE
13	K	122	LEU
13	K	131	ASN
13	K	142	ILE
14	L	21	CYS
14	L	42	THR

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Mol	Chain	Res	Type
14	L	49	ARG
14	L	56	ASP
14	L	58	LEU
14	L	65	THR
14	L	84	CYS
14	L	116	ILE
15	M	14	LYS
15	M	46	VAL
15	M	47	ARG
15	M	55	MET
15	M	59	ARG
15	M	86	GLU
15	M	91	ASP
15	M	101	ILE
15	M	126	ARG
15	M	141	LYS
15	M	143	GLU
16	N	6	ARG
16	N	7	THR
16	N	12	MET
16	N	25	ASP
16	N	54	THR
16	N	58	LYS
16	N	81	ARG
16	N	115	GLU
16	N	133	LYS
16	N	135	VAL
17	O	14	SER
17	O	33	ILE
17	O	36	THR
17	O	69	ARG
17	O	74	GLU
17	O	75	ILE
17	O	100	CYS
18	P	2	ASP
18	P	5	SER
18	P	16	ARG
18	P	18	LEU
18	P	19	GLN
18	P	20	GLU
18	P	31	THR
18	P	36	TYR

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Mol	Chain	Res	Type
18	P	43	ASN
18	P	49	VAL
18	P	55	GLU
18	P	56	LYS
18	P	58	ILE
18	P	61	GLN
18	P	69	ASP
18	P	78	VAL
18	P	98	GLN
19	Q	3	ASN
19	Q	7	GLN
19	Q	21	ARG
19	Q	26	VAL
19	Q	51	ARG
19	Q	65	SER
19	Q	68	GLU
19	Q	92	VAL
19	Q	94	LYS
19	Q	102	GLU
19	Q	115	ASN
20	R	6	ARG
20	R	17	ILE
20	R	24	TYR
20	R	31	VAL
20	R	39	VAL
20	R	40	ILE
20	R	51	ARG
20	R	74	ILE
20	R	80	ILE
20	R	109	LEU
21	S	4	VAL
21	S	10	LYS
21	S	20	VAL
21	S	25	LEU
21	S	38	VAL
21	S	45	GLU
21	S	60	LYS
21	S	72	VAL
21	S	83	TYR
21	S	85	LYS
21	S	101	ILE
22	T	12	SER

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Mol	Chain	Res	Type
22	T	20	VAL
22	T	28	LYS
22	T	55	ILE
22	T	68	ASP
22	T	74	ILE
22	T	95	ARG
22	T	96	ILE
22	T	98	LYS
23	U	7	LEU
23	U	16	VAL
23	U	17	SER
23	U	48	GLN
23	U	72	GLN
24	V	7	ARG
24	V	28	VAL
24	V	34	VAL
24	V	41	LEU
24	V	42	VAL
24	V	68	SER
24	V	83	VAL
24	V	102	THR
25	W	7	GLU
25	W	12	GLN
25	W	61	LEU
25	W	77	VAL
25	W	78	GLN
25	W	92	VAL
26	X	11	ARG
26	X	12	ASN
26	X	21	LEU
26	X	35	SER
26	X	38	VAL
26	X	41	ARG
26	X	56	ASP
26	X	58	THR
26	X	72	LYS
26	X	85	GLU
27	Y	2	SER
27	Y	4	VAL
27	Y	13	VAL
27	Y	42	SER
27	Y	44	LYS

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Mol	Chain	Res	Type
27	Y	71	LEU
27	Y	74	ARG
27	Y	77	LYS
28	Z	2	LYS
28	Z	16	THR
28	Z	28	LEU
28	Z	44	LYS
28	Z	45	GLN
28	Z	48	ARG
28	Z	56	LEU
29	a	30	ARG
29	a	36	VAL
29	a	56	LYS
30	b	4	GLN
30	b	9	THR
30	b	15	MET
30	b	18	SER
30	b	25	VAL
30	b	26	THR
30	b	28	LEU
30	b	36	GLU
30	b	40	ARG
30	b	46	ASP
30	b	52	ARG
31	c	5	ILE
31	c	6	ARG
31	c	22	THR
31	c	42	VAL
31	c	47	VAL
32	d	1	MET
32	d	12	ARG
32	d	24	THR
32	d	25	LYS
32	d	34	ARG
32	d	41	ARG
32	d	42	LEU
33	e	8	ARG
33	e	32	ILE
33	e	50	VAL
33	e	51	SER
34	f	1	MET
34	f	2	LYS

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Mol	Chain	Res	Type
34	f	12	ARG
37	i	23	THR
37	i	27	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
5	C	86	ASN
5	C	90	ASN
5	C	251	GLN
6	D	136	ASN
6	D	140	HIS
7	E	24	ASN
7	E	165	HIS
8	F	37	ASN
8	F	63	GLN
8	F	81	GLN
8	F	127	ASN
9	G	30	ASN
9	G	48	ASN
10	H	33	GLN
12	J	31	GLN
13	K	76	HIS
13	K	80	HIS
13	K	86	GLN
14	L	3	GLN
14	L	89	ASN
15	M	104	GLN
16	N	3	GLN
18	P	43	ASN
18	P	100	HIS
19	Q	3	ASN
19	Q	52	ASN
19	Q	56	HIS
19	Q	75	GLN
20	R	37	GLN
20	R	81	ASN
21	S	82	HIS
22	T	7	HIS
22	T	102	HIS
23	U	48	GLN
23	U	59	ASN

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Mol	Chain	Res	Type
23	U	92	ASN
25	W	12	GLN
26	X	46	HIS
28	Z	25	GLN
28	Z	39	GLN
28	Z	58	ASN
29	a	20	HIS
30	b	6	ASN
32	d	29	GLN
37	i	91	GLN
37	i	332	ASN
37	i	419	GLN
40	l	161	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	103/104 (99%)	22 (21%)	0
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	518 (17%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3102/3130 (99%)	554 (17%)	19 (0%)

All (554) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	27	G
1	1	29	U
1	1	30	A
1	1	33	C
1	1	34	U
1	1	37	U
1	1	38	U
1	1	39	A
1	1	41	C
1	1	42	A
1	1	46	C
1	1	57	G
1	1	75	U
1	1	76	G
1	1	83	G

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Mol	Chain	Res	Type
1	1	87	C
1	1	88	G
1	1	90	G
1	1	94	U
1	1	95	A
1	1	102	A
1	1	107	C
2	2	76	A
3	A	10	A
3	A	12	U
3	A	33	C
3	A	34	U
3	A	35	G
3	A	45	G
3	A	46	G
3	A	49	A
3	A	50	U
3	A	51	G
3	A	62	U
3	A	63	A
3	A	65	U
3	A	71	A
3	A	72	U
3	A	74	A
3	A	75	G
3	A	84	A
3	A	93	G
3	A	96	C
3	A	101	A
3	A	102	U
3	A	103	A
3	A	110	G
3	A	118	A
3	A	119	A
3	A	120	U
3	A	136	G
3	A	137	U
3	A	138	U
3	A	139	U
3	A	142	A
3	A	156	A
3	A	162	U

