



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:54 PM UTC

PDB ID : 6O8X / pdb_00006o8x
EMDB ID : EMD-0657
Title : Cryo-EM image reconstruction of the 70S Ribosome *Enterococcus faecalis* Class02
Authors : Jogl, G.; Khayat, R.
Deposited on : 2019-03-12
Resolution : 3.68 Å (reported)
Based on initial models : 4YBB, 5LI0

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

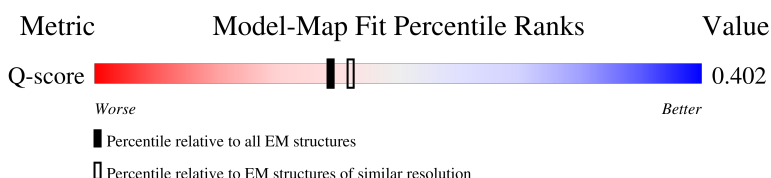
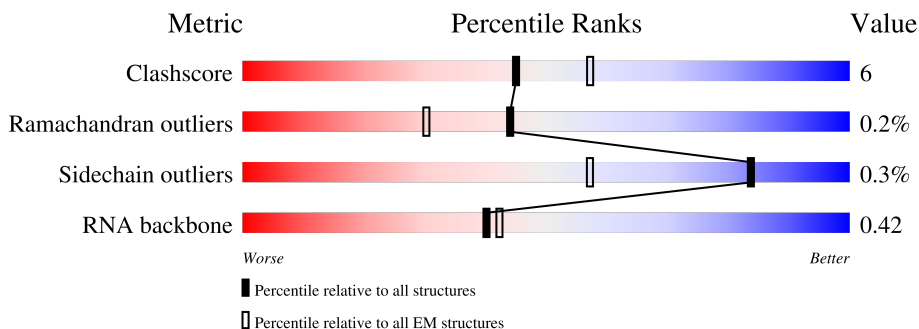
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.68 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	11376 (3.18 - 4.18)

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

Mol	Chain	Length	Quality of chain
1	a	1528	
2	c	204	
3	d	201	

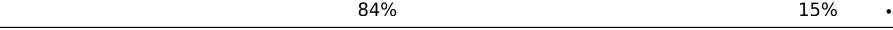
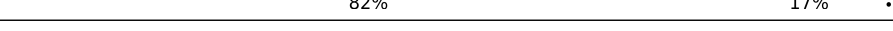
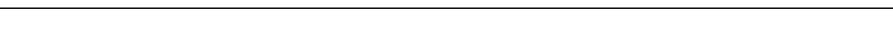
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	e	163	
5	f	97	
6	g	154	
7	h	131	
8	i	128	
9	j	99	
10	k	117	
11	l	136	
12	m	112	
13	n	60	
14	o	88	
15	p	89	
16	q	83	
17	r	66	
18	s	78	
19	t	81	
20	A	2903	
21	B	116	
22	C	275	
23	D	207	
24	E	206	
25	F	177	
26	G	176	
27	K	145	
28	L	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	M	146	 82% 16% .
30	N	141	 7% 76% 24% .
31	O	123	 89% 11% .
32	P	117	 84% 15% .
33	Q	114	 78% 22% .
34	R	118	 86% 12% .
35	S	102	 75% 25% .
36	T	112	 89% 11% .
37	U	89	 69% 28% ..
38	V	101	 82% 15% ..
39	W	94	 67% 82% 17% .
40	X	76	 83% 17% .
41	Y	54	 81% 17% .
42	Z	61	 80% 20% .
43	0	58	 86% 14% .
44	1	60	 5% 82% 18% .
45	2	56	 84% 16% .
46	3	49	 82% 18% .
47	4	44	 80% 18% .
48	5	64	 84% 16% .
49	6	38	 79% 21% .

2 Entry composition [i](#)

There are 50 unique types of molecules in this entry. The entry contains 138230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1528	Total	C	N	O	P	0	0
			32746	14609	5979	10630	1528		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	204	Total	C	N	O	S	0	0
			1610	1012	303	292	3		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	201	Total	C	N	O	S	0	0
			1620	1016	303	297	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	163	Total	C	N	O	S	0	0
			1204	759	222	221	2		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	97	Total	C	N	O	S	0	0
			795	501	137	154	3		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	154	Total	C	N	O	S	0	0
			1229	765	236	222	6		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	131	Total	C	N	O	S	0	0
			1041	662	184	193	2		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	128	Total	C	N	O	S	0	0
			990	615	197	177	1		

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	99	Total	C	N	O	S	0	0
			800	504	147	147	2		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	117	Total	C	N	O	S	0	0
			863	533	165	161	4		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	l	136	Total	C	N	O	S	0	0
			1065	661	214	188	2		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	112	Total	C	N	O	S	0	0
			884	540	180	163	1		

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	60	Total	C	N	O	S	0	0
			492	310	100	77	5		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	88	Total	C	N	O	S	0	0
			741	455	152	133	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	p	89	Total	C	N	O	S	0	0
			708	448	131	127	2		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	83	Total	C	N	O	S	0	0
			681	427	127	124	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	r	66	Total	C	N	O	S	0	0
			537	343	99	94	1		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	s	78	Total	C	N	O	S	0	0
			634	410	113	109	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	t	81	Total	C	N	O	S	0	0
			610	372	119	117	2		

- Molecule 20 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A	2898	Total	C	N	O	P	0	0
			62196	27761	11436	20101	2898		

- Molecule 21 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	116	Total	C	N	O	P	0	0
			2478	1105	444	813	116		

- Molecule 22 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	C	275	Total	C	N	O	S	0	0
			2114	1310	416	381	7		

- Molecule 23 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	207	Total	C	N	O	S	0	0
			1578	993	292	289	4		

- Molecule 24 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	206	Total	C	N	O	S	0	0
			1572	984	289	297	2		

- Molecule 25 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	177	Total	C	N	O	S	0	0
			1391	886	239	260	6		

- Molecule 26 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	G	176	Total	C	N	O	S	0	0
			1344	841	244	255	4		

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	K	145	Total	C	N	O	S	0	0
			1129	713	205	207	4		

- Molecule 28 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L	122	Total	C	N	O	S	0	0
			922	574	176	170	2		

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	M	146	Total	C	N	O	S	0	0
			1094	676	212	205	1		

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	141	Total	C	N	O	S	0	0
			1117	709	216	185	7		

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	O	123	Total	C	N	O	S	0	0
			978	603	189	183	3		

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P	117	Total	C	N	O	S	0	0
			898	555	175	167	1		

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Q	114	Total	C	N	O	0	0
			924	582	185	157		

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R	115	Total	C	N	O	S	0	0
			913	580	172	157	4		

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S	102	Total	C	N	O	S	0	0
			783	500	138	143	2		

- Molecule 36 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	T	112	Total	C	N	O	S	0	0
			849	532	156	159	2		

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	U	89	Total	C	N	O	S	0	0
			719	457	127	132	3		

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	V	101	Total	C	N	O	S	0	0
			763	486	135	140	2		

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	W	94	Total	C	N	O	S	0	0
			757	478	135	140	4		

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	X	76	Total	C	N	O	0	0
			572	351	109	112		

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Y	54	Total	C	N	O	S	0	0
			424	265	86	71	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	51	ALA	THR	conflict	UNP A0A1B4XRZ8

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Z	61	Total	C	N	O	S	0	0
			504	314	94	95	1		

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	0	58	Total	C	N	O	S	0	0
			435	271	81	82	1		

- Molecule 44 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	60	Total	C	N	O	S	0	0
			475	301	75	97	2		

- Molecule 45 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	56	Total	C	N	O	S	0	0
			429	262	88	73	6		

- Molecule 46 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3	49	Total	C	N	O	S	0	0
			419	253	86	76	4		

- Molecule 47 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4	44	Total	C	N	O	S	0	0
			373	226	91	54	2		

- Molecule 48 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	64	Total	C	N	O	S	0	0
			522	320	122	78	2		

- Molecule 49 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	6	38	Total	C	N	O	S	0	0
			304	188	66	44	6		

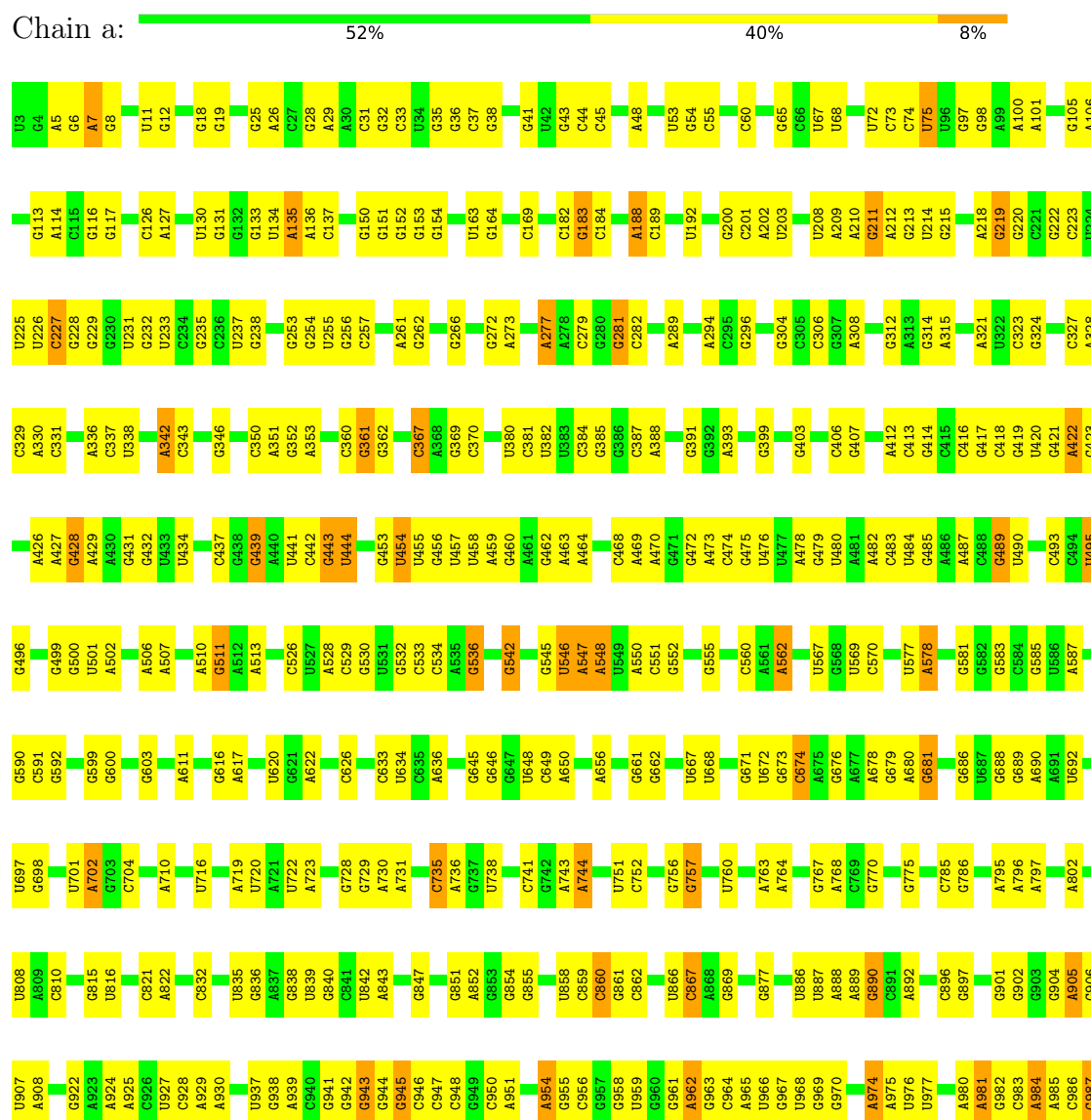
- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

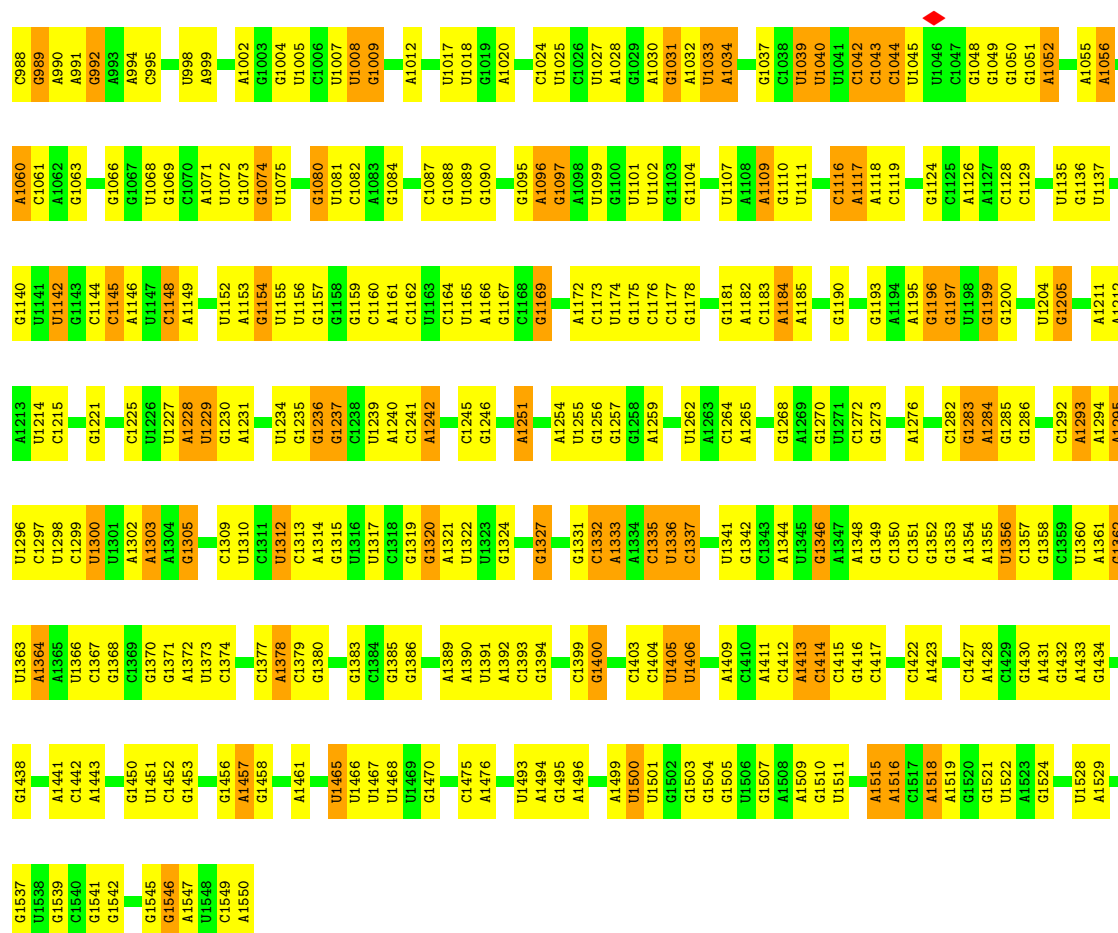
Mol	Chain	Residues	Atoms		AltConf
50	n	1	Total	Zn	0
			1	1	
50	2	1	Total	Zn	0
			1	1	
50	3	1	Total	Zn	0
			1	1	
50	6	1	Total	Zn	0
			1	1	