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Mol	Chain	Res	Type
3	A	181	A
3	A	188	G
3	A	196	A
3	A	199	A
3	A	215	G
3	A	216	A
3	A	220	G
3	A	221	A
3	A	222	A
3	A	226	A
3	A	248	G
3	A	266	G
3	A	272	A
3	A	275	C
3	A	276	U
3	A	285	G
3	A	291	G
3	A	302	C
3	A	311	A
3	A	329	G
3	A	330	A
3	A	335	C
3	A	349	U
3	A	353	C
3	A	356	G
3	A	361	G
3	A	362	A
3	A	372	G
3	A	386	G
3	A	396	G
3	A	399	U
3	A	411	G
3	A	419	U
3	A	424	G
3	A	454	A
3	A	455	C
3	A	475	C
3	A	477	A
3	A	479	A
3	A	480	A
3	A	481	G
3	A	491	G

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Mol	Chain	Res	Type
3	A	504	A
3	A	505	A
3	A	509	C
3	A	510	C
3	A	513	A
3	A	518	G
3	A	529	A
3	A	531	C
3	A	532	A
3	A	533	G
3	A	543	G
3	A	544	C
3	A	550	C
3	A	552	U
3	A	558	U
3	A	563	A
3	A	567	U
3	A	568	U
3	A	573	U
3	A	575	A
3	A	586	A
3	A	603	A
3	A	613	A
3	A	614	A
3	A	615	U
3	A	627	A
3	A	632	A
3	A	634	C
3	A	637	A
3	A	645	C
3	A	646	U
3	A	647	G
3	A	653	U
3	A	654	A
3	A	655	A
3	A	668	A
3	A	685	A
3	A	686	U
3	A	711	G
3	A	712	G
3	A	713	G
3	A	718	A

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Mol	Chain	Res	Type
3	A	730	A
3	A	747	U
3	A	753	A
3	A	757	G
3	A	763	G
3	A	764	A
3	A	765	C
3	A	775	G
3	A	777	G
3	A	782	A
3	A	784	G
3	A	785	G
3	A	788	A
3	A	789	A
3	A	790	U
3	A	791	C
3	A	793	A
3	A	794	A
3	A	801	G
3	A	805	G
3	A	812	C
3	A	827	U
3	A	828	U
3	A	831	G
3	A	846	U
3	A	859	G
3	A	865	C
3	A	869	G
3	A	878	A
3	A	896	A
3	A	897	C
3	A	899	A
3	A	907	G
3	A	910	A
3	A	914	G
3	A	915	C
3	A	932	U
3	A	933	A
3	A	946	C
3	A	953	G
3	A	957	C
3	A	961	C

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Mol	Chain	Res	Type
3	A	974	G
3	A	983	A
3	A	990	A
3	A	996	A
3	A	999	U
3	A	1005	C
3	A	1009	A
3	A	1012	U
3	A	1013	C
3	A	1022	G
3	A	1023	U
3	A	1027	A
3	A	1033	U
3	A	1040	A
3	A	1046	A
3	A	1056	G
3	A	1057	A
3	A	1070	A
3	A	1071	G
3	A	1073	A
3	A	1083	U
3	A	1087	G
3	A	1088	A
3	A	1090	A
3	A	1101	U
3	A	1111	A
3	A	1112	G
3	A	1116	G
3	A	1129	A
3	A	1130	U
3	A	1132	U
3	A	1133	A
3	A	1135	C
3	A	1136	G
3	A	1139	G
3	A	1142	A
3	A	1143	A
3	A	1155	A
3	A	1173	U
3	A	1179	G
3	A	1182	G
3	A	1206	G

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Mol	Chain	Res	Type
3	A	1212	G
3	A	1218	G
3	A	1236	G
3	A	1238	G
3	A	1247	A
3	A	1249	U
3	A	1252	G
3	A	1253	A
3	A	1256	G
3	A	1262	A
3	A	1271	G
3	A	1272	A
3	A	1294	U
3	A	1300	G
3	A	1301	A
3	A	1302	A
3	A	1308	A
3	A	1329	U
3	A	1332	G
3	A	1337	G
3	A	1338	G
3	A	1345	C
3	A	1346	G
3	A	1365	A
3	A	1379	U
3	A	1383	A
3	A	1395	A
3	A	1403	A
3	A	1416	G
3	A	1417	C
3	A	1424	G
3	A	1428	C
3	A	1434	A
3	A	1437	C
3	A	1449	G
3	A	1451	C
3	A	1452	G
3	A	1453	A
3	A	1482	G
3	A	1489	C
3	A	1491	G
3	A	1493	C

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Mol	Chain	Res	Type
3	A	1494	A
3	A	1495	A
3	A	1497	U
3	A	1498	C
3	A	1509	A
3	A	1510	G
3	A	1515	A
3	A	1524	G
3	A	1529	G
3	A	1533	C
3	A	1535	A
3	A	1536	C
3	A	1537	G
3	A	1554	U
3	A	1560	G
3	A	1566	A
3	A	1569	A
3	A	1576	U
3	A	1578	U
3	A	1581	G
3	A	1583	A
3	A	1585	C
3	A	1606	C
3	A	1607	C
3	A	1608	A
3	A	1616	A
3	A	1634	A
3	A	1639	C
3	A	1647	U
3	A	1648	U
3	A	1649	G
3	A	1660	G
3	A	1674	G
3	A	1677	A
3	A	1715	G
3	A	1722	A
3	A	1725	U
3	A	1729	U
3	A	1730	C
3	A	1738	G
3	A	1744	A
3	A	1757	A

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Mol	Chain	Res	Type
3	A	1764	C
3	A	1773	A
3	A	1782	U
3	A	1786	A
3	A	1791	A
3	A	1800	C
3	A	1801	A
3	A	1802	A
3	A	1808	A
3	A	1809	A
3	A	1811	G
3	A	1816	C
3	A	1829	A
3	A	1847	A
3	A	1849	G
3	A	1850	G
3	A	1870	C
3	A	1871	A
3	A	1872	A
3	A	1876	A
3	A	1896	G
3	A	1906	G
3	A	1920	C
3	A	1927	A
3	A	1929	G
3	A	1930	G
3	A	1931	U
3	A	1934	C
3	A	1936	A
3	A	1937	A
3	A	1939	U
3	A	1955	U
3	A	1956	U
3	A	1960	A
3	A	1962	C
3	A	1966	A
3	A	1967	C
3	A	1970	A
3	A	1971	U
3	A	1972	G
3	A	1974	C
3	A	1982	U

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Mol	Chain	Res	Type
3	A	1991	U
3	A	1992	G
3	A	1993	U
3	A	1997	C
3	A	2021	C
3	A	2023	C
3	A	2030	A
3	A	2031	A
3	A	2033	A
3	A	2043	C
3	A	2050	C
3	A	2054	A
3	A	2055	C
3	A	2056	G
3	A	2060	A
3	A	2061	G
3	A	2062	A
3	A	2069	G
3	A	2072	C
3	A	2093	G
3	A	2097	A
3	A	2101	A
3	A	2103	C
3	A	2104	C
3	A	2105	U
3	A	2106	U
3	A	2111	U
3	A	2112	G
3	A	2113	U
3	A	2116	G
3	A	2117	A
3	A	2118	U
3	A	2119	A
3	A	2120	G
3	A	2123	G
3	A	2126	A
3	A	2128	G
3	A	2131	U
3	A	2132	U
3	A	2133	G
3	A	2134	A
3	A	2145	C

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Mol	Chain	Res	Type
3	A	2146	C
3	A	2147	A
3	A	2148	G
3	A	2159	G
3	A	2160	C
3	A	2161	C
3	A	2163	A
3	A	2164	C
3	A	2165	C
3	A	2167	U
3	A	2168	G
3	A	2169	A
3	A	2170	A
3	A	2171	A
3	A	2172	U
3	A	2173	A
3	A	2174	C
3	A	2177	C
3	A	2178	C
3	A	2185	U
3	A	2187	U
3	A	2190	G
3	A	2198	A
3	A	2203	U
3	A	2204	G
3	A	2211	A
3	A	2212	A
3	A	2225	A
3	A	2238	G
3	A	2239	G
3	A	2250	G
3	A	2268	A
3	A	2278	A
3	A	2280	G
3	A	2283	C
3	A	2287	A
3	A	2288	A
3	A	2297	A
3	A	2305	U
3	A	2308	G
3	A	2322	A
3	A	2325	G

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Mol	Chain	Res	Type
3	A	2331	G
3	A	2336	A
3	A	2345	G
3	A	2347	C
3	A	2350	C
3	A	2354	C
3	A	2357	G
3	A	2366	A
3	A	2383	G
3	A	2385	C
3	A	2402	U
3	A	2403	C
3	A	2406	A
3	A	2420	C
3	A	2421	G
3	A	2422	C
3	A	2423	U
3	A	2424	C
3	A	2425	A
3	A	2427	C
3	A	2429	G
3	A	2430	A
3	A	2431	U
3	A	2432	A
3	A	2434	A
3	A	2435	A
3	A	2440	C
3	A	2441	U
3	A	2445	G
3	A	2448	A
3	A	2464	G
3	A	2475	C
3	A	2476	A
3	A	2478	A
3	A	2491	U
3	A	2492	U
3	A	2497	A
3	A	2502	G
3	A	2504	U
3	A	2505	G
3	A	2506	U
3	A	2507	C

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Mol	Chain	Res	Type
3	A	2513	A
3	A	2514	U
3	A	2518	A
3	A	2520	C
3	A	2529	G
3	A	2566	A
3	A	2567	G
3	A	2578	G
3	A	2582	G
3	A	2585	U
3	A	2586	U
3	A	2602	A
3	A	2603	G
3	A	2609	U
3	A	2613	U
3	A	2615	U
3	A	2621	G
3	A	2623	G
3	A	2624	G
3	A	2629	U
3	A	2630	G
3	A	2636	C
3	A	2638	G
3	A	2669	G
3	A	2682	A
3	A	2689	U
3	A	2690	U
3	A	2714	G
3	A	2716	C
3	A	2726	A
3	A	2733	A
3	A	2739	U
3	A	2744	G
3	A	2748	A
3	A	2757	A
3	A	2765	A
3	A	2778	A
3	A	2779	U
3	A	2780	G
3	A	2791	G
3	A	2792	A
3	A	2798	U

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Mol	Chain	Res	Type
3	A	2799	A
3	A	2801	G
3	A	2820	A
3	A	2821	A
3	A	2825	G
3	A	2833	U
3	A	2835	A
3	A	2836	U
3	A	2849	U
3	A	2860	A
3	A	2861	U
3	A	2867	G
3	A	2870	C
3	A	2873	A
3	A	2879	A
3	A	2880	C
3	A	2883	A
3	A	2884	U
3	A	2885	G
3	A	2886	A
3	A	2888	C
3	A	2891	U
4	B	24	G
4	B	25	U
4	B	35	C
4	B	41	G
4	B	45	A
4	B	56	G
4	B	66	A
4	B	67	G
4	B	71	C
4	B	88	C
4	B	89	U
4	B	90	C
4	B	109	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	100	U
3	A	613	A
3	A	645	C

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Mol	Chain	Res	Type
3	A	653	U
3	A	784	G
3	A	827	U
3	A	830	G
3	A	1110	G
3	A	1344	U
3	A	1494	A
3	A	1721	G
3	A	1939	U
3	A	2127	G
3	A	2158	A
3	A	2422	C
3	A	2424	C
3	A	2430	A
3	A	2602	A
3	A	2756	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
42	ALF	l	1001	44	0,4,4	-	-	-		
44	GDP	i	1003	42,43	28,30,30	1.13	3 (10%)	44,47,47	1.87	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	ALF	i	1001	44	0,4,4	-	-	-		
44	GDP	l	1003	42,43	28,30,30	1.14	3 (10%)	44,47,47	1.85	8 (18%)

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
44	GDP	i	1003	42,43	-	4/16/32/32	0/3/3/3
44	GDP	l	1003	42,43	-	7/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	i	1003	GDP	C5-C4	3.12	1.47	1.38
44	l	1003	GDP	C5-C4	3.10	1.47	1.38
44	l	1003	GDP	C6-N1	-2.48	1.34	1.38
44	i	1003	GDP	C6-N1	-2.40	1.34	1.38
44	l	1003	GDP	C5-N7	-2.14	1.34	1.39
44	i	1003	GDP	C5-N7	-2.10	1.35	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	i	1003	GDP	C5-C4-N3	-6.16	118.46	128.46
44	l	1003	GDP	C5-C4-N3	-6.08	118.59	128.46
44	i	1003	GDP	C2-N3-C4	4.96	121.14	112.30
44	l	1003	GDP	C2-N3-C4	4.93	121.09	112.30
44	i	1003	GDP	N9-C4-N3	4.59	135.15	125.94
44	l	1003	GDP	N9-C4-N3	4.49	134.96	125.94
44	i	1003	GDP	PA-O3A-PB	-3.78	119.86	132.83
44	l	1003	GDP	PA-O3A-PB	-3.67	120.23	132.83
44	l	1003	GDP	C6-C5-N7	3.26	136.31	130.25
44	i	1003	GDP	C6-C5-N7	3.18	136.16	130.25
44	l	1003	GDP	C4-C5-N7	-2.64	106.55	110.72
44	i	1003	GDP	C4-C5-N7	-2.63	106.55	110.72
44	i	1003	GDP	C3'-C2'-C1'	2.14	105.49	101.43
44	l	1003	GDP	C3'-C2'-C1'	2.09	105.40	101.43
44	i	1003	GDP	O6-C6-C5	-2.09	121.06	126.60
44	l	1003	GDP	O6-C6-C5	-2.09	121.06	126.60

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	i	1003	GDP	C5'-O5'-PA-O3A
44	i	1003	GDP	O4'-C4'-C5'-O5'
44	i	1003	GDP	C3'-C4'-C5'-O5'
44	l	1003	GDP	PA-O3A-PB-O2B
44	l	1003	GDP	C5'-O5'-PA-O1A
44	l	1003	GDP	C5'-O5'-PA-O2A
44	l	1003	GDP	O4'-C4'-C5'-O5'
44	l	1003	GDP	C3'-C4'-C5'-O5'
44	i	1003	GDP	C5'-O5'-PA-O1A
44	l	1003	GDP	PA-O3A-PB-O1B
44	l	1003	GDP	C5'-O5'-PA-O3A

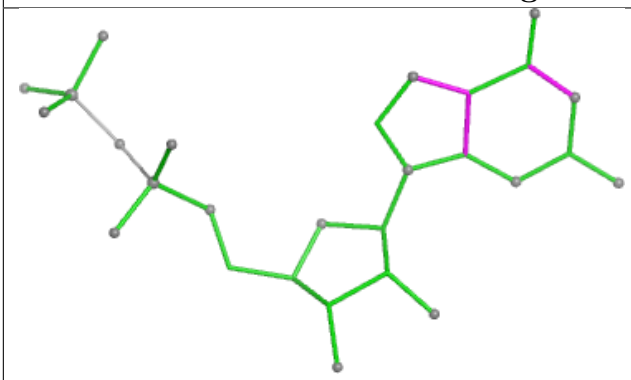
There are no ring outliers.