3 Residue-property plots

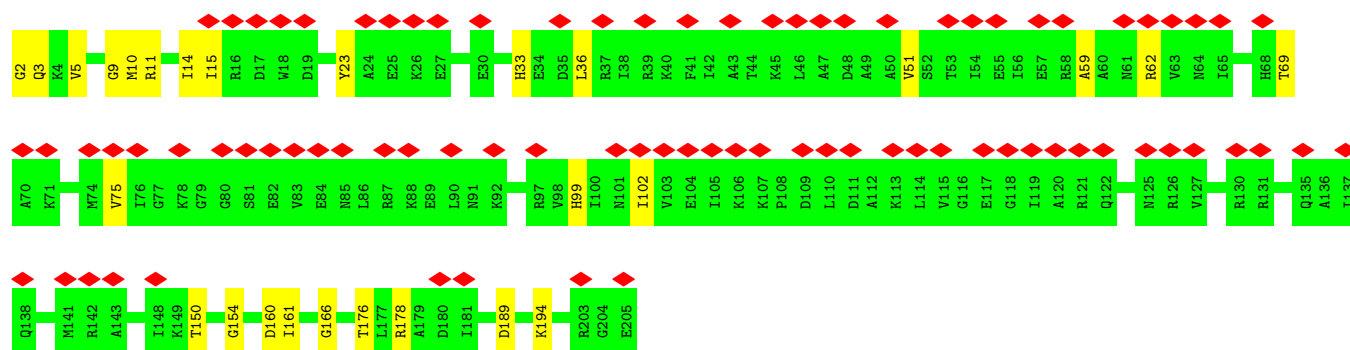
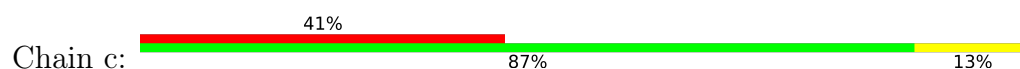
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

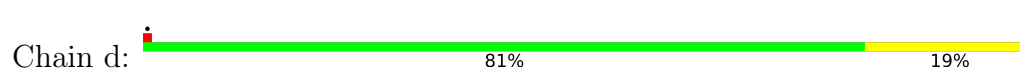




• Molecule 2: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S4





- Molecule 4: 30S ribosomal protein S5

Chain e: 85% 15%



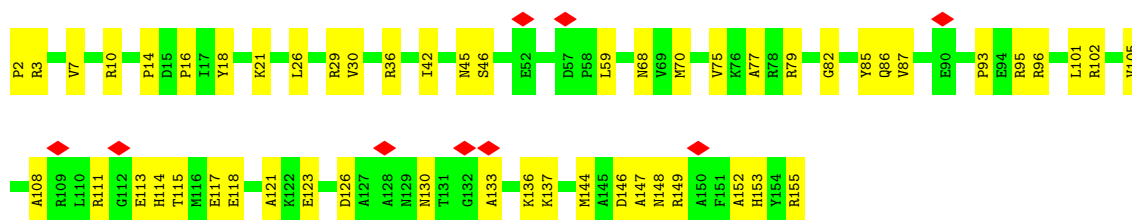
- Molecule 5: 30S ribosomal protein S6

Chain f: 77% 23%



- Molecule 6: 30S ribosomal protein S7

Chain g: 6% 66% 34%



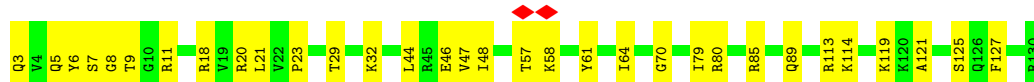
- Molecule 7: 30S ribosomal protein S8

Chain h: 84% 16%



- Molecule 8: 30S ribosomal protein S9

Chain i: 75% 25%

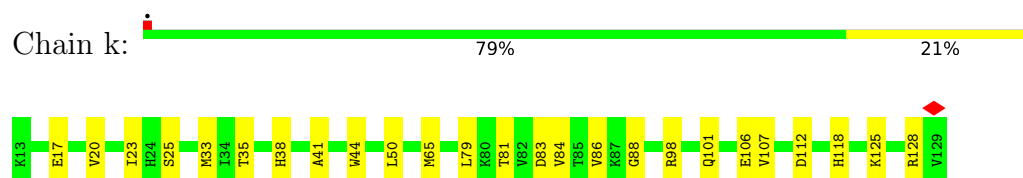


- Molecule 9: 30S ribosomal protein S10

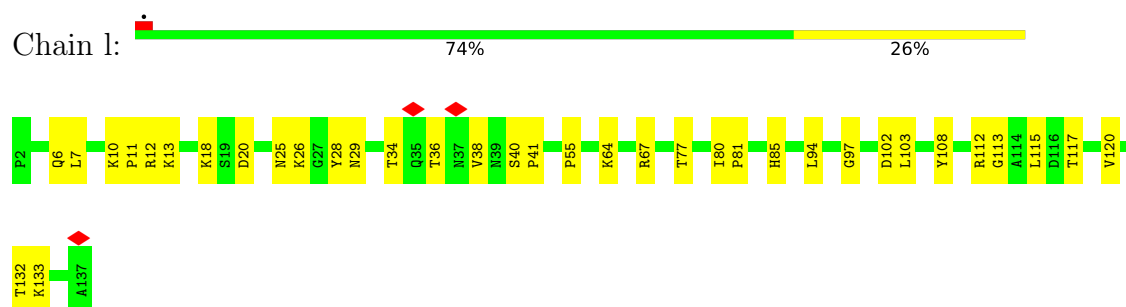
Chain j: 8% 79% 21%



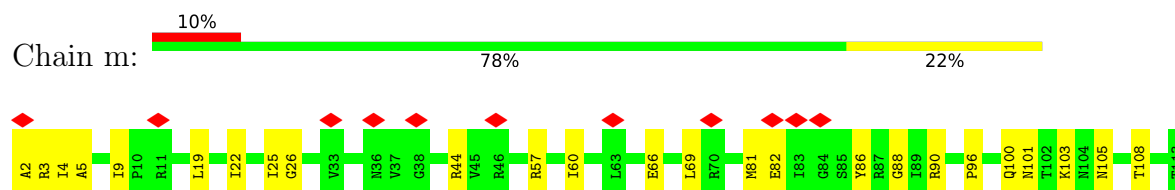
- Molecule 10: 30S ribosomal protein S11



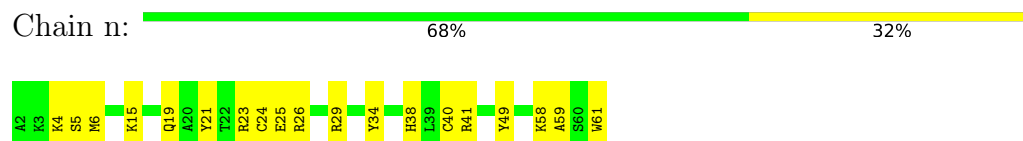
- Molecule 11: 30S ribosomal protein S12



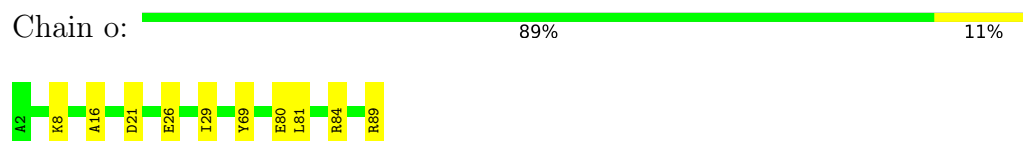
- Molecule 12: 30S ribosomal protein S13



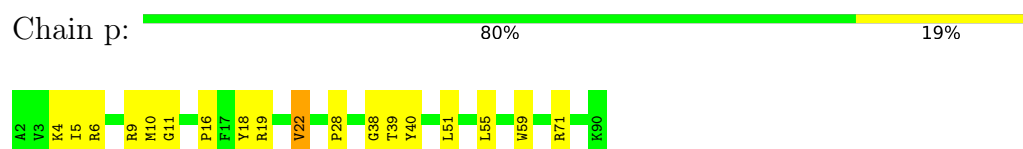
- Molecule 13: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17

Chain q:  83% 17%



- Molecule 17: 30S ribosomal protein S18

Chain r:  88% 11%



- Molecule 18: 30S ribosomal protein S19

Chain s:  6% 71% 29%



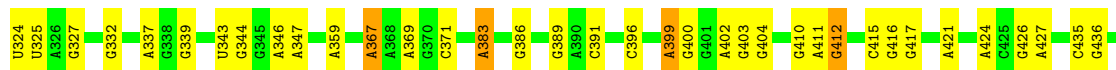
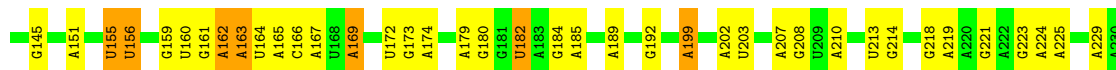
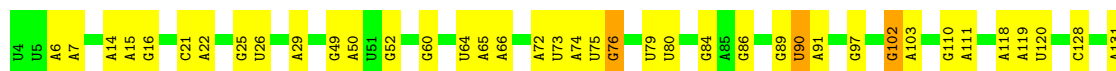
- Molecule 19: 30S ribosomal protein S20

Chain t:  85% 12%

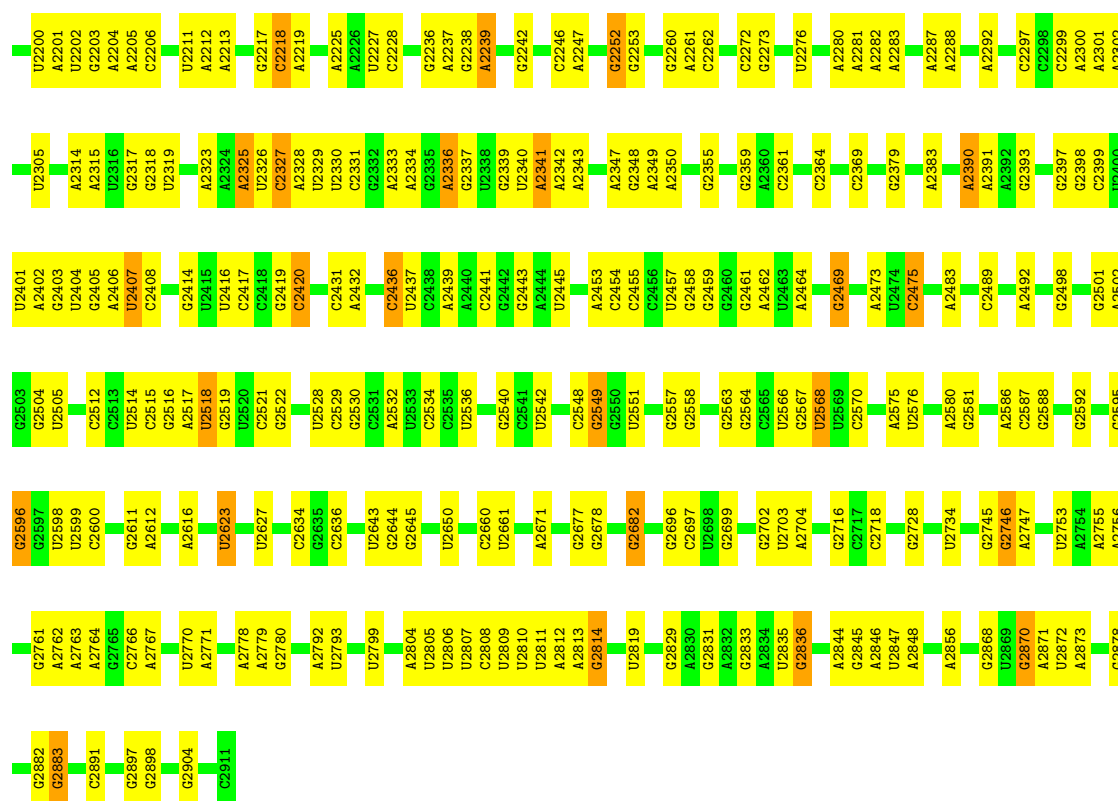


- Molecule 20: 23S rRNA

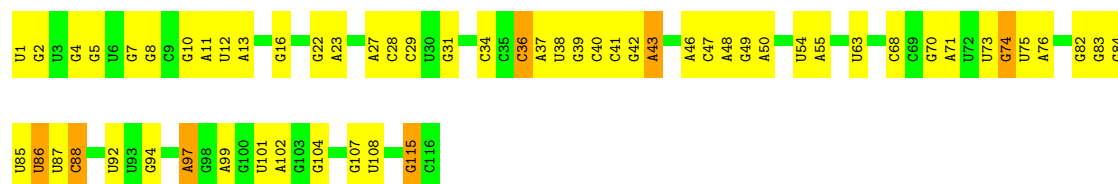
Chain A:  61% 32% 6%



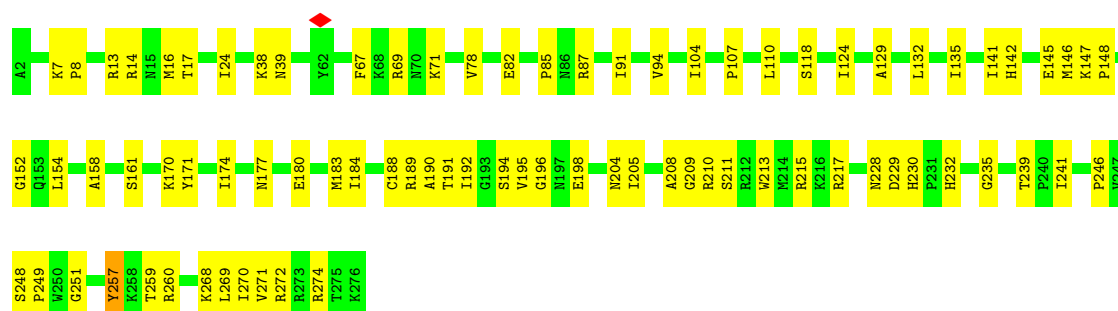




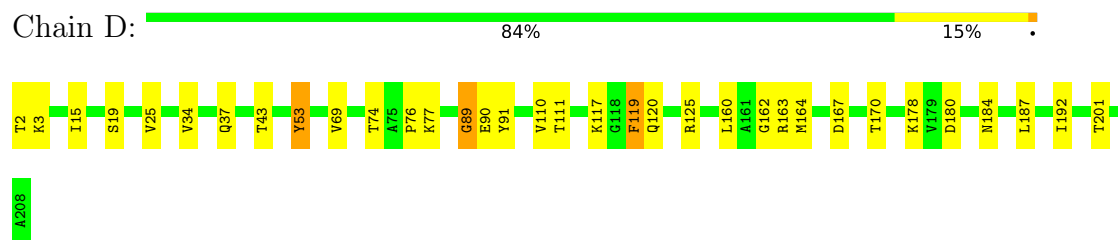
• Molecule 21: 5S rRNA



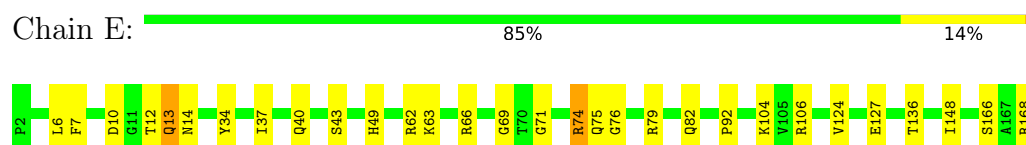
• Molecule 22: 50S ribosomal protein L2



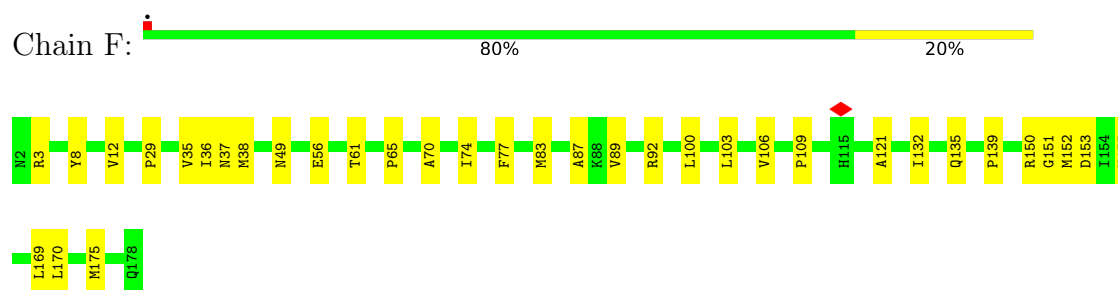
• Molecule 23: 50S ribosomal protein L3



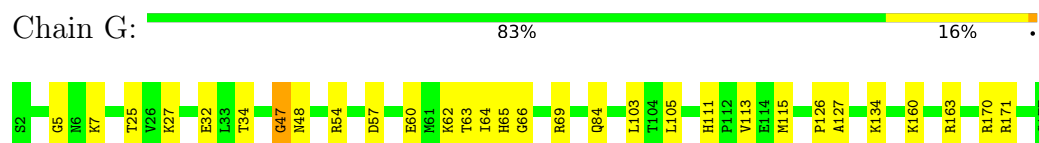
- Molecule 24: 50S ribosomal protein L4



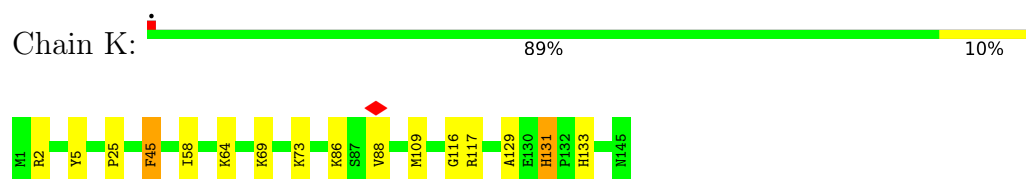
- Molecule 25: 50S ribosomal protein L5



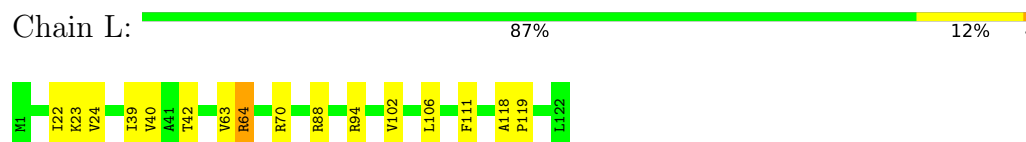
- Molecule 26: 50S ribosomal protein L6



- Molecule 27: 50S ribosomal protein L13



- Molecule 28: 50S ribosomal protein L14



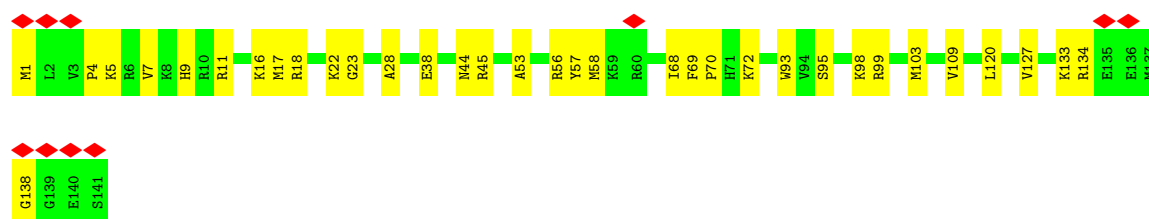
- Molecule 29: 50S ribosomal protein L15

Chain M:  82% 16%



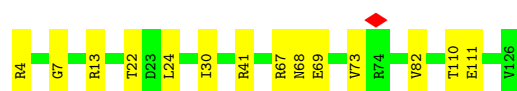
- Molecule 30: 50S ribosomal protein L16

Chain N:  7% 76% 24%



- Molecule 31: 50S ribosomal protein L17

Chain O:  89% 11%



- Molecule 32: 50S ribosomal protein L18

Chain P:  84% 15%



- Molecule 33: 50S ribosomal protein L19

Chain Q:  78% 22%



- Molecule 34: 50S ribosomal protein L20

Chain R:  86% 12%



- Molecule 35: 50S ribosomal protein L21

Chain S:  75% 25%



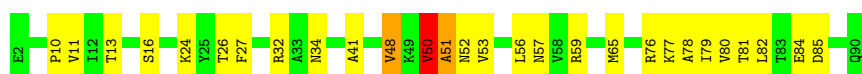
- Molecule 36: 50S ribosomal protein L22

Chain T: 89% 11%



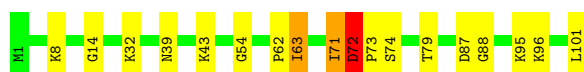
- Molecule 37: 50S ribosomal protein L23

Chain U: 69% 28% ..



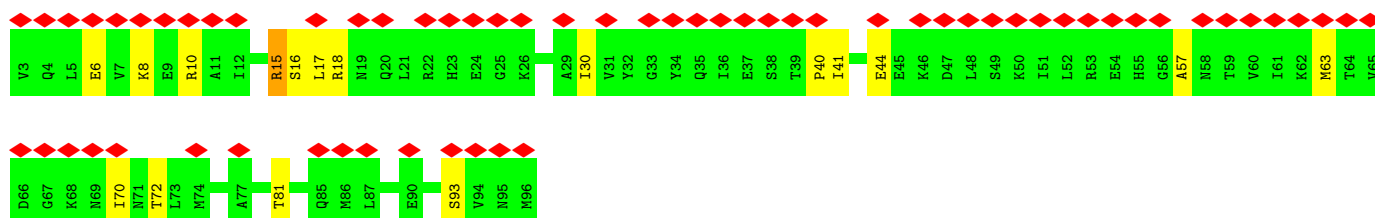
- Molecule 38: 50S ribosomal protein L24

Chain V: 82% 15% ..



- Molecule 39: 50S ribosomal protein L25

Chain W: 67% 82% 17% .



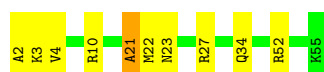
- Molecule 40: 50S ribosomal protein L27

Chain X: 83% 17%

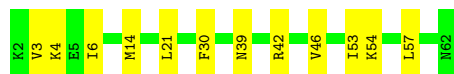


- Molecule 41: 50S ribosomal protein L28

Chain Y: 81% 17% .



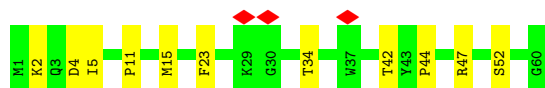
• Molecule 42: 50S ribosomal protein L29

Chain Z:  80% 20%

• Molecule 43: 50S ribosomal protein L30

Chain 0:  86% 14%

• Molecule 44: 50S ribosomal protein L31 type B

Chain 1:  5% 82% 18%

• Molecule 45: 50S ribosomal protein L32

Chain 2:  84% 16%

• Molecule 46: 50S ribosomal protein L33

Chain 3:  82% 18%

• Molecule 47: 50S ribosomal protein L34

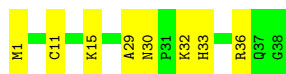
Chain 4:  80% 18% .

• Molecule 48: 50S ribosomal protein L35

Chain 5:  84% 16%

- Molecule 49: 50S ribosomal protein L36

Chain 6:  79% 21%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32689	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.890	Depositor
Minimum map value	-0.723	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.238	Depositor
Map size (Å)	482.68, 482.68, 482.68	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.097, 1.097, 1.097	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.31	0/36657	0.43	0/57173
2	c	0.21	0/1635	0.57	0/2197
3	d	0.27	0/1650	0.61	0/2217
4	e	0.27	0/1217	0.60	0/1641
5	f	0.29	0/807	0.54	0/1087
6	g	0.25	0/1249	0.58	0/1682
7	h	0.32	0/1054	0.55	0/1417
8	i	0.22	0/1003	0.57	0/1343
9	j	0.24	0/812	0.60	0/1093
10	k	0.29	0/878	0.60	2/1185 (0.2%)
11	l	0.30	0/1082	0.69	0/1453
12	m	0.23	0/890	0.58	0/1195
13	n	0.22	0/504	0.66	0/669
14	o	0.34	0/751	0.58	0/1001
15	p	0.35	0/720	0.65	0/966
16	q	0.31	0/689	0.60	0/920
17	r	0.32	0/544	0.61	0/728
18	s	0.23	0/650	0.55	0/872
19	t	0.30	0/612	0.53	0/818
20	A	0.41	0/69661	0.48	2/108645 (0.0%)
21	B	0.34	0/2769	0.46	0/4310
22	C	0.46	0/2147	0.76	0/2885
23	D	0.46	0/1598	0.77	0/2145
24	E	0.41	0/1594	0.63	0/2155
25	F	0.30	0/1408	0.58	0/1890
26	G	0.32	0/1362	0.66	2/1833 (0.1%)
27	K	0.47	0/1148	0.73	0/1549
28	L	0.45	0/929	0.70	1/1247 (0.1%)
29	M	0.40	0/1103	0.82	4/1470 (0.3%)
30	N	0.42	0/1140	0.75	2/1518 (0.1%)
31	O	0.44	0/985	0.84	2/1318 (0.2%)
32	P	0.40	0/907	0.66	0/1214

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Q	0.45	0/938	0.67	0/1262
34	R	0.46	0/923	0.63	0/1227
35	S	0.39	0/794	0.65	0/1064
36	T	0.41	0/858	0.66	0/1157
37	U	0.39	0/724	0.82	4/966 (0.4%)
38	V	0.33	0/772	0.79	2/1035 (0.2%)
39	W	0.23	0/766	0.61	0/1030
40	X	0.45	0/578	0.66	0/773
41	Y	0.28	0/430	0.57	0/573
42	Z	0.34	0/505	0.61	0/672
43	0	0.42	0/437	0.64	0/589
44	1	0.28	0/487	0.74	0/662
45	2	0.43	0/436	0.62	0/578
46	3	0.27	0/423	0.53	0/563
47	4	0.42	0/374	0.76	0/485
48	5	0.41	0/528	0.69	0/689
49	6	0.42	0/309	0.61	0/409
All	All	0.37	0/150437	0.52	21/225570 (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
3	d	0	2
7	h	0	1
16	q	0	1
19	t	0	1
22	C	0	2
23	D	0	2
24	E	0	1
25	F	0	1
26	G	0	2
27	K	0	2
29	M	0	2
30	N	0	1
32	P	0	1
35	S	0	1
37	U	0	2
38	V	0	2
39	W	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
40	X	0	2
41	Y	0	1
47	4	0	1
All	All	0	29

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	V	71	ILE	CA-C-N	6.42	137.46	121.80
38	V	71	ILE	C-N-CA	6.42	137.46	121.80
31	O	41	ARG	CA-CB-CG	6.09	126.29	114.10
29	M	15	VAL	CA-C-N	5.91	132.83	121.54
29	M	15	VAL	C-N-CA	5.91	132.83	121.54
37	U	51	ALA	CA-C-N	5.76	132.55	121.54
37	U	51	ALA	C-N-CA	5.76	132.55	121.54
31	O	41	ARG	CB-CG-CD	-5.68	98.23	111.30
10	k	38	HIS	CA-C-N	5.56	131.70	121.70
10	k	38	HIS	C-N-CA	5.56	131.70	121.70
30	N	9	HIS	CA-C-N	5.53	132.10	121.54
30	N	9	HIS	C-N-CA	5.53	132.10	121.54
37	U	50	VAL	CA-C-N	5.31	131.69	121.54
37	U	50	VAL	C-N-CA	5.31	131.69	121.54
28	L	64	ARG	CA-CB-CG	5.21	124.52	114.10
20	A	1604	A	P-O3'-C3'	5.21	128.01	120.20
20	A	1584	G	P-O3'-C3'	5.14	127.92	120.20
29	M	94	VAL	CA-C-N	5.12	131.19	121.97
29	M	94	VAL	C-N-CA	5.12	131.19	121.97
26	G	60	GLU	CA-C-N	5.00	131.10	121.54
26	G	60	GLU	C-N-CA	5.00	131.10	121.54

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	4	3	ARG	Peptide
22	C	154	LEU	Peptide
22	C	198	GLU	Peptide
23	D	53	TYR	Peptide
23	D	89	GLY	Peptide
24	E	13	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	F	121	ALA	Peptide
26	G	47	GLY	Peptide
26	G	57	ASP	Peptide
27	K	131	HIS	Peptide
27	K	45	PHE	Peptide
29	M	30	THR	Peptide
29	M	85	PHE	Peptide
30	N	133	LYS	Peptide
32	P	30	ARG	Peptide
35	S	50	ALA	Peptide
37	U	50	VAL	Peptide
37	U	84	GLU	Peptide
38	V	72	ASP	Peptide
38	V	87	ASP	Peptide
39	W	15	ARG	Peptide
40	X	28	LYS	Peptide
40	X	49	GLN	Peptide
41	Y	21	ALA	Peptide
3	d	189	GLU	Peptide
3	d	29	ARG	Peptide
7	h	22	HIS	Peptide
16	q	73	THR	Peptide
19	t	66	ILE	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	a	32746	0	16491	369	0
2	c	1610	0	1653	19	0
3	d	1620	0	1641	25	0
4	e	1204	0	1280	15	0
5	f	795	0	789	13	0
6	g	1229	0	1259	38	0
7	h	1041	0	1092	13	0
8	i	990	0	1035	23	0
9	j	800	0	846	17	0
10	k	863	0	882	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	l	1065	0	1133	24	0
12	m	884	0	932	19	0
13	n	492	0	510	16	0
14	o	741	0	756	7	0
15	p	708	0	746	15	0
16	q	681	0	719	11	0
17	r	537	0	572	8	0
18	s	634	0	649	18	0
19	t	610	0	640	10	0
20	A	62196	0	31247	463	0
21	B	2478	0	1246	34	0
22	C	2114	0	2201	56	0
23	D	1578	0	1655	25	0
24	E	1572	0	1619	22	0
25	F	1391	0	1450	23	0
26	G	1344	0	1373	19	0
27	K	1129	0	1166	13	0
28	L	922	0	985	13	0
29	M	1094	0	1144	13	0
30	N	1117	0	1175	21	0
31	O	978	0	1017	8	0
32	P	898	0	928	13	0
33	Q	924	0	979	18	0
34	R	913	0	955	12	0
35	S	783	0	823	17	0
36	T	849	0	906	11	0
37	U	719	0	767	24	0
38	V	763	0	824	10	0
39	W	757	0	775	18	0
40	X	572	0	580	7	0
41	Y	424	0	457	7	0
42	Z	504	0	538	8	0
43	0	435	0	472	5	0
44	1	475	0	441	9	0
45	2	429	0	446	8	0
46	3	419	0	435	7	0
47	4	373	0	418	9	0
48	5	522	0	576	9	0
49	6	304	0	338	7	0
50	2	1	0	0	0	0
50	3	1	0	0	0	0
50	6	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	n	1	0	0	0	0
All	All	138230	0	91561	1363	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 6.