4 monomers are involved in 5 short contacts:

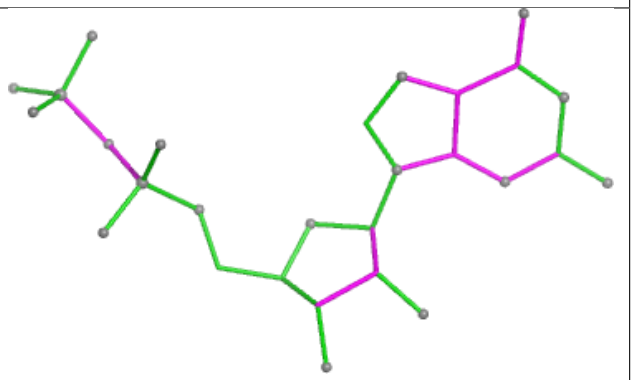
Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	l	1001	ALF	1	0
44	i	1003	GDP	3	0
42	i	1001	ALF	2	0
44	l	1003	GDP	1	0

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

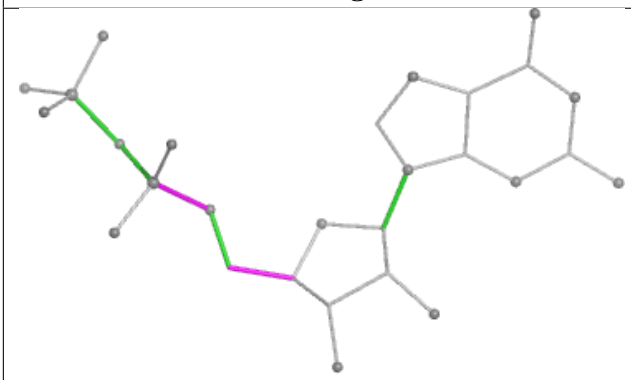
Ligand GDP i 1003



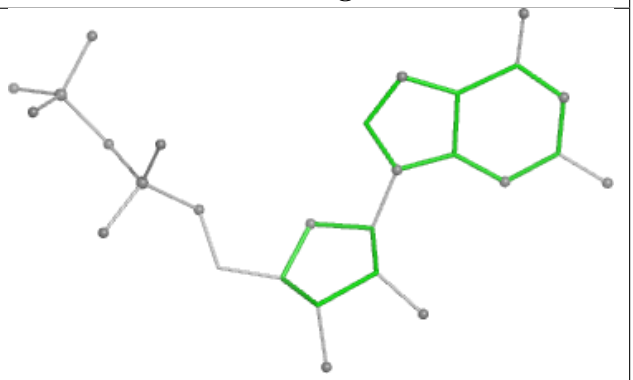
Bond lengths



Bond angles

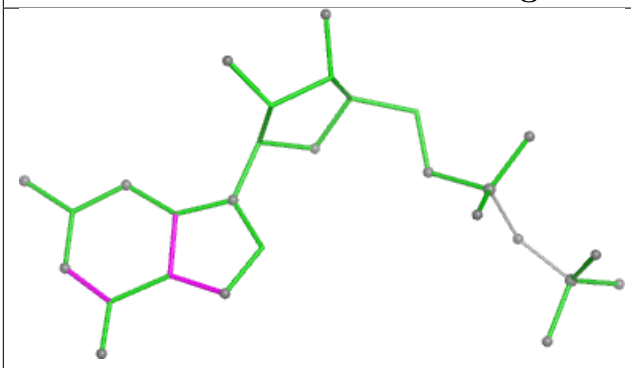


Torsions

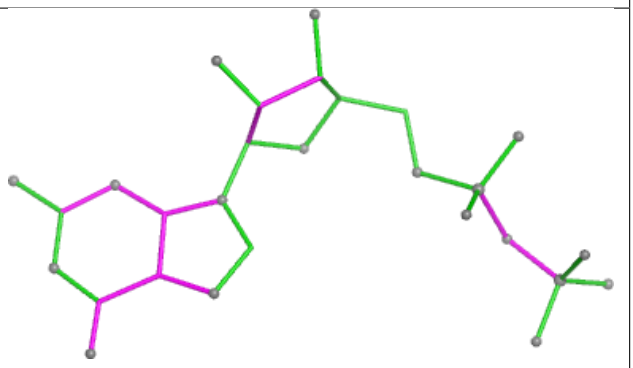


Rings

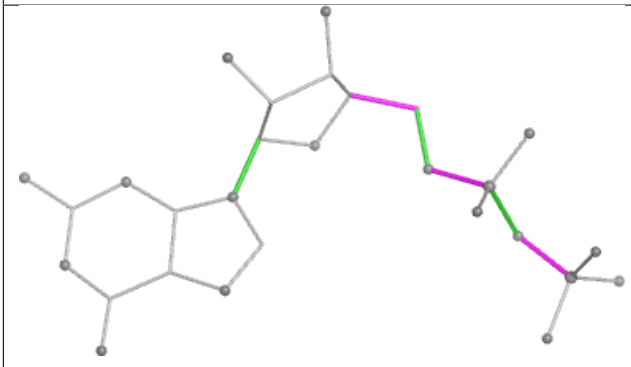
Ligand GDP l 1003



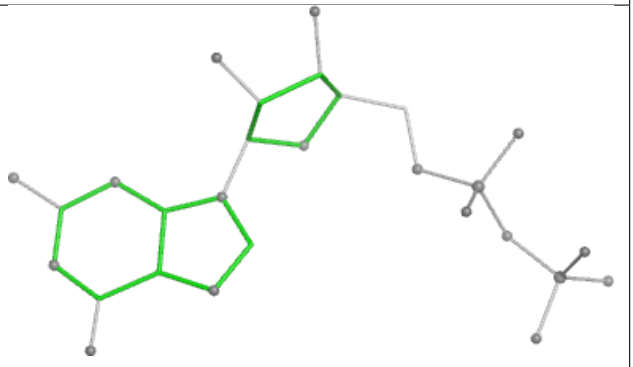
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

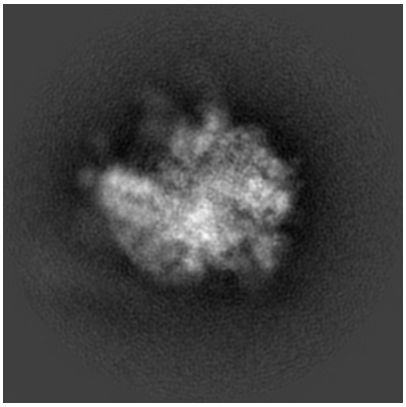
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3617. These allow visual inspection of the internal detail of the map and identification of artifacts.

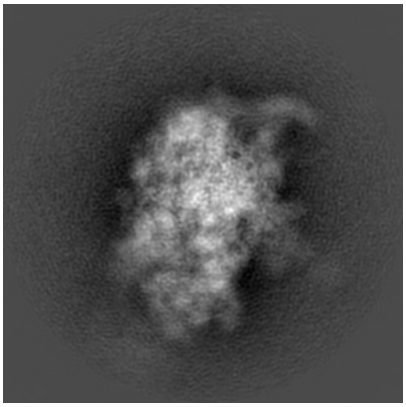
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

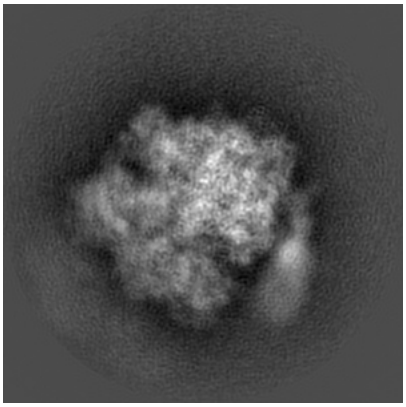
6.1.1 Primary map



X



Y

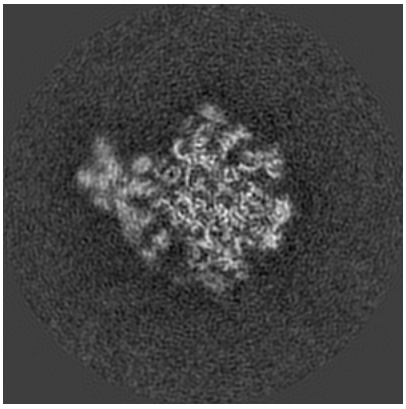


Z

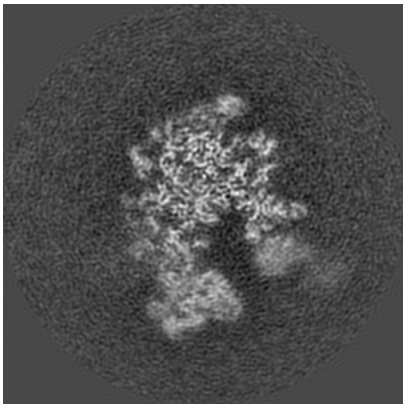
The images above show the map projected in three orthogonal directions.

6.2 Central slices

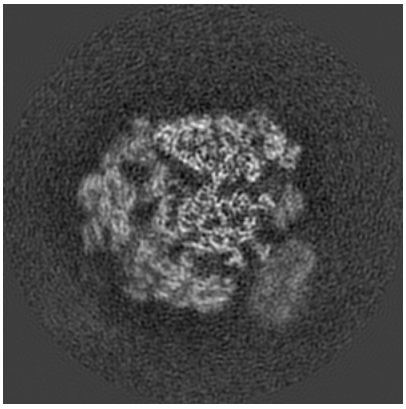
6.2.1 Primary map



X Index: 160



Y Index: 160

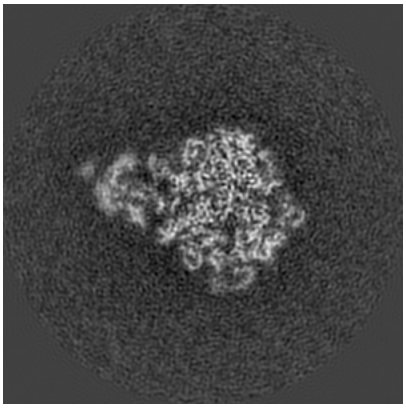


Z Index: 160

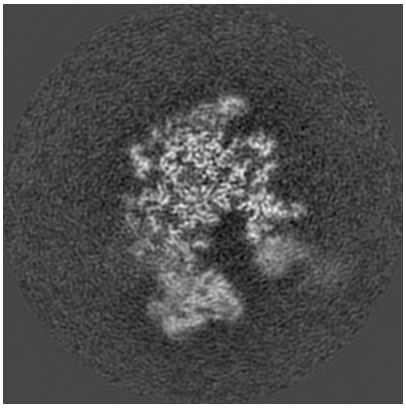
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

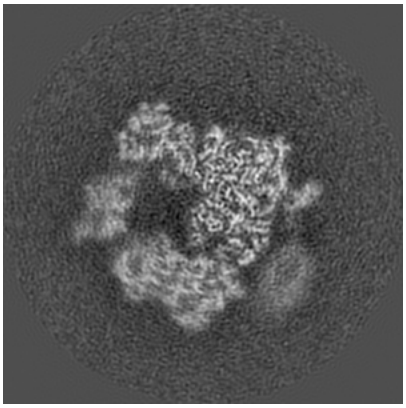
6.3.1 Primary map



X Index: 170



Y Index: 159

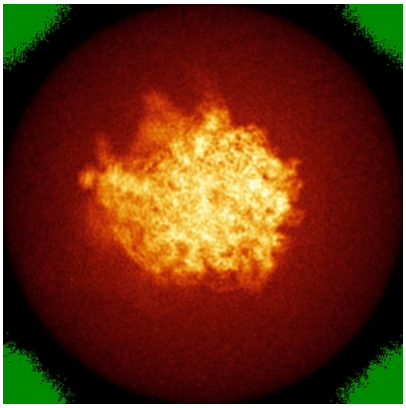


Z Index: 175

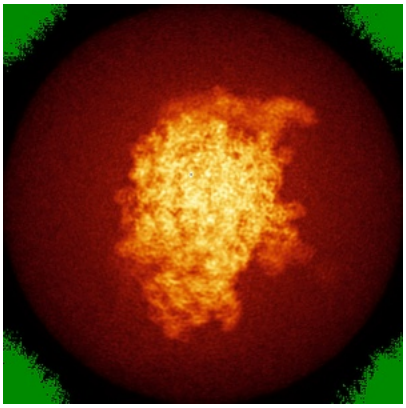
The images above show the largest variance slices of the map in three orthogonal directions.