All (1363) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:994:A:H2	1:a:1331:G:N2	1.35	1.25
20:A:2596:G:C4	20:A:2596:G:C2	2.23	1.21
1:a:994:A:C2	1:a:1331:G:N2	2.07	1.19
20:A:2536:U:C6	20:A:2536:U:C2	2.38	1.05
1:a:1321:A:N6	1:a:1346:G:C2	2.25	1.04
20:A:2761:G:N2	20:A:2771:A:H62	1.55	1.04
20:A:2761:G:H21	20:A:2771:A:N6	1.57	1.01
20:A:2536:U:C2	20:A:2536:U:C1'	2.43	1.00
1:a:943:G:H1	1:a:1405:U:H3	0.97	0.97
20:A:2536:U:C6	20:A:2536:U:C1'	2.48	0.96
20:A:1039:U:H3	20:A:1195:A:H62	0.99	0.95
20:A:2115:G:H1	20:A:2202:U:H3	0.96	0.95
1:a:1071:A:H62	1:a:1215:C:N4	1.64	0.94
20:A:1396:G:H22	20:A:2228:C:H42	0.95	0.94
1:a:1372:A:H61	1:a:1380:G:H1	1.00	0.93
20:A:343:U:H3	20:A:347:A:H62	1.13	0.92
31:O:68:ASN:C	31:O:69:GLU:CA	2.43	0.92
1:a:1071:A:H62	1:a:1215:C:H42	1.05	0.91
29:M:18:ARG:CA	29:M:18:ARG:CG	2.49	0.91
21:B:108:U:C5	21:B:108:U:N1	2.38	0.90
35:S:86:GLN:C	35:S:87:GLY:CA	2.44	0.90
20:A:2414:G:C5	20:A:2414:G:N1	2.32	0.90
23:D:43:THR:CA	23:D:43:THR:CG2	2.49	0.90
1:a:1372:A:N6	1:a:1380:G:H1	1.68	0.90
20:A:325:U:H3	20:A:389:G:H1	1.16	0.90
21:B:48:A:C3'	21:B:49:G:P	2.60	0.90
20:A:2464:A:H62	20:A:2515:C:H42	1.20	0.89
1:a:338:U:H3	1:a:342:A:H62	0.90	0.88
21:B:16:G:H1	21:B:63:U:H3	1.18	0.88
1:a:1135:U:H3	1:a:1169:G:H1	1.18	0.88
20:A:1396:G:N2	20:A:2228:C:H42	1.71	0.88
1:a:961:G:H1	1:a:1251:A:H61	1.21	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:75:U:H3	21:B:97:A:H62	1.21	0.87
20:A:1396:G:H22	20:A:2228:C:N4	1.71	0.87
25:F:135:GLN:CB	25:F:135:GLN:C	2.47	0.87
1:a:1071:A:N6	1:a:1215:C:H42	1.73	0.86
47:4:1:MET:CB	47:4:1:MET:C	2.49	0.85
20:A:275:A:H62	20:A:296:G:N2	1.74	0.85
20:A:343:U:H3	20:A:347:A:N6	1.75	0.84
20:A:1039:U:H3	20:A:1195:A:N6	1.74	0.84
20:A:1883:U:O2	20:A:1886:G:N1	2.09	0.84
37:U:41:ALA:CB	37:U:41:ALA:C	2.51	0.84
27:K:116:GLY:CA	27:K:117:ARG:N	2.42	0.82
1:a:338:U:H3	1:a:342:A:N6	1.74	0.82
1:a:220:G:H1	1:a:233:U:H3	1.26	0.81
20:A:2898:G:N2	20:A:2898:G:N3	2.29	0.81
37:U:41:ALA:CB	37:U:41:ALA:N	2.43	0.81
39:W:18:ARG:NH1	39:W:18:ARG:NE	2.29	0.81
20:A:2898:G:N2	20:A:2898:G:N1	2.29	0.81
39:W:18:ARG:NH1	39:W:18:ARG:NH2	2.29	0.80
20:A:1100:U:N3	20:A:1128:A:C8	2.49	0.80
25:F:135:GLN:CB	25:F:135:GLN:N	2.44	0.80
26:G:126:PRO:CA	26:G:127:ALA:N	2.45	0.79
47:4:1:MET:CB	47:4:1:MET:N	2.45	0.79
39:W:18:ARG:NE	39:W:18:ARG:NH2	2.29	0.79
21:B:75:U:O2	21:B:97:A:N6	2.16	0.79
20:A:164:U:O2	20:A:167:A:N6	2.12	0.78
22:C:147:LYS:CA	22:C:148:PRO:N	2.45	0.78
1:a:961:G:H1	1:a:1251:A:N6	1.81	0.78
20:A:2414:G:C5	20:A:2414:G:O6	2.37	0.77
20:A:275:A:N6	20:A:296:G:H21	1.81	0.77
1:a:1137:U:H3	1:a:1167:G:H1	0.85	0.77
47:4:1:MET:C	47:4:1:MET:N	2.44	0.76
14:o:80:GLU:O	14:o:84:ARG:HB2	1.86	0.76
20:A:1100:U:C2	20:A:1128:A:C8	2.74	0.75
20:A:2542:U:H3	20:A:2549:G:H1	1.33	0.75
20:A:2150:A:H2	20:A:2170:G:H1	1.34	0.74
44:1:4:ASP:OD1	44:1:4:ASP:CB	2.37	0.73
20:A:1793:U:C2	20:A:1797:A:N7	2.56	0.73
37:U:41:ALA:C	37:U:41:ALA:N	2.46	0.73
20:A:2763:A:H4'	26:G:62:LYS:HB3	1.68	0.73
20:A:2114:U:H3	20:A:2203:G:H1	1.37	0.73
1:a:838:G:HO2'	7:h:2:VAL:N	1.86	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:F:135:GLN:C	25:F:135:GLN:N	2.47	0.73
44:1:4:ASP:CB	44:1:4:ASP:OD2	2.37	0.73
21:B:75:U:C2	21:B:97:A:N6	2.57	0.72
1:a:994:A:N1	1:a:1331:G:N3	2.38	0.72
1:a:468:C:H41	1:a:495:U:H3	1.37	0.71
20:A:1100:U:N3	20:A:1128:A:N7	2.38	0.71
20:A:2898:G:N3	20:A:2898:G:N1	2.37	0.71
22:C:147:LYS:CA	22:C:147:LYS:O	2.38	0.71
22:C:147:LYS:O	22:C:148:PRO:N	2.24	0.71
27:K:116:GLY:CA	27:K:116:GLY:O	2.38	0.71
20:A:275:A:H62	20:A:296:G:H21	1.38	0.71
26:G:126:PRO:CA	26:G:126:PRO:O	2.39	0.70
23:D:43:THR:CG2	23:D:43:THR:OG1	2.39	0.70
34:R:16:LYS:O	34:R:17:VAL:N	2.25	0.70
1:a:225:U:HO2'	1:a:228:G:H1	1.35	0.70
26:G:126:PRO:O	26:G:127:ALA:N	2.25	0.70
27:K:116:GLY:O	27:K:117:ARG:N	2.24	0.69
1:a:192:U:H3	1:a:211:G:H1	1.40	0.69
23:D:43:THR:CA	23:D:43:THR:OG1	2.41	0.68
20:A:2154:G:H1	20:A:2165:U:H3	1.36	0.68
1:a:692:U:H3	1:a:728:G:H22	1.42	0.68
20:A:1499:G:H22	20:A:2716:G:H22	1.42	0.68
20:A:2761:G:H21	20:A:2771:A:H62	0.76	0.68
20:A:1100:U:C4	20:A:1128:A:N7	2.61	0.68
20:A:2414:G:N1	20:A:2414:G:O6	2.26	0.68
20:A:2718:C:C4'	20:A:2718:C:O5'	2.42	0.68
1:a:1344:A:H5''	12:m:26:GLY:H	1.58	0.68
23:D:120:GLN:H	23:D:125:ARG:HH22	1.42	0.68
20:A:1883:U:O2	20:A:1886:G:C6	2.47	0.67
1:a:679:G:H22	1:a:756:G:H1	1.38	0.67
20:A:1531:G:H21	20:A:1532:A:H61	1.42	0.67
9:j:9:ARG:HB2	9:j:99:GLU:HB3	1.76	0.67
7:h:12:THR:HG22	7:h:15:ARG:HH21	1.60	0.67
21:B:75:U:H3	21:B:97:A:N6	1.90	0.67
10:k:81:THR:HA	10:k:106:GLU:HB2	1.77	0.66
31:O:7:GLY:H	31:O:13:ARG:HE	1.42	0.66
35:S:14:VAL:HG13	35:S:97:ILE:HD13	1.76	0.66
20:A:2475:C:O3'	20:A:2475:C:C4'	2.43	0.66
1:a:994:A:H61	1:a:1331:G:H1'	1.61	0.66
20:A:497:A:N7	20:A:512:A:N6	2.44	0.66
1:a:133:G:O2'	16:q:8:ARG:NH1	2.28	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:902:G:H1	1:a:927:U:H3	1.44	0.65
1:a:958:G:N2	1:a:1356:U:O2	2.29	0.65
1:a:1362:G:N2	1:a:1389:A:OP2	2.30	0.65
20:A:346:A:N7	20:A:367:A:N6	2.44	0.65
20:A:510:A:OP1	24:E:79:ARG:NH2	2.30	0.65
6:g:79:ARG:HA	6:g:85:TYR:HB2	1.78	0.65
1:a:1135:U:H2'	1:a:1136:G:H8	1.62	0.64
20:A:2475:C:O3'	20:A:2475:C:C2'	2.45	0.64
1:a:338:U:O4	1:a:342:A:N7	2.30	0.64
1:a:1319:G:H21	1:a:1348:A:H62	1.45	0.64
20:A:2132:U:H3	20:A:2163:U:H5'	1.63	0.64
1:a:444:U:OP1	3:d:9:TRP:NE1	2.31	0.64
20:A:275:A:N6	20:A:296:G:N2	2.40	0.64
12:m:66:GLU:HB2	12:m:69:LEU:HB2	1.80	0.64
1:a:958:G:N1	1:a:1356:U:N3	2.44	0.63
13:n:29:ARG:HH11	13:n:40:CYS:HB2	1.61	0.63
29:M:75:ALA:HB2	29:M:106:LYS:H	1.63	0.63
1:a:1335:C:H42	18:s:36:ARG:HH11	1.44	0.63
20:A:1390:A:H5''	22:C:38:LYS:HE2	1.81	0.63
1:a:434:U:H3	1:a:439:G:H1	1.47	0.63
5:f:92:ARG:NH1	17:r:68:ILE:O	2.31	0.63
20:A:607:G:N2	20:A:2044:A:O2'	2.31	0.63
20:A:785:G:H21	20:A:790:A:H61	1.47	0.63
26:G:5:GLY:HA3	26:G:65:HIS:HB3	1.80	0.63
20:A:84:G:H1	20:A:102:G:HO2'	1.46	0.63
1:a:1257:G:N2	1:a:1310:U:O2	2.31	0.63
20:A:2150:A:N1	20:A:2170:G:O6	2.32	0.63
3:d:178:THR:HG22	3:d:179:ARG:HG3	1.82	0.62
17:r:54:LYS:HA	17:r:57:ARG:HE	1.63	0.62
1:a:1073:G:H1'	2:c:194:LYS:HD2	1.81	0.61
23:D:125:ARG:NE	23:D:162:GLY:O	2.34	0.61
1:a:1181:G:N2	1:a:1184:A:OP2	2.33	0.61
4:e:163:GLU:HG3	4:e:164:ILE:HG13	1.82	0.61
5:f:9:ILE:HG12	5:f:95:ILE:HG12	1.80	0.61
20:A:2130:G:N2	20:A:2175:C:OP1	2.33	0.61
20:A:435:C:H2'	20:A:436:G:H8	1.65	0.61
20:A:1453:U:H4'	20:A:1454:U:H5'	1.81	0.61
1:a:994:A:N1	1:a:1331:G:C2	2.68	0.61
20:A:2671:A:O2'	26:G:160:LYS:NZ	2.34	0.61
30:N:28:ALA:O	30:N:134:ARG:NH2	2.33	0.61
47:4:34:ARG:HH11	47:4:39:ARG:HD2	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:939:A:O2'	1:a:1413:A:O2'	2.19	0.61
1:a:1087:C:H2'	1:a:1088:G:H8	1.66	0.61
20:A:2636:C:O2'	20:A:2836:G:N2	2.33	0.61
6:g:18:TYR:HB3	6:g:59:LEU:HD21	1.81	0.61
1:a:1175:G:N7	1:a:1197:G:N1	2.47	0.61
20:A:2027:A:N3	36:T:93:ARG:NH2	2.49	0.61
9:j:10:LEU:HB2	9:j:72:ARG:HB2	1.82	0.61
20:A:1359:G:OP1	36:T:103:LYS:NZ	2.34	0.61
20:A:1487:U:N3	20:A:1503:U:OP2	2.33	0.61
1:a:532:G:N1	1:a:548:A:OP1	2.34	0.60
1:a:1322:U:OP1	12:m:100:GLN:NE2	2.35	0.60
6:g:149:ARG:HA	6:g:152:ALA:HB3	1.81	0.60
8:i:20:ARG:HB3	8:i:64:ILE:HB	1.82	0.60
20:A:2305:U:H3	20:A:2355:G:H1	1.49	0.60
37:U:48:VAL:HG13	37:U:85:ASP:HB2	1.83	0.60
1:a:1236:G:H4'	18:s:77:THR:HG21	1.82	0.60
20:A:2699:G:OP2	33:Q:51:ARG:NH2	2.35	0.60
37:U:57:ASN:HD21	37:U:76:ARG:HH21	1.49	0.60
21:B:1:U:H3	21:B:115:G:H1	1.49	0.60
1:a:1390:A:O2'	6:g:102:ARG:NH2	2.34	0.60
20:A:2390:A:N3	32:P:112:ARG:NH2	2.49	0.60
1:a:346:G:O2'	19:t:3:ASN:N	2.34	0.60
11:l:28:TYR:HB2	11:l:34:THR:H	1.66	0.60
1:a:983:C:H3'	1:a:984:A:H2'	1.84	0.60
7:h:106:ILE:HG12	7:h:127:VAL:HG22	1.84	0.60
6:g:75:VAL:HG11	6:g:148:ASN:HD21	1.67	0.60
20:A:610:G:OP2	35:S:79:LYS:NZ	2.35	0.60
26:G:163:ARG:HH22	26:G:171:ARG:HH21	1.49	0.60
45:2:37:LYS:NZ	45:2:46:CYS:SG	2.75	0.60
14:o:29:ILE:HD11	14:o:81:LEU:HD13	1.83	0.60
20:A:182:U:H5''	47:4:36:ARG:HH21	1.66	0.60
1:a:1392:A:OP1	6:g:95:ARG:NH2	2.35	0.60
1:a:419:G:O2'	1:a:454:U:N3	2.35	0.59
1:a:1090:G:H1	1:a:1099:U:H3	1.49	0.59
1:a:1363:U:H2'	1:a:1364:A:H8	1.67	0.59
35:S:49:GLY:HA3	35:S:53:VAL:HG22	1.84	0.59
5:f:12:ILE:HB	5:f:91:ILE:HB	1.83	0.59
20:A:2529:C:H2'	20:A:2530:G:H8	1.66	0.59
21:B:75:U:OP2	39:W:18:ARG:NH1	2.34	0.59
1:a:1262:U:C2	1:a:1305:G:O6	2.55	0.59
3:d:17:ILE:HG22	3:d:19:LEU:H	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:15:MET:HB2	44:1:47:ARG:HG2	1.83	0.59
1:a:406:C:OP1	15:p:9:ARG:NH2	2.35	0.59
1:a:562:A:OP1	3:d:66:ARG:NH2	2.32	0.59
6:g:77:ALA:HA	6:g:86:GLN:HB3	1.84	0.59
10:k:25:SER:H	10:k:88:GLY:HA3	1.67	0.59
20:A:632:U:H2'	20:A:633:G:H8	1.66	0.59
20:A:2299:C:OP2	46:3:22:ASN:ND2	2.35	0.59
44:1:4:ASP:OD1	44:1:4:ASP:OD2	2.19	0.59
1:a:925:A:OP1	11:l:18:LYS:NZ	2.35	0.59
1:a:225:U:O2'	1:a:228:G:N1	2.27	0.59
20:A:1212:A:N7	20:A:1216:G:N2	2.50	0.59
3:d:50:GLN:HG2	3:d:194:LEU:HB3	1.85	0.59
15:p:11:GLY:HA3	15:p:16:PRO:HA	1.83	0.59
20:A:1793:U:O2	20:A:1797:A:C6	2.56	0.59
16:q:71:SER:HB2	16:q:74:LYS:HG2	1.84	0.59
20:A:2147:G:N2	20:A:2172:A:OP2	2.35	0.59
20:A:192:G:H21	20:A:210:A:H62	1.50	0.59
30:N:38:GLU:HB2	30:N:127:VAL:HG13	1.85	0.59
20:A:922:G:H21	20:A:936:U:H5	1.50	0.59
25:F:109:PRO:HG3	44:1:52:SER:HB3	1.84	0.59
1:a:1044:C:OP2	1:a:1051:G:N2	2.36	0.58
2:c:51:VAL:HA	2:c:69:THR:HA	1.85	0.58
22:C:107:PRO:HD2	22:C:110:LEU:HD12	1.86	0.58
22:C:135:ILE:HG21	22:C:141:ILE:HD11	1.85	0.58
24:E:63:LYS:HG2	24:E:76:GLY:HA2	1.84	0.58
9:j:26:VAL:HG13	9:j:36:VAL:HG21	1.86	0.58
11:l:11:PRO:HB2	11:l:13:LYS:HG3	1.84	0.58
20:A:359:A:OP1	24:E:168:ARG:NH1	2.36	0.58
20:A:508:G:OP2	47:4:37:LYS:NZ	2.36	0.58
20:A:1050:A:OP1	34:R:66:ASN:ND2	2.36	0.58
20:A:2457:U:H2'	20:A:2458:G:H8	1.68	0.58
1:a:542:G:O2'	1:a:550:A:N1	2.29	0.58
20:A:874:U:H2'	20:A:875:A:H8	1.68	0.58
20:A:1793:U:O2	20:A:1797:A:C5	2.57	0.58
21:B:74:G:OP1	39:W:10:ARG:NH1	2.37	0.58
1:a:1084:G:H5'	1:a:1403:C:H5'	1.86	0.58
9:j:46:ARG:NH1	9:j:66:GLU:OE1	2.37	0.58
20:A:1133:G:H22	20:A:1138:A:H5''	1.68	0.58
20:A:1871:G:N2	20:A:1900:U:O4	2.37	0.58
21:B:12:U:OP2	40:X:83:ARG:NH2	2.37	0.58
1:a:418:C:H5''	3:d:130:PRO:HD2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1087:G:O2'	20:A:1151:A:N6	2.37	0.58
20:A:2152:C:N4	20:A:2153:G:O6	2.37	0.58
21:B:75:U:N3	21:B:97:A:N6	2.44	0.58
23:D:34:VAL:HG21	23:D:74:THR:HG21	1.85	0.58
1:a:279:C:O2'	16:q:68:ARG:NH1	2.36	0.58
1:a:312:G:N2	1:a:315:A:OP2	2.35	0.58
20:A:570:A:OP1	20:A:598:G:N2	2.35	0.58
42:Z:14:MET:HE3	42:Z:53:ILE:HG23	1.86	0.58
2:c:23:TYR:HB3	9:j:97:ASN:HD22	1.67	0.58
20:A:1178:G:H21	27:K:109:MET:HE1	1.69	0.58
6:g:26:LEU:HD13	6:g:101:LEU:HD22	1.85	0.57
20:A:1452:G:H21	20:A:1454:U:H1'	1.69	0.57
35:S:67:LYS:HB3	35:S:89:ARG:HG2	1.85	0.57
20:A:731:C:OP1	22:C:217:ARG:NH2	2.37	0.57
32:P:25:THR:HG21	32:P:30:ARG:HG3	1.86	0.57
1:a:314:G:N2	1:a:581:G:O6	2.37	0.57
12:m:81:MET:HG3	12:m:82:GLU:HG3	1.85	0.57
18:s:47:PHE:HB2	18:s:62:ILE:HD12	1.86	0.57
20:A:416:G:H2'	20:A:417:G:H8	1.68	0.57
20:A:1491:U:O4	20:A:1506:A:N6	2.38	0.57
1:a:821:C:H2'	1:a:822:A:H8	1.69	0.57
1:a:1042:C:H4'	1:a:1043:C:H5'	1.86	0.57
20:A:273:A:OP2	20:A:297:G:N1	2.38	0.57
20:A:1831:G:OP1	22:C:87:ARG:NH2	2.37	0.57
20:A:2025:U:OP2	36:T:21:LYS:NZ	2.34	0.57
1:a:227:C:H3'	1:a:228:G:H8	1.70	0.57
1:a:281:G:H3'	16:q:72:ALA:HB2	1.85	0.57
30:N:4:PRO:HD2	30:N:44:ASN:HB3	1.87	0.57
20:A:1014:A:OP2	35:S:80:LYS:NZ	2.37	0.57
21:B:75:U:H2'	21:B:76:A:H8	1.70	0.57
22:C:94:VAL:HG21	22:C:104:ILE:HD12	1.85	0.57
24:E:14:ASN:ND2	24:E:127:GLU:OE2	2.37	0.57
26:G:27:LYS:HG2	26:G:32:GLU:HG2	1.87	0.57
1:a:967:G:N7	12:m:103:LYS:NZ	2.51	0.57
11:l:25:ASN:HB3	11:l:36:THR:HG21	1.87	0.57
20:A:520:A:H4'	38:V:43:LYS:HG2	1.86	0.57
20:A:653:G:N1	20:A:655:G:OP2	2.37	0.57
20:A:939:C:O2'	20:A:940:G:N7	2.32	0.57
20:A:2090:U:OP2	20:A:2252:G:N2	2.38	0.57
45:2:46:CYS:HB3	45:2:48:HIS:HD2	1.69	0.57
20:A:1301:G:H5''	45:2:16:ARG:HH22	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1499:G:H1	20:A:2716:G:H1	1.52	0.57
1:a:1516:A:H5''	1:a:1524:G:H5''	1.84	0.57
20:A:1612:A:OP2	22:C:210:ARG:NH2	2.38	0.57
1:a:904:G:H21	1:a:925:A:H62	1.53	0.56
2:c:189:ASP:HB2	2:c:194:LYS:HA	1.87	0.56
20:A:248:G:N7	48:5:8:ARG:NH1	2.52	0.56
20:A:2218:C:H2'	20:A:2219:A:H8	1.70	0.56
43:0:10:ARG:HB3	43:0:53:LEU:HD23	1.87	0.56
1:a:1074:G:N2	1:a:1214:U:O2	2.36	0.56
21:B:34:C:N4	21:B:47:C:O2	2.34	0.56
25:F:170:LEU:HB3	25:F:175:MET:HG3	1.86	0.56
37:U:53:VAL:HG13	37:U:80:VAL:HG22	1.87	0.56
37:U:48:VAL:HG11	37:U:82:LEU:HD13	1.88	0.56
1:a:1231:A:H5''	13:n:5:SER:HB3	1.86	0.56
8:i:29:THR:HB	8:i:32:LYS:HA	1.87	0.56
20:A:1039:U:C2	20:A:1195:A:N6	2.74	0.56
20:A:2202:U:H2'	20:A:2203:G:H8	1.71	0.56
1:a:1371:G:H2'	1:a:1372:A:H8	1.71	0.56
22:C:145:GLU:HB2	22:C:188:CYS:HB3	1.87	0.56
20:A:343:U:N3	20:A:347:A:N6	2.39	0.56
25:F:70:ALA:HB2	25:F:83:MET:H	1.70	0.56
1:a:431:G:H2'	1:a:432:G:H8	1.71	0.56
1:a:1107:U:O2'	1:a:1109:A:N6	2.39	0.56
3:d:18:SER:HB2	3:d:22:THR:H	1.71	0.56
20:A:60:G:H1'	20:A:74:A:H2'	1.88	0.56
20:A:1361:C:O2	36:T:91:ARG:NH2	2.39	0.56
20:A:1730:G:H21	20:A:1744:A:H62	1.53	0.56
20:A:2045:A:HO2'	20:A:2469:G:HO2'	1.53	0.56
1:a:116:G:H5''	15:p:28:PRO:HG3	1.88	0.56
1:a:442:C:OP1	3:d:13:ARG:NH1	2.39	0.56
1:a:1457:A:HO2'	33:Q:114:ARG:HH12	1.54	0.56
20:A:568:A:H2	20:A:2055:U:H3	1.52	0.56
20:A:626:U:H2'	20:A:627:A:H8	1.71	0.56
21:B:86:U:O2	21:B:88:C:N4	2.38	0.56
1:a:1149:A:N6	1:a:1157:G:O6	2.39	0.56
20:A:1120:A:N6	20:A:1128:A:OP2	2.31	0.55
20:A:2143:C:H2'	20:A:2173:G:H1	1.70	0.55
22:C:161:SER:H	22:C:177:ASN:HD21	1.53	0.55
33:Q:53:ALA:H	33:Q:57:GLU:HG2	1.71	0.55
1:a:133:G:H3'	16:q:5:ARG:HH21	1.70	0.55
20:A:128:C:OP2	37:U:32:ARG:NH2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:162:A:O2'	20:A:169:A:N6	2.38	0.55
20:A:203:U:H4'	41:Y:22:MET:HB2	1.87	0.55
33:Q:60:THR:HG22	33:Q:73:THR:HG22	1.88	0.55
6:g:29:ARG:HB3	6:g:105:VAL:HG21	1.87	0.55
8:i:9:THR:H	8:i:85:ARG:HD2	1.71	0.55
20:A:2179:G:N7	20:A:2180:G:N2	2.53	0.55
35:S:56:ALA:HA	35:S:101:ASN:HD21	1.72	0.55
1:a:1257:G:C2	1:a:1310:U:O2	2.60	0.55
18:s:55:ARG:HG2	18:s:56:LYS:HG2	1.88	0.55
20:A:544:A:HO2'	20:A:548:C:HO2'	1.51	0.55
20:A:1030:A:O2'	20:A:1032:C:OP2	2.21	0.55
20:A:2767:A:O2'	49:6:15:LYS:NZ	2.39	0.55
22:C:241:ILE:HD13	22:C:246:PRO:HB3	1.88	0.55
1:a:1177:C:H2'	1:a:1178:G:H8	1.72	0.55
1:a:1270:G:H2'	1:a:1294:A:H61	1.71	0.55
20:A:996:G:OP2	30:N:16:LYS:NZ	2.37	0.55
20:A:1309:A:O5'	20:A:1689:A:N6	2.39	0.55
20:A:2047:A:O2'	20:A:2049:G:OP2	2.24	0.55
20:A:2114:U:O2	20:A:2203:G:N2	2.37	0.55
20:A:500:A:H62	20:A:509:G:H8	1.55	0.55
38:V:79:THR:HG22	38:V:96:LYS:HB2	1.89	0.55
1:a:324:G:O2'	1:a:622:A:N1	2.36	0.55
1:a:1144:C:O2'	1:a:1162:C:N3	2.39	0.55
20:A:900:G:O2'	20:A:957:G:O6	2.19	0.55
20:A:934:G:N2	20:A:935:U:O4	2.39	0.55
20:A:2390:A:N6	32:P:100:TYR:OH	2.39	0.55
1:a:1432:G:O2'	1:a:1499:A:N6	2.39	0.55
14:o:89:ARG:HH11	20:A:754:U:H2'	1.72	0.55
20:A:769:G:H22	22:C:208:ALA:HB3	1.71	0.55
20:A:1319:G:N2	20:A:1322:A:OP2	2.39	0.55
33:Q:62:ARG:HH22	33:Q:101:ARG:HG3	1.70	0.55
20:A:1396:G:O6	20:A:2228:C:O2	2.24	0.55
1:a:1162:C:O2	8:i:18:ARG:NH1	2.38	0.55
20:A:2361:C:HO2'	46:3:17:TYR:HH	1.52	0.55
1:a:785:C:H2'	1:a:786:G:H8	1.72	0.54
4:e:98:PRO:HG2	7:h:99:ASN:HD21	1.72	0.54
8:i:6:TYR:HB2	8:i:21:LEU:HB3	1.88	0.54
20:A:2836:G:H1	23:D:163:ARG:HH22	1.55	0.54
26:G:170:ARG:NH1	49:6:29:ALA:O	2.40	0.54
34:R:52:GLN:HG2	34:R:55:ARG:HD2	1.88	0.54
4:e:24:VAL:HG23	4:e:29:ARG:HG2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:W:72:THR:HA	39:W:93:SER:HA	1.88	0.54
11:l:80:ILE:HD13	11:l:85:HIS:HB3	1.88	0.54
14:o:26:GLU:HG2	14:o:81:LEU:HD11	1.88	0.54
20:A:79:U:OP1	42:Z:4:LYS:NZ	2.40	0.54
1:a:1430:G:H2'	1:a:1431:A:H8	1.71	0.54
20:A:84:G:N1	20:A:102:G:O2'	2.37	0.54
20:A:1396:G:N1	20:A:2228:C:N3	2.44	0.54
22:C:71:LYS:O	22:C:118:SER:OG	2.25	0.54
1:a:1234:U:OP1	13:n:15:LYS:NZ	2.39	0.54
1:a:1357:C:H2'	1:a:1358:G:C8	2.42	0.54
22:C:174:ILE:HD12	22:C:184:ILE:HD12	1.88	0.54
37:U:56:LEU:HD12	37:U:77:LYS:HD2	1.89	0.54
1:a:453:G:N2	1:a:511:G:N7	2.43	0.54
21:B:68:C:H5	21:B:104:G:H22	1.55	0.54
25:F:74:ILE:HG22	25:F:77:PHE:H	1.71	0.54
20:A:73:U:OP2	42:Z:54:LYS:NZ	2.41	0.54
20:A:1143:A:N6	20:A:1144:C:N3	2.56	0.54
11:l:81:PRO:O	11:l:112:ARG:NH1	2.41	0.54
39:W:15:ARG:O	39:W:17:LEU:N	2.41	0.54
1:a:1148:C:OP1	8:i:3:GLN:NE2	2.41	0.54
1:a:1164:C:OP2	8:i:11:ARG:NH2	2.41	0.54
20:A:699:U:H2'	20:A:700:G:H8	1.72	0.54
20:A:2158:G:O2'	20:A:2161:A:N6	2.41	0.54
39:W:10:ARG:HD3	39:W:40:PRO:HB2	1.89	0.54
1:a:650:A:O3'	16:q:9:LYS:NZ	2.41	0.54
1:a:1193:G:N2	1:a:1196:G:OP2	2.41	0.54
1:a:1295:A:OP2	9:j:9:ARG:NH2	2.41	0.54
20:A:1457:A:N6	20:A:1630:G:OP2	2.39	0.53
20:A:2006:G:N2	20:A:2010:C:O2'	2.40	0.53
6:g:79:ARG:HD3	6:g:82:GLY:HA2	1.90	0.53
10:k:86:VAL:HB	10:k:112:ASP:HA	1.90	0.53
20:A:145:G:OP1	37:U:34:ASN:ND2	2.41	0.53
1:a:470:A:OP1	15:p:71:ARG:NH2	2.37	0.53
20:A:1724:G:H21	20:A:1776:A:H3'	1.73	0.53
24:E:12:THR:HG22	24:E:13:GLN:HG3	1.89	0.53
27:K:2:ARG:HH22	35:S:10:LYS:HZ2	1.55	0.53
28:L:106:LEU:HB3	28:L:111:PHE:HB2	1.89	0.53
1:a:939:A:HO2'	1:a:1413:A:HO2'	1.57	0.53
1:a:1475:C:OP1	19:t:26:ASN:ND2	2.39	0.53
5:f:50:ARG:HA	5:f:60:GLU:HA	1.90	0.53
6:g:16:PRO:HB3	8:i:46:GLU:H	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:681:G:N2	20:A:684:U:OP2	2.39	0.53
33:Q:48:ILE:HG23	33:Q:97:LEU:H	1.72	0.53
36:T:9:LYS:HG2	36:T:111:VAL:HG22	1.89	0.53
1:a:987:G:HO2'	1:a:1380:G:HO2'	1.55	0.53
20:A:2704:A:OP1	31:O:4:ARG:NH1	2.40	0.53
22:C:39:ASN:OD1	22:C:215:ARG:NH1	2.41	0.53
36:T:87:MET:HB2	36:T:103:LYS:HB2	1.91	0.53
4:e:18:ILE:HG22	4:e:35:ALA:HA	1.90	0.53
1:a:361:G:OP1	33:Q:39:ARG:NH1	2.42	0.53
1:a:1493:U:H2'	1:a:1494:A:H8	1.74	0.53
3:d:61:TYR:HE1	3:d:97:ASN:HD21	1.56	0.53