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

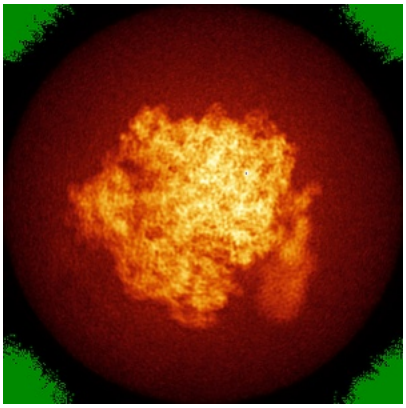
6.4.1 Primary map



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

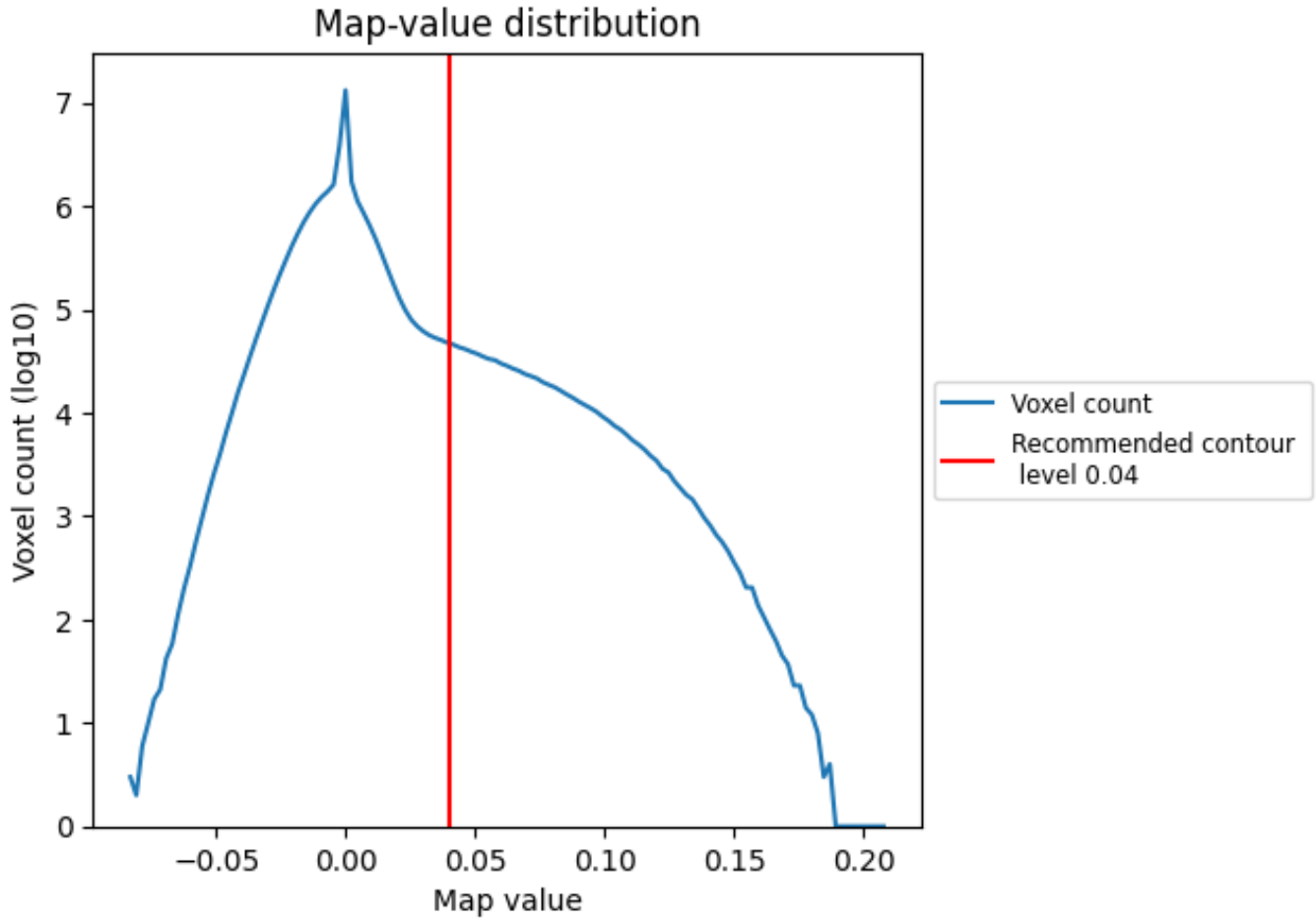
6.6 Mask visualisation (i)

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

7 Map analysis

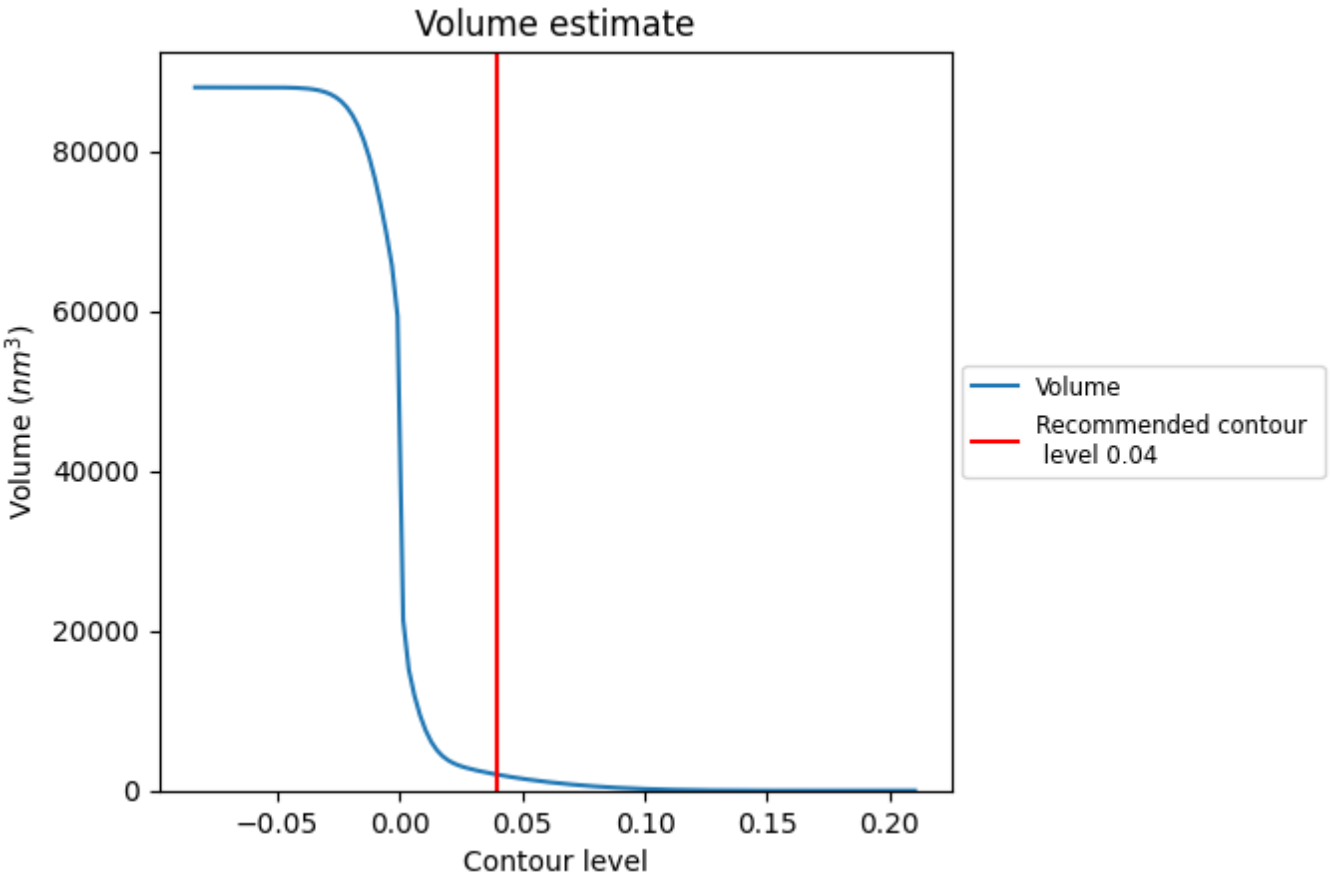
This section contains the results of statistical analysis of the map.

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.

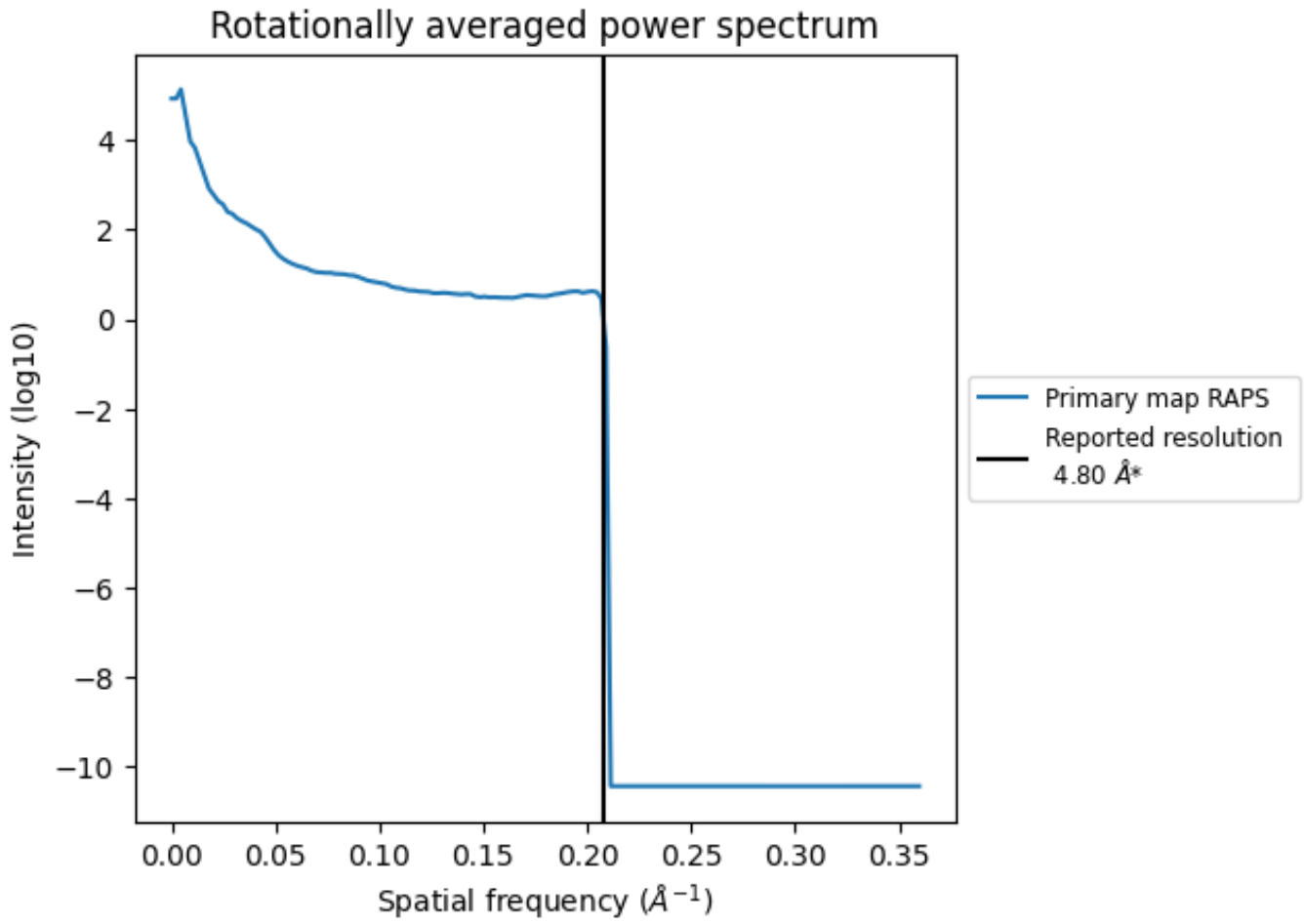
7.2 Volume estimate (i)



The volume at the recommended contour level is 1992 nm^3; this corresponds to an approximate mass of 1799 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 0.208 Å^{-1}

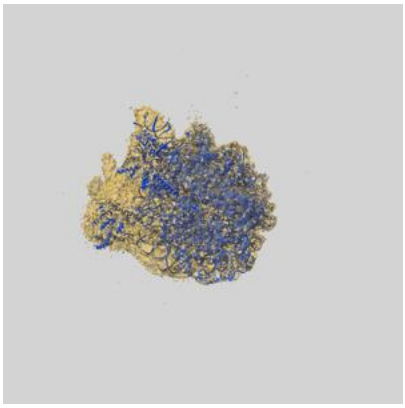
8 Fourier-Shell correlation (i)

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

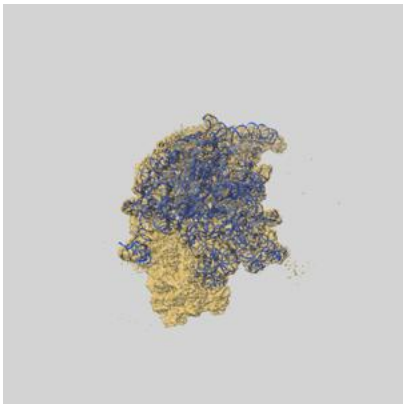
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3617 and PDB model 5NCO. Per-residue inclusion information can be found in section 3 on page 13.

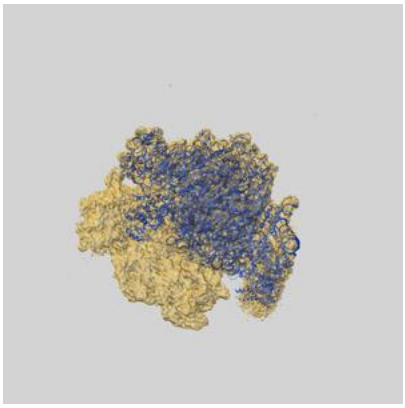
9.1 Map-model overlay



X



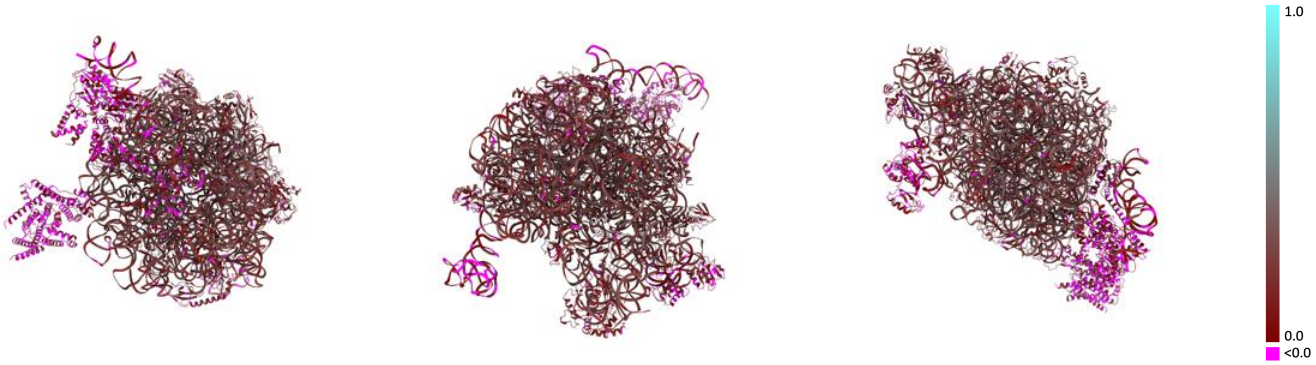
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