20:A:2272:C:O2'	20:A:2441:C:OP2	2.26	0.53
1:a:545:G:N2	1:a:545:G:OP2	2.40	0.53
8:i:7:SER:O	8:i:89:GLN:NE2	2.42	0.53
20:A:610:G:N1	20:A:2045:A:OP1	2.38	0.53
20:A:1502:G:H1'	20:A:1503:U:H3'	1.91	0.53
20:A:1955:C:N4	20:A:1979:C:O4'	2.41	0.53
1:a:795:A:H5''	10:k:125:LYS:HD2	1.91	0.53
20:A:343:U:C2	20:A:347:A:N6	2.76	0.53
20:A:2154:G:O6	20:A:2165:U:O4	2.27	0.53
1:a:943:G:N1	1:a:1405:U:N3	2.42	0.52
3:d:112:ARG:O	3:d:116:ASN:HB2	2.09	0.52
1:a:667:U:O4	1:a:767:G:O2'	2.28	0.52
1:a:697:U:H2'	1:a:698:G:H8	1.74	0.52
20:A:746:A:OP1	22:C:7:LYS:NZ	2.32	0.52
20:A:830:A:N1	20:A:834:A:O2'	2.42	0.52
20:A:1645:U:OP1	37:U:59:ARG:NH2	2.42	0.52
20:A:2115:G:N2	20:A:2202:U:O2	2.33	0.52
27:K:131:HIS:HB3	27:K:133:HIS:H	1.73	0.52
32:P:33:ILE:HD13	32:P:104:VAL:HG13	1.90	0.52
37:U:51:ALA:O	37:U:81:THR:OG1	2.27	0.52
37:U:53:VAL:HG22	37:U:80:VAL:HG13	1.91	0.52
1:a:966:U:OP1	12:m:101:ASN:ND2	2.42	0.52
3:d:25:GLU:HG3	3:d:29:ARG:HD2	1.91	0.52
20:A:1151:A:H8	20:A:1152:G:H1'	1.74	0.52
23:D:2:THR:OG1	23:D:3:LYS:N	2.42	0.52
38:V:32:LYS:HB3	38:V:62:PRO:HB2	1.91	0.52
1:a:213:G:O2'	19:t:58:ASP:OD2	2.28	0.52
1:a:367:C:O2	1:a:370:C:N4	2.42	0.52
1:a:943:G:O6	1:a:1405:U:O4	2.28	0.52
1:a:998:U:H3'	13:n:6:MET:HE1	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:320:U:H3'	20:A:321:C:H4'	1.91	0.52
25:F:29:PRO:HB2	25:F:169:LEU:HD11	1.91	0.52
25:F:65:PRO:HB2	25:F:87:ALA:HB1	1.92	0.52
1:a:1128:C:O2	2:c:178:ARG:NE	2.42	0.52
12:m:5:ALA:HA	12:m:57:ARG:HG3	1.92	0.52
20:A:836:U:OP2	24:E:62:ARG:NH1	2.40	0.52
20:A:905:G:OP1	20:A:906:C:N4	2.40	0.52
20:A:1375:G:H21	20:A:1646:A:H1'	1.75	0.52
1:a:192:U:O2	1:a:211:G:N2	2.40	0.52
1:a:1237:G:N7	1:a:1337:C:N4	2.57	0.52
1:a:1442:C:H2'	1:a:1443:A:H8	1.74	0.52
6:g:70:MET:HG3	6:g:96:ARG:HD3	1.90	0.52
20:A:782:U:H2'	20:A:783:A:C8	2.44	0.52
20:A:1262:G:OP1	35:S:70:LYS:NZ	2.43	0.52
20:A:1883:U:O2	20:A:1886:G:O6	2.26	0.52
33:Q:31:LYS:HD2	33:Q:80:ARG:HA	1.91	0.52
40:X:27:SER:O	40:X:29:ARG:NH1	2.42	0.52
1:a:1145:C:N4	1:a:1154:G:O2'	2.42	0.52
20:A:65:A:H2'	20:A:66:A:H8	1.75	0.52
8:i:5:GLN:OE1	8:i:20:ARG:NE	2.41	0.52
20:A:993:A:OP2	30:N:18:ARG:NH1	2.43	0.52
20:A:2762:A:H2'	20:A:2763:A:H8	1.75	0.52
1:a:18:G:H21	1:a:930:A:H62	1.57	0.52
1:a:562:A:OP2	3:d:2:SER:N	2.43	0.52
12:m:3:ARG:HG3	12:m:4:ILE:HG23	1.92	0.52
16:q:23:THR:OG1	16:q:74:LYS:NZ	2.43	0.52
20:A:451:G:OP2	20:A:2420:C:O2'	2.27	0.52
20:A:1632:A:N1	20:A:1634:A:N6	2.58	0.52
20:A:2176:G:OP1	20:A:2180:G:N2	2.43	0.52
1:a:135:A:O2'	1:a:203:U:O4	2.28	0.52
1:a:851:G:H1	1:a:866:U:H3	1.57	0.52
20:A:824:U:O4	22:C:228:ASN:ND2	2.25	0.52
24:E:7:PHE:HD1	24:E:13:GLN:H	1.58	0.52
1:a:1002:A:H1'	18:s:55:ARG:HA	1.91	0.51
1:a:1283:G:O2'	1:a:1341:U:O2'	2.23	0.51
8:i:47:VAL:HA	8:i:80:ARG:HH21	1.73	0.51
10:k:17:GLU:HA	10:k:79:LEU:HA	1.92	0.51
11:l:94:LEU:HB2	11:l:115:LEU:HD12	1.91	0.51
20:A:1572:A:H62	20:A:1589:G:H8	1.58	0.51
20:A:2150:A:C2	20:A:2170:G:N1	2.73	0.51
22:C:171:TYR:HB2	22:C:183:MET:HE3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:10:MET:SD	15:p:19:ARG:NE	2.83	0.51
15:p:55:LEU:O	15:p:59:TRP:HB2	2.10	0.51
20:A:1039:U:O4	20:A:1195:A:N7	2.42	0.51
32:P:45:ILE:HG12	32:P:52:THR:HG22	1.92	0.51
1:a:475:G:N2	1:a:489:G:O2'	2.41	0.51
1:a:688:G:H2'	1:a:689:G:C8	2.45	0.51
20:A:674:C:O2'	20:A:678:U:OP1	2.28	0.51
20:A:2157:C:O2	20:A:2162:G:N2	2.41	0.51
29:M:97:LYS:HG3	29:M:98:GLU:H	1.75	0.51
33:Q:14:ARG:HG2	33:Q:16:ASP:H	1.75	0.51
1:a:1546:G:N2	1:a:1547:A:N1	2.58	0.51
2:c:36:LEU:HD21	13:n:26:ARG:HB3	1.93	0.51
20:A:1104:C:N3	20:A:1115:C:N4	2.57	0.51
20:A:2246:C:OP2	41:Y:27:ARG:NH2	2.44	0.51
30:N:99:ARG:O	39:W:81:THR:OG1	2.25	0.51
1:a:1137:U:O4	1:a:1167:G:O6	2.28	0.51
1:a:1235:G:N2	18:s:54:GLY:O	2.44	0.51
3:d:84:GLY:HA3	3:d:192:GLU:HB2	1.93	0.51
20:A:343:U:O4	20:A:347:A:N7	2.43	0.51
20:A:708:A:H2'	20:A:710:A:H62	1.76	0.51
21:B:68:C:H41	21:B:104:G:H1	1.59	0.51
25:F:100:LEU:HD23	25:F:103:LEU:HD12	1.91	0.51
1:a:391:G:H5''	15:p:6:ARG:HD2	1.92	0.51
2:c:9:GLY:HA3	13:n:49:TYR:HD1	1.76	0.51
20:A:2150:A:N1	20:A:2170:G:C6	2.79	0.51
23:D:167:ASP:N	23:D:167:ASP:OD1	2.40	0.51
6:g:144:MET:HA	6:g:147:ALA:HB3	1.92	0.51
13:n:24:CYS:SG	13:n:25:GLU:N	2.84	0.51
20:A:1096:G:H3'	20:A:1127:G:H22	1.75	0.51
22:C:142:HIS:O	22:C:191:THR:N	2.39	0.51
24:E:124:VAL:HG21	24:E:148:ILE:HD11	1.92	0.51
1:a:1074:G:N1	1:a:1214:U:N3	2.46	0.51
1:a:1175:G:O6	1:a:1197:G:O6	2.28	0.51
4:e:85:VAL:HB	4:e:96:MET:HB2	1.93	0.51
5:f:38:ALA:HB2	5:f:76:ALA:HB1	1.92	0.51
20:A:638:C:O2'	24:E:104:LYS:NZ	2.44	0.51
20:A:961:G:N2	20:A:2283:A:OP2	2.44	0.51
20:A:1422:C:H2'	20:A:1423:A:C8	2.46	0.51
1:a:735:C:O2'	17:r:56:GLN:NE2	2.44	0.51
1:a:743:A:H2'	1:a:744:A:C8	2.46	0.51
1:a:1299:C:H3'	1:a:1300:U:H2'	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:31:ILE:HD12	18:s:49:ILE:HG12	1.92	0.51
20:A:199:A:H61	20:A:871:G:H21	1.58	0.51
23:D:15:ILE:HD12	23:D:25:VAL:HG21	1.92	0.51
25:F:132:ILE:HB	25:F:152:MET:HB2	1.93	0.51
35:S:5:ILE:HD12	35:S:14:VAL:HG21	1.92	0.51
1:a:1225:C:H1'	1:a:1229:U:H3	1.75	0.51
1:a:1500:U:HO2'	20:A:1974:A:HO2'	1.53	0.51
15:p:5:ILE:HG22	15:p:22:VAL:HB	1.93	0.51
20:A:2501:G:H2'	20:A:2502:A:H8	1.76	0.51
25:F:8:TYR:HA	25:F:12:VAL:HB	1.93	0.51
1:a:1204:U:H5''	2:c:5:VAL:HG21	1.93	0.50
20:A:539:G:N1	20:A:542:A:OP2	2.40	0.50
25:F:36:ILE:HB	25:F:89:VAL:HB	1.92	0.50
45:2:30:CYS:HB2	45:2:33:CYS:H	1.75	0.50
1:a:689:G:H2'	1:a:690:A:H8	1.76	0.50
1:a:1428:A:H2	1:a:1503:G:H22	1.59	0.50
6:g:108:ALA:HB2	6:g:123:GLU:HG2	1.93	0.50
20:A:498:G:H22	20:A:509:G:H2'	1.75	0.50
20:A:2756:A:OP2	49:6:36:ARG:NH1	2.45	0.50
1:a:346:G:HO2'	19:t:3:ASN:N	2.10	0.50
1:a:1142:U:N3	1:a:1295:A:OP1	2.44	0.50
1:a:1262:U:O2	1:a:1305:G:O6	2.29	0.50
20:A:2369:C:O2'	40:X:33:LYS:NZ	2.43	0.50
22:C:230:HIS:CE1	22:C:232:HIS:HD2	2.28	0.50
43:0:6:ILE:HG23	43:0:54:VAL:HG11	1.94	0.50
48:5:33:PHE:O	48:5:41:ARG:NH2	2.44	0.50
1:a:729:G:H2'	1:a:730:A:C8	2.47	0.50
20:A:1710:G:O2'	20:A:2005:U:O4	2.30	0.50
20:A:2327:C:O2'	25:F:37:ASN:ND2	2.45	0.50
22:C:158:ALA:HA	22:C:195:VAL:HB	1.93	0.50
1:a:690:A:H1'	10:k:118:HIS:CD2	2.47	0.50
1:a:1264:C:N4	1:a:1303:A:N7	2.59	0.50
20:A:346:A:H4'	38:V:14:GLY:HA2	1.93	0.50
20:A:485:C:OP1	34:R:2:ALA:N	2.45	0.50
20:A:2325:A:O2'	20:A:2326:U:O4'	2.30	0.50
20:A:2809:U:O2	20:A:2814:G:N2	2.45	0.50
22:C:271:VAL:HG12	22:C:272:ARG:HG3	1.94	0.50
1:a:877:G:O2'	1:a:890:G:O2'	2.30	0.50
1:a:1294:A:OP1	9:j:11:LYS:NZ	2.44	0.50
11:l:113:GLY:H	11:l:117:THR:HG23	1.76	0.50
27:K:5:TYR:O	34:R:64:ARG:NH2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S:2:TYR:HB2	35:S:42:GLY:H	1.77	0.50
1:a:797:A:H62	1:a:815:G:H21	1.58	0.50
1:a:1292:C:O2'	1:a:1294:A:N7	2.36	0.50
1:a:1539:G:H5''	10:k:125:LYS:HE3	1.94	0.50
2:c:2:GLY:N	2:c:3:GLN:OE1	2.45	0.50
12:m:96:PRO:HD2	12:m:100:GLN:HB2	1.92	0.50
20:A:192:G:H2'	20:A:208:G:H22	1.76	0.50
1:a:441:U:OP1	3:d:28:ARG:NE	2.43	0.50
1:a:877:G:HO2'	1:a:890:G:HO2'	1.60	0.50
4:e:6:PRO:HB2	4:e:8:HIS:HD2	1.75	0.50
6:g:133:ALA:O	6:g:137:LYS:N	2.45	0.50
13:n:21:TYR:HE2	13:n:23:ARG:HH21	1.58	0.50
20:A:516:G:N1	20:A:519:A:OP2	2.41	0.50
20:A:1455:U:O4	20:A:1457:A:N6	2.45	0.50
20:A:2699:G:OP1	33:Q:49:LYS:NZ	2.45	0.50
1:a:839:U:H2'	1:a:840:G:H8	1.76	0.50
1:a:1007:U:O2	1:a:1228:A:N7	2.44	0.50
1:a:1312:U:H5''	12:m:44:ARG:HH22	1.77	0.50
1:a:1357:C:H2'	1:a:1358:G:H8	1.77	0.50
20:A:337:A:OP2	38:V:95:LYS:NZ	2.42	0.50
20:A:1256:G:OP1	34:R:22:LYS:NZ	2.45	0.50
20:A:2145:A:OP1	20:A:2146:U:N3	2.45	0.50
33:Q:14:ARG:NH2	33:Q:78:THR:O	2.45	0.50
1:a:134:U:OP2	16:q:5:ARG:NH2	2.45	0.49
1:a:897:G:OP2	11:l:6:GLN:NE2	2.45	0.49
6:g:115:THR:HB	6:g:118:GLU:HB2	1.94	0.49
11:l:28:TYR:N	11:l:34:THR:O	2.45	0.49
20:A:1657:A:N6	36:T:97:SER:O	2.42	0.49
1:a:434:U:O2	1:a:439:G:N2	2.41	0.49
1:a:616:G:H2'	1:a:617:A:H8	1.77	0.49
20:A:938:C:C4	20:A:939:C:H1'	2.48	0.49
20:A:2045:A:O2'	20:A:2469:G:O2'	2.28	0.49
1:a:352:G:H2'	1:a:353:A:H8	1.76	0.49
15:p:19:ARG:HA	15:p:39:THR:HA	1.93	0.49
15:p:22:VAL:HG21	15:p:59:TRP:HE1	1.76	0.49
20:A:782:U:H2'	20:A:783:A:H8	1.77	0.49
20:A:1039:U:N3	20:A:1195:A:N6	2.43	0.49
30:N:22:LYS:HG3	30:N:98:LYS:HD2	1.94	0.49
1:a:219:G:H2'	1:a:220:G:H8	1.77	0.49
1:a:1357:C:H4'	8:i:127:PHE:HB3	1.95	0.49
20:A:1400:G:OP2	41:Y:2:ALA:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:2361:C:O2'	46:3:17:TYR:OH	2.20	0.49
20:A:2833:G:O2'	20:A:2836:G:O6	2.30	0.49
23:D:110:VAL:HG11	23:D:192:ILE:HG12	1.95	0.49
1:a:327:C:H2'	1:a:328:A:H8	1.77	0.49
1:a:1361:A:H2'	6:g:10:ARG:HH22	1.77	0.49
4:e:58:GLU:HG3	4:e:61:ARG:HH21	1.77	0.49
19:t:51:ASN:HB3	19:t:55:LYS:HZ3	1.77	0.49
20:A:80:U:O2'	20:A:383:A:N3	2.45	0.49
21:B:43:A:O4'	25:F:92:ARG:NH1	2.36	0.49
32:P:36:SER:OG	32:P:39:ASN:N	2.40	0.49
24:E:37:ILE:HG23	24:E:184:LEU:HD21	1.95	0.49
27:K:58:ILE:HG23	27:K:129:ALA:HA	1.95	0.49
29:M:79:LEU:HD21	29:M:117:LEU:HB2	1.95	0.49
37:U:26:THR:HG22	37:U:79:ILE:HG12	1.94	0.49
41:Y:10:ARG:HH22	41:Y:52:ARG:HG2	1.78	0.49
1:a:974:A:OP1	18:s:55:ARG:NH1	2.45	0.49
1:a:1095:G:H2'	1:a:1096:A:C8	2.48	0.49
9:j:53:ARG:NH2	9:j:63:GLU:OE1	2.46	0.49
20:A:1867:A:H2'	20:A:1868:A:C8	2.48	0.49
20:A:2807:U:H3	20:A:2814:G:H22	1.61	0.49
1:a:506:A:H2'	1:a:507:A:H8	1.77	0.49
1:a:1495:G:H2'	1:a:1496:A:H8	1.78	0.49
2:c:10:MET:SD	13:n:58:LYS:NZ	2.85	0.49
18:s:36:ARG:NH2	18:s:75:ALA:O	2.44	0.49
20:A:1068:A:H2'	20:A:1069:A:C8	2.48	0.49
22:C:205:ILE:HG21	22:C:211:SER:HB3	1.94	0.49
26:G:103:LEU:HB2	26:G:115:MET:HB2	1.93	0.49
1:a:350:C:H2'	1:a:351:A:H8	1.77	0.49
20:A:412:G:O2'	20:A:440:G:O6	2.27	0.49
21:B:39:G:OP1	21:B:41:C:N4	2.39	0.49
22:C:69:ARG:O	22:C:189:ARG:NH1	2.39	0.49
37:U:13:THR:N	37:U:16:SER:OG	2.42	0.49
44:1:2:LYS:HB3	44:1:5:ILE:HD11	1.95	0.49
1:a:1068:U:O2	1:a:1221:G:O6	2.31	0.49
1:a:1442:C:H2'	1:a:1443:A:C8	2.48	0.49
11:l:55:PRO:HB3	11:l:102:ASP:HB2	1.95	0.49
20:A:2342:A:H2'	20:A:2343:A:C8	2.48	0.49
23:D:15:ILE:HD11	23:D:187:LEU:HD13	1.94	0.49
1:a:208:U:H2'	1:a:209:A:C8	2.48	0.48
1:a:257:C:OP1	11:l:13:LYS:NZ	2.35	0.48
1:a:760:U:OP1	1:a:867:C:O2'	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:31:ILE:HB	18:s:49:ILE:HG23	1.94	0.48
20:A:526:C:O2'	36:T:65:ASN:ND2	2.42	0.48
20:A:2483:A:O2'	30:N:56:ARG:NH1	2.44	0.48
1:a:906:G:O2'	1:a:922:G:O6	2.29	0.48
1:a:1135:U:H2'	1:a:1136:G:C8	2.45	0.48
1:a:1504:G:H2'	1:a:1505:G:H8	1.77	0.48
2:c:11:ARG:NH2	2:c:176:THR:O	2.46	0.48
9:j:10:LEU:HG	9:j:98:ILE:HG22	1.95	0.48
20:A:730:C:O2'	20:A:820:G:OP1	2.28	0.48
21:B:83:G:H2'	21:B:84:G:C8	2.47	0.48
22:C:87:ARG:HD2	22:C:91:ILE:HD11	1.94	0.48
1:a:961:G:N2	1:a:1349:G:O2'	2.46	0.48
7:h:10:PHE:HD1	7:h:27:VAL:HG11	1.78	0.48
7:h:41:LYS:HD3	7:h:49:VAL:HG22	1.95	0.48
20:A:231:A:H1'	20:A:232:U:H2'	1.94	0.48
20:A:2431:C:H2'	20:A:2432:A:H8	1.78	0.48
1:a:567:U:O2'	11:l:41:PRO:O	2.31	0.48
20:A:487:A:OP1	34:R:5:LYS:NZ	2.41	0.48
20:A:1875:G:H2'	20:A:1876:G:H8	1.78	0.48
20:A:2644:G:H2'	20:A:2645:G:H8	1.78	0.48
22:C:248:SER:OG	22:C:251:GLY:O	2.26	0.48
23:D:34:VAL:H	23:D:77:LYS:HZ2	1.61	0.48
25:F:37:ASN:H	25:F:153:ASP:HB2	1.78	0.48
1:a:1475:C:H2'	1:a:1476:A:H8	1.78	0.48
8:i:113:ARG:NH1	8:i:114:LYS:O	2.47	0.48
18:s:36:ARG:NH1	18:s:72:GLY:O	2.47	0.48
20:A:311:A:O2'	20:A:399:A:N6	2.47	0.48
20:A:913:U:H2'	20:A:914:G:C8	2.49	0.48
24:E:74:ARG:H	24:E:74:ARG:HD3	1.78	0.48
1:a:688:G:O3'	5:f:92:ARG:NH2	2.46	0.48
1:a:1193:G:O2'	1:a:1195:A:N7	2.39	0.48
6:g:42:ILE:HB	6:g:117:GLU:HB3	1.95	0.48
20:A:281:A:H2'	20:A:282:A:C8	2.49	0.48
28:L:63:VAL:HG12	28:L:64:ARG:HG2	1.95	0.48
46:3:14:GLU:OE2	46:3:38:ARG:NH1	2.47	0.48
1:a:1237:G:OP1	1:a:1336:U:O2'	2.27	0.48
2:c:14:ILE:HG22	2:c:15:ILE:HG23	1.94	0.48
1:a:796:A:N7	1:a:816:U:O4	2.46	0.48
1:a:907:U:H2'	1:a:908:A:H8	1.79	0.48
20:A:1029:G:H5''	43:0:13:ILE:HD11	1.96	0.48
24:E:49:HIS:HD2	24:E:92:PRO:HB2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Q:87:VAL:HG12	33:Q:88:ARG:HG3	1.95	0.48
40:X:58:VAL:HB	40:X:89:SER:HB2	1.96	0.48
1:a:130:U:H2'	1:a:131:G:C8	2.49	0.48
1:a:965:A:OP1	12:m:105:ASN:ND2	2.46	0.48
9:j:9:ARG:HE	9:j:11:LYS:HE3	1.78	0.48
15:p:4:LYS:HE2	15:p:6:ARG:HD3	1.95	0.48
20:A:1823:A:H2'	20:A:1824:A:C8	2.48	0.48
1:a:360:C:O2	1:a:361:G:N2	2.47	0.48
1:a:768:A:OP1	14:o:69:TYR:OH	2.31	0.48
1:a:928:C:H2'	1:a:929:A:C8	2.49	0.48
1:a:1372:A:N1	1:a:1380:G:N2	2.55	0.48
6:g:86:GLN:O	6:g:155:ARG:NH1	2.47	0.48
20:A:571:A:H3'	34:R:38:GLN:HE22	1.79	0.48
20:A:967:C:H2'	20:A:968:A:H8	1.77	0.48
20:A:1097:A:N6	20:A:1127:G:OP2	2.44	0.48
20:A:1214:U:O4	20:A:1216:G:N2	2.41	0.48
20:A:2246:C:H2'	20:A:2247:A:H8	1.78	0.48
20:A:2436:C:H41	48:5:31:HIS:HE1	1.62	0.48
1:a:7:A:H2'	1:a:8:G:H8	1.79	0.47
1:a:131:G:OP1	1:a:620:U:O2'	2.32	0.47
1:a:1422:C:H2'	1:a:1423:A:H8	1.79	0.47
20:A:493:A:N3	20:A:497:A:O2'	2.47	0.47
20:A:1421:A:O2'	20:A:1432:U:O2	2.32	0.47
1:a:272:G:H2'	1:a:273:A:H8	1.79	0.47
20:A:2085:A:H2'	20:A:2086:G:H8	1.77	0.47
27:K:25:PRO:HD3	27:K:64:LYS:HD2	1.95	0.47
30:N:68:ILE:HD12	30:N:103:MET:HA	1.96	0.47
42:Z:3:VAL:HA	42:Z:6:ILE:HD12	1.96	0.47
1:a:551:C:H2'	1:a:552:G:H8	1.79	0.47
1:a:924:A:H2'	1:a:925:A:H8	1.78	0.47
5:f:42:GLU:OE2	5:f:44:LYS:NZ	2.39	0.47
24:E:49:HIS:CD2	24:E:92:PRO:HB2	2.50	0.47
26:G:54:ARG:HH12	26:G:65:HIS:N	2.12	0.47
33:Q:62:ARG:NH1	33:Q:71:GLU:OE2	2.47	0.47
1:a:661:G:H2'	1:a:662:G:H8	1.79	0.47
1:a:722:U:H2'	1:a:723:A:H8	1.79	0.47
1:a:1008:U:C2	1:a:1060:A:N6	2.82	0.47
1:a:1283:G:H21	1:a:1342:G:H1'	1.78	0.47
1:a:1366:U:H3	1:a:1386:G:H1	1.63	0.47
5:f:6:LYS:HG2	5:f:69:THR:HG22	1.96	0.47
25:F:61:THR:HG21	25:F:89:VAL:HG11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S:5:ILE:HG12	35:S:38:VAL:HG22	1.96	0.47
1:a:672:U:H3	1:a:673:G:H21	1.62	0.47
1:a:1043:C:N4	1:a:1052:A:N3	2.62	0.47
1:a:1245:C:H2'	1:a:1246:G:H8	1.80	0.47
10:k:23:ILE:HD12	10:k:86:VAL:HG22	1.96	0.47
12:m:4:ILE:HG12	12:m:9:ILE:HG21	1.96	0.47
20:A:654:A:H1'	20:A:655:G:H5''	1.95	0.47
20:A:868:U:O2'	20:A:871:G:O6	2.31	0.47
20:A:890:A:H2'	20:A:891:A:C8	2.50	0.47
20:A:2576:U:H1'	28:L:23:LYS:HE2	1.97	0.47
35:S:68:GLN:O	35:S:89:ARG:NH1	2.47	0.47
38:V:8:LYS:HB3	38:V:71:ILE:HD12	1.95	0.47
43:0:7:THR:HG22	43:0:34:THR:HG22	1.97	0.47
1:a:31:C:H2'	1:a:32:G:H8	1.79	0.47
10:k:33:MET:HG3	10:k:44:TRP:HB3	1.96	0.47
20:A:523:A:O2'	38:V:54:GLY:O	2.33	0.47
20:A:820:G:N1	22:C:229:ASP:OD2	2.44	0.47
1:a:209:A:H2'	1:a:210:A:H8	1.79	0.47
1:a:992:G:OP2	1:a:1373:U:O2'	2.32	0.47
1:a:1027:U:O4	1:a:1028:A:N6	2.48	0.47
1:a:1116:C:C4	1:a:1118:A:H5'	2.50	0.47
1:a:1319:G:N2	1:a:1348:A:H62	2.13	0.47
1:a:1456:G:H21	1:a:1476:A:H62	1.63	0.47
3:d:41:ARG:NH1	3:d:43:LYS:O	2.42	0.47
6:g:133:ALA:HA	6:g:136:LYS:HB2	1.97	0.47
13:n:34:TYR:O	13:n:38:HIS:N	2.45	0.47
20:A:302:A:H2'	20:A:303:G:H8	1.79	0.47
20:A:1081:U:O2	20:A:1154:G:O6	2.32	0.47
20:A:1134:U:H4'	20:A:1138:A:H62	1.79	0.47
20:A:1193:C:OP1	34:R:92:ARG:NH2	2.47	0.47
20:A:1515:C:H2'	20:A:1516:A:H8	1.78	0.47
20:A:1576:A:OP2	20:A:1584:G:N2	2.44	0.47
20:A:2061:C:H2'	20:A:2062:G:H8	1.80	0.47
21:B:46:A:H4'	32:P:101:HIS:HB2	1.94	0.47
23:D:111:THR:HG22	23:D:170:THR:HG22	1.96	0.47
23:D:180:ASP:O	23:D:184:ASN:N	2.46	0.47
30:N:58:MET:HE1	30:N:109:VAL:HG21	1.96	0.47
39:W:8:LYS:H	39:W:41:ILE:HG23	1.80	0.47
1:a:459:A:H2'	1:a:460:G:H8	1.79	0.47
10:k:35:THR:HG22	10:k:41:ALA:HA	1.97	0.47
20:A:90:U:H3'	20:A:91:A:H8	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1335:G:N2	20:A:1683:A:N7	2.63	0.47
20:A:1814:C:H5'	22:C:146:MET:HE2	1.96	0.47
1:a:237:U:H2'	1:a:238:G:H8	1.80	0.47
1:a:413:C:H2'	1:a:414:G:H8	1.79	0.47
1:a:1257:G:N1	1:a:1310:U:C2	2.79	0.47
1:a:1371:G:H2'	1:a:1372:A:C8	2.49	0.47
2:c:59:ALA:HB3	2:c:62:ARG:HB2	1.95	0.47
16:q:60:ASP:OD1	16:q:85:ALA:N	2.39	0.47
18:s:52:TYR:HA	18:s:57:HIS:HA	1.97	0.47
20:A:2762:A:H4'	26:G:66:GLY:HA3	1.96	0.47
20:A:2883:G:H21	31:O:4:ARG:NH2	2.13	0.47
1:a:75:U:OP2	1:a:98:G:N2	2.48	0.47
1:a:200:G:N2	1:a:203:U:OP2	2.44	0.47
1:a:384:C:H2'	1:a:385:G:H8	1.80	0.47
1:a:1090:G:N2	1:a:1099:U:O2	2.40	0.47
1:a:1332:C:O2'	1:a:1333:A:O4'	2.33	0.47
21:B:27:A:OP2	32:P:37:ASN:N	2.44	0.47
30:N:70:PRO:HA	30:N:95:SER:HB3	1.97	0.47
31:O:73:VAL:HG22	31:O:82:VAL:HA	1.97	0.47
1:a:352:G:H2'	1:a:353:A:C8	2.50	0.46
1:a:1321:A:N6	1:a:1346:G:N2	2.61	0.46
20:A:172:U:H2'	20:A:173:G:H8	1.80	0.46
20:A:2563:G:H2'	20:A:2564:G:H8	1.80	0.46
36:T:40:ILE:HG23	45:2:24:ILE:HD12	1.96	0.46
1:a:428:G:N2	1:a:443:G:O2'	2.46	0.46
1:a:474:C:H2'	1:a:475:G:C8	2.51	0.46
1:a:1063:G:OP1	13:n:4:LYS:NZ	2.48	0.46
10:k:50:LEU:HD23	10:k:65:MET:HE2	1.98	0.46
11:l:7:LEU:HA	11:l:10:LYS:HG2	1.97	0.46
20:A:1441:C:H2'	20:A:1442:A:H8	1.79	0.46
1:a:626:C:H42	1:a:645:G:H22	1.63	0.46
1:a:1097:G:H5'	4:e:23:LYS:HD2	1.96	0.46
7:h:52:ILE:O	7:h:59:VAL:N	2.41	0.46
20:A:703:G:N2	20:A:980:G:OP1	2.49	0.46
20:A:785:G:O2'	20:A:788:G:O2'	2.27	0.46
20:A:1303:G:O2'	20:A:2026:G:O6	2.33	0.46
20:A:2762:A:H2'	20:A:2763:A:C8	2.50	0.46
20:A:2807:U:H3	20:A:2814:G:H1	1.63	0.46
22:C:17:THR:HG1	22:C:204:ASN:H	1.63	0.46
32:P:16:ARG:O	32:P:20:ASN:ND2	2.48	0.46
4:e:82:PRO:HD2	4:e:147:LEU:HD21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:23:PRO:HA	8:i:61:TYR:CG	2.50	0.46
12:m:22:ILE:HD11	12:m:25:ILE:HB	1.98	0.46
18:s:36:ARG:HH21	18:s:53:ASP:HA	1.81	0.46
20:A:998:U:H5'	30:N:16:LYS:HD3	1.98	0.46
20:A:1119:C:H2'	20:A:1120:A:C4	2.51	0.46
20:A:1452:G:H22	20:A:1456:G:H22	1.63	0.46
20:A:2682:G:O2'	26:G:111:HIS:NE2	2.36	0.46
22:C:67:PHE:HB3	22:C:152:GLY:H	1.79	0.46
1:a:1515:A:H2'	1:a:1516:A:H8	1.79	0.46
5:f:29:PHE:HA	5:f:32:ILE:HG12	1.98	0.46
20:A:892:U:O2'	43:O:42:ALA:O	2.31	0.46
20:A:2204:A:H2'	20:A:2205:A:H8	1.79	0.46
38:V:72:ASP:O	38:V:74:SER:N	2.48	0.46
39:W:18:ARG:NH1	39:W:18:ARG:CD	2.78	0.46
42:Z:14:MET:HG3	42:Z:57:LEU:HD21	1.96	0.46
47:4:8:ASN:HD22	47:4:11:LYS:HD2	1.80	0.46
20:A:1753:G:H2'	20:A:1754:A:C8	2.51	0.46