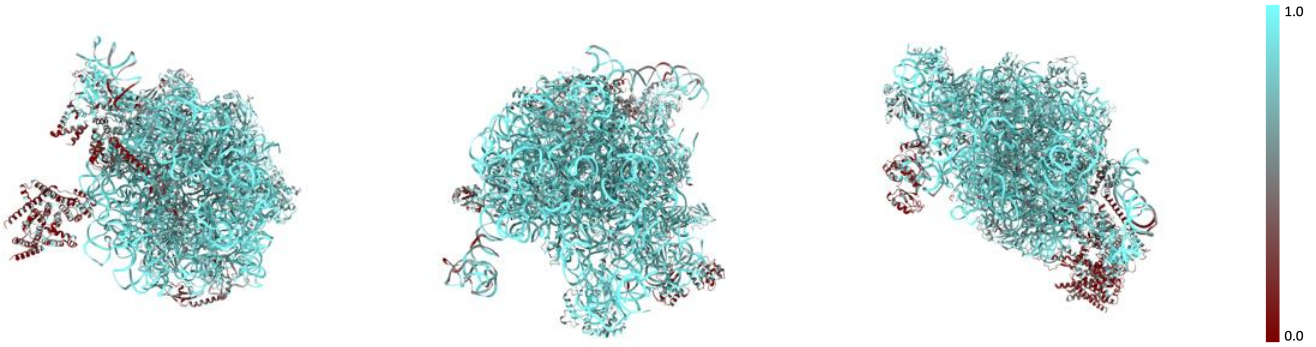
9.2 Q-score mapped to coordinate model (i)



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.

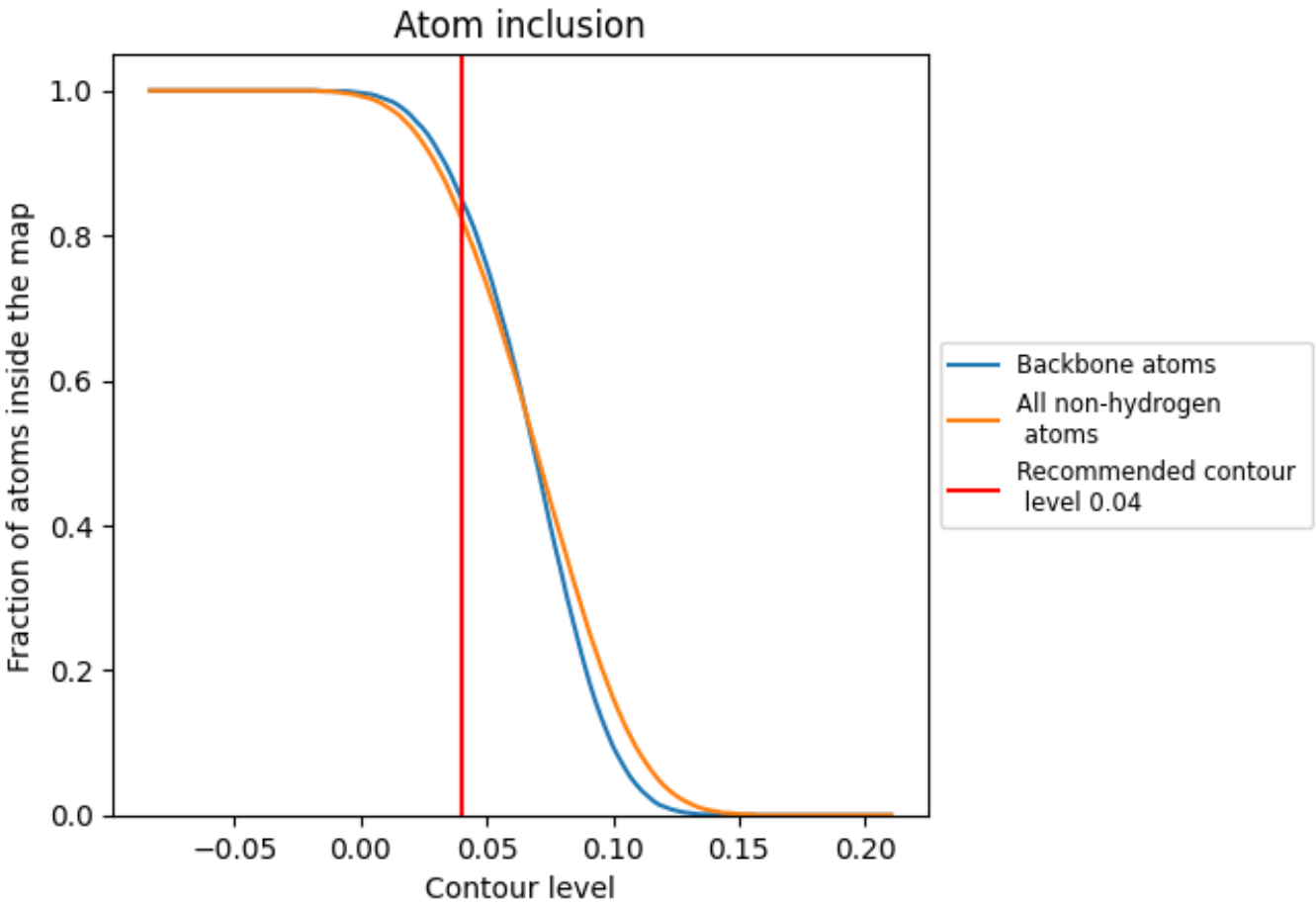
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.2180
1	0.7470	0.0820
2	0.9030	0.2780
A	0.9270	0.2540
B	0.9510	0.2450
C	0.7000	0.2090
D	0.7160	0.2310
E	0.7210	0.2080
F	0.6910	0.1350
G	0.7310	0.2130
H	0.4340	0.1410
I	0.4080	0.0570
J	0.3230	0.0500
K	0.7270	0.2280
L	0.6250	0.2120
M	0.7440	0.2090
N	0.7420	0.2390
O	0.6560	0.2170
P	0.7800	0.1880
Q	0.6840	0.2320
R	0.7880	0.2280
S	0.7340	0.2260
T	0.6670	0.2230
U	0.6860	0.2060
V	0.7080	0.2070
W	0.7130	0.2120
X	0.7500	0.1850
Y	0.7010	0.2080
Z	0.6910	0.1640
a	0.7730	0.2340
b	0.7240	0.2260
c	0.6670	0.1380
d	0.7160	0.2070
e	0.6930	0.2100
f	0.7750	0.1990



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Chain	Atom inclusion	Q-score
g	0.2910	0.0050
h	0.1560	-0.0410
i	0.5010	0.0590
j	0.2820	0.0170
k	0.6670	0.1140
l	0.6440	0.0390