20:A:2147:G:H21	20:A:2172:A:H8	1.63	0.46
20:A:2276:U:OP1	20:A:2401:U:O2'	2.31	0.46
23:D:111:THR:OG1	23:D:201:THR:OG1	2.26	0.46
41:Y:3:LYS:HG3	41:Y:4:VAL:HG22	1.98	0.46
46:3:31:GLU:HB3	46:3:44:LEU:HD21	1.97	0.46
9:j:42:LEU:HB2	9:j:71:LYS:HB2	1.97	0.46
25:F:49:ASN:O	25:F:150:ARG:NH2	2.41	0.46
28:L:63:VAL:HG11	28:L:102:VAL:HG22	1.98	0.46
30:N:17:MET:HE2	30:N:72:LYS:HZ3	1.79	0.46
30:N:53:ALA:HB1	30:N:120:LEU:HB3	1.96	0.46
1:a:1008:U:N3	1:a:1060:A:N6	2.64	0.46
1:a:1090:G:O2'	1:a:1117:A:N1	2.41	0.46
20:A:199:A:H61	20:A:871:G:N2	2.14	0.46
20:A:325:U:O4	20:A:389:G:O6	2.34	0.46
20:A:1347:U:O2	37:U:59:ARG:NH1	2.49	0.46
1:a:419:G:O5'	3:d:116:ASN:ND2	2.48	0.46
1:a:1073:G:H5'	2:c:154:GLY:HA2	1.97	0.46
1:a:1144:C:H1'	1:a:1162:C:H42	1.81	0.46
15:p:18:TYR:O	15:p:39:THR:OG1	2.25	0.46
20:A:155:U:O2'	20:A:156:U:O4'	2.33	0.46
20:A:584:U:OP1	20:A:1256:G:O2'	2.33	0.46
37:U:24:LYS:HG2	37:U:81:THR:HG22	1.97	0.46
1:a:689:G:H2'	1:a:690:A:C8	2.51	0.46
1:a:1321:A:H62	1:a:1346:G:N2	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:623:A:H62	20:A:1288:A:H2	1.64	0.46
20:A:1453:U:N3	20:A:1629:A:O3'	2.48	0.46
41:Y:21:ALA:O	41:Y:23:ASN:N	2.49	0.46
1:a:37:C:H2'	1:a:38:G:H8	1.80	0.45
1:a:968:U:H2'	1:a:969:G:H8	1.81	0.45
1:a:1465:U:O4	1:a:1470:G:N2	2.49	0.45
7:h:54:ASP:OD1	7:h:54:ASP:N	2.46	0.45
10:k:20:VAL:HG22	10:k:83:ASP:HB2	1.97	0.45
18:s:42:PRO:HG3	18:s:67:VAL:HG23	1.97	0.45
20:A:2202:U:H2'	20:A:2203:G:C8	2.49	0.45
22:C:260:ARG:HH22	22:C:270:ILE:HD13	1.80	0.45
1:a:797:A:OP1	1:a:1537:G:N2	2.50	0.45
9:j:52:ILE:HG12	13:n:41:ARG:HD3	1.98	0.45
20:A:234:C:O2'	20:A:235:G:O4'	2.35	0.45
20:A:246:U:H5''	48:5:65:MET:HG3	1.99	0.45
20:A:415:C:H2'	20:A:416:G:H8	1.81	0.45
20:A:883:A:H2'	20:A:884:A:C8	2.51	0.45
20:A:1465:A:H2'	20:A:1466:G:H8	1.81	0.45
23:D:19:SER:O	33:Q:80:ARG:NH2	2.49	0.45
49:6:11:CYS:SG	49:6:33:HIS:NE2	2.90	0.45
1:a:327:C:H2'	1:a:328:A:C8	2.51	0.45
1:a:1320:G:N1	1:a:1346:G:O2'	2.50	0.45
8:i:57:THR:HA	8:i:58:LYS:HA	1.73	0.45
20:A:1796:C:H1'	20:A:2623:U:H5'	1.98	0.45
20:A:626:U:H2'	20:A:627:A:C8	2.50	0.45
20:A:2407:U:OP2	48:5:30:SER:OG	2.32	0.45
24:E:10:ASP:OD1	24:E:10:ASP:N	2.49	0.45
1:a:941:G:O2'	1:a:943:G:OP1	2.29	0.45
1:a:1004:G:N2	1:a:1032:A:N3	2.59	0.45
20:A:1307:C:H5''	20:A:1308:G:H5'	1.99	0.45
20:A:1314:C:H2'	20:A:1315:A:H8	1.81	0.45
20:A:1498:G:H2'	20:A:1499:G:C8	2.52	0.45
20:A:2336:A:N6	20:A:2347:A:N7	2.65	0.45
33:Q:29:HIS:HD2	33:Q:83:GLN:HB2	1.81	0.45
12:m:81:MET:HA	12:m:88:GLY:HA3	1.98	0.45
20:A:163:A:N6	20:A:169:A:N7	2.65	0.45
24:E:136:THR:HG22	24:E:166:SER:HA	1.99	0.45
35:S:3:ALA:HB3	35:S:14:VAL:HB	1.98	0.45
1:a:472:G:O6	1:a:473:A:N6	2.50	0.45
1:a:678:A:H61	1:a:757:G:H1	1.64	0.45
19:t:66:ILE:HG21	19:t:70:LYS:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1391:G:OP2	22:C:38:LYS:NZ	2.36	0.45
20:A:1434:C:O3'	37:U:24:LYS:NZ	2.49	0.45
20:A:1576:A:N6	20:A:1579:U:O4	2.49	0.45
1:a:422:A:OP1	3:d:109:ARG:NH2	2.49	0.45
1:a:704:C:HO2'	1:a:720:U:HO2'	1.61	0.45
1:a:1541:G:H2'	1:a:1542:G:H8	1.81	0.45
10:k:101:GLN:HE21	10:k:107:VAL:HB	1.81	0.45
11:l:120:VAL:O	11:l:132:THR:OG1	2.34	0.45
20:A:172:U:H2'	20:A:173:G:C8	2.52	0.45
20:A:221:G:H22	20:A:238:U:H4'	1.82	0.45
20:A:302:A:H2'	20:A:303:G:C8	2.51	0.45
20:A:1689:A:H2	20:A:1690:G:H4'	1.81	0.45
20:A:2872:U:H2'	20:A:2873:A:H8	1.81	0.45
1:a:980:A:N7	1:a:981:A:N6	2.64	0.45
1:a:1184:A:H2'	1:a:1185:A:C8	2.51	0.45
12:m:5:ALA:HB1	12:m:60:ILE:HD12	1.99	0.45
20:A:632:U:H2'	20:A:633:G:C8	2.50	0.45
20:A:1611:C:O2'	20:A:1613:A:N7	2.47	0.45
25:F:3:ARG:HH21	44:1:23:PHE:HB2	1.81	0.45
1:a:943:G:N1	1:a:1406:U:O4	2.50	0.45
1:a:1031:G:H2'	1:a:1032:A:H8	1.82	0.45
3:d:107:THR:HG23	3:d:110:GLN:H	1.81	0.45
20:A:1101:U:N3	20:A:1110:A:OP2	2.50	0.45
20:A:2341:A:H2'	20:A:2342:A:C8	2.52	0.45
21:B:1:U:H2'	21:B:2:G:C8	2.52	0.45
1:a:1374:C:O2'	1:a:1377:C:N4	2.48	0.44
3:d:140:ILE:HG22	3:d:175:GLY:H	1.82	0.44
3:d:167:SER:OG	3:d:176:SER:OG	2.35	0.44
19:t:74:ASP:HA	19:t:77:ARG:HG2	1.99	0.44
20:A:213:U:H2'	20:A:214:G:H8	1.83	0.44
20:A:280:C:H2'	20:A:281:A:C8	2.52	0.44
1:a:277:A:H4'	19:t:67:HIS:HE1	1.82	0.44
1:a:810:C:O2'	10:k:128:ARG:O	2.29	0.44
19:t:49:LEU:H	19:t:49:LEU:HG	1.59	0.44
21:B:7:G:OP2	32:P:19:ARG:NH1	2.51	0.44
29:M:101:ILE:HG22	29:M:102:VAL:HG23	1.99	0.44
44:1:34:THR:HG23	44:1:44:PRO:HG3	1.99	0.44
1:a:67:U:H2'	1:a:68:U:H6	1.81	0.44
20:A:1643:C:OP1	37:U:76:ARG:NH2	2.50	0.44
23:D:69:VAL:HG21	23:D:76:PRO:HA	1.98	0.44
35:S:42:GLY:HA2	35:S:46:THR:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:231:U:H2'	1:a:232:G:H8	1.82	0.44
1:a:272:G:H2'	1:a:273:A:C8	2.52	0.44
1:a:970:G:H21	1:a:1242:A:H62	1.65	0.44
1:a:989:G:O3'	13:n:41:ARG:NH1	2.46	0.44
6:g:111:ARG:NH2	6:g:126:ASP:OD2	2.35	0.44
20:A:2745:G:N1	20:A:2746:G:O6	2.51	0.44
1:a:954:A:N3	1:a:1391:U:O2'	2.43	0.44
6:g:146:ASP:HA	6:g:149:ARG:HB2	1.99	0.44
20:A:872:G:H2'	20:A:873:C:C6	2.53	0.44
20:A:1453:U:O4	20:A:1457:A:N6	2.51	0.44
22:C:78:VAL:HG22	22:C:94:VAL:HG22	1.99	0.44
1:a:416:C:H2'	1:a:417:G:H8	1.83	0.44
1:a:674:C:OP2	14:o:8:LYS:NZ	2.50	0.44
1:a:1414:C:H5''	1:a:1518:A:H62	1.81	0.44
2:c:33:HIS:CE1	13:n:25:GLU:HB2	2.52	0.44
20:A:76:G:H22	20:A:111:A:H2	1.65	0.44
20:A:728:U:H2'	20:A:729:A:H8	1.82	0.44
20:A:1010:U:H2'	20:A:1011:C:H6	1.83	0.44
20:A:1388:U:H1'	20:A:1616:A:H2	1.81	0.44
20:A:1512:A:H2'	20:A:1513:A:H8	1.82	0.44
20:A:2436:C:H41	48:5:31:HIS:CE1	2.35	0.44
21:B:4:G:H2'	21:B:5:G:H8	1.82	0.44
21:B:92:U:H5'	39:W:17:LEU:HD23	2.00	0.44
27:K:69:LYS:HD2	27:K:73:LYS:HD2	2.00	0.44
28:L:88:ARG:HE	28:L:94:ARG:HG2	1.82	0.44
31:O:110:THR:OG1	31:O:111:GLU:N	2.51	0.44
33:Q:26:VAL:HG13	33:Q:84:ILE:HG23	1.99	0.44
33:Q:94:ARG:HA	33:Q:94:ARG:HD3	1.75	0.44
36:T:43:PHE:HB3	45:2:38:LYS:HE3	1.98	0.44
1:a:328:A:H2'	1:a:329:C:C6	2.53	0.44
1:a:337:C:H2'	1:a:338:U:C6	2.53	0.44
1:a:1008:U:H4'	1:a:1009:G:H5''	1.99	0.44
13:n:59:ALA:HB1	13:n:61:TRP:HZ3	1.83	0.44
20:A:25:G:H2'	20:A:26:U:C6	2.53	0.44
20:A:246:U:OP2	48:5:8:ARG:NH2	2.50	0.44
20:A:1336:U:C2	20:A:1669:G:C6	3.06	0.44
20:A:2540:G:H1	20:A:2551:U:H3	1.64	0.44
22:C:230:HIS:CD2	22:C:249:PRO:HB3	2.52	0.44
24:E:40:GLN:O	24:E:43:SER:OG	2.33	0.44
20:A:2204:A:H2'	20:A:2205:A:C8	2.53	0.44
20:A:2342:A:H2'	20:A:2343:A:H8	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:45:HIS:HB3	4:e:71:LEU:HB3	1.99	0.44
20:A:2168:G:N2	20:A:2169:A:N7	2.66	0.44
32:P:15:HIS:CE1	32:P:96:GLY:HA2	2.53	0.44
1:a:209:A:H2'	1:a:210:A:C8	2.53	0.43
1:a:983:C:OP2	1:a:984:A:O2'	2.29	0.43
20:A:2242:G:H22	41:Y:34:GLN:HE22	1.66	0.43
20:A:2540:G:O2'	49:6:1:MET:N	2.47	0.43
23:D:117:LYS:HB2	23:D:164:MET:HB2	1.98	0.43
28:L:22:ILE:HG22	28:L:23:LYS:HG3	1.98	0.43
30:N:138:GLY:HA2	39:W:57:ALA:HB1	1.98	0.43
6:g:30:VAL:HG22	6:g:105:VAL:HG13	1.99	0.43
11:l:26:LYS:NZ	11:l:29:ASN:OD1	2.48	0.43
11:l:38:VAL:O	11:l:40:SER:N	2.51	0.43
20:A:678:U:H2'	20:A:679:C:C6	2.53	0.43
20:A:898:A:OP1	40:X:86:LYS:NZ	2.42	0.43
20:A:940:G:H2'	20:A:941:A:C4	2.53	0.43
20:A:1345:G:OP1	47:4:9:LYS:N	2.49	0.43
20:A:1422:C:H2'	20:A:1423:A:H8	1.83	0.43
20:A:2261:A:H2'	20:A:2262:C:H6	1.82	0.43
21:B:4:G:H2'	21:B:5:G:C8	2.54	0.43
22:C:124:ILE:HG23	22:C:192:ILE:HD13	1.99	0.43
38:V:39:ASN:HD21	38:V:63:ILE:HG13	1.82	0.43
38:V:72:ASP:HA	38:V:101:LEU:HD21	2.00	0.43
1:a:253:G:H2'	1:a:254:G:C8	2.53	0.43
1:a:633:C:N4	1:a:636:A:OP2	2.52	0.43
1:a:730:A:H2'	1:a:731:A:H8	1.82	0.43
1:a:1234:U:H2'	1:a:1235:G:C8	2.53	0.43
10:k:23:ILE:HB	10:k:86:VAL:HA	2.00	0.43
20:A:223:G:H22	20:A:467:U:H2'	1.83	0.43
20:A:502:C:H2'	20:A:503:G:H8	1.82	0.43
20:A:1023:A:N6	20:A:1024:G:O6	2.51	0.43
20:A:2260:G:H2'	20:A:2261:A:H8	1.82	0.43
20:A:2644:G:H2'	20:A:2645:G:C8	2.54	0.43
23:D:178:LYS:HB2	23:D:187:LEU:HD12	2.00	0.43
28:L:22:ILE:HD12	28:L:40:VAL:HG12	1.99	0.43
42:Z:21:LEU:HD22	42:Z:46:VAL:HG13	2.00	0.43
1:a:422:A:H2'	1:a:423:G:C8	2.54	0.43
5:f:51:LEU:HD12	5:f:59:ARG:HA	2.01	0.43
8:i:6:TYR:HD2	8:i:21:LEU:HD23	1.83	0.43
20:A:699:U:H2'	20:A:700:G:C8	2.52	0.43
22:C:13:ARG:HD3	22:C:16:MET:HG3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:57:ARG:HG3	48:5:58:ILE:HG13	1.99	0.43
1:a:201:C:N4	16:q:4:GLU:OE1	2.51	0.43
1:a:599:G:H2'	1:a:600:G:H8	1.84	0.43
1:a:892:A:H1'	7:h:12:THR:HG21	2.00	0.43
17:r:25:ILE:H	17:r:25:ILE:HG13	1.54	0.43
20:A:922:G:N2	20:A:935:U:OP2	2.35	0.43
20:A:1125:A:H2'	20:A:1126:A:C8	2.53	0.43
20:A:1185:C:H2'	20:A:1186:A:H8	1.83	0.43
20:A:2314:A:H2'	20:A:2315:A:H8	1.84	0.43
21:B:27:A:H2'	21:B:28:C:H6	1.84	0.43
22:C:235:GLY:HA3	22:C:239:THR:HG21	2.00	0.43
22:C:257:TYR:HB3	22:C:259:THR:HG23	2.01	0.43
1:a:555:G:O2'	3:d:35:GLN:NE2	2.41	0.43
6:g:117:GLU:O	6:g:121:ALA:N	2.46	0.43
9:j:42:LEU:HD23	9:j:42:LEU:HA	1.88	0.43
14:o:16:ALA:HB1	14:o:21:ASP:HB2	2.00	0.43
20:A:2144:G:H4'	20:A:2172:A:C4	2.54	0.43
48:5:2:PRO:HB2	48:5:3:LYS:H	1.62	0.43
1:a:1528:U:H2'	1:a:1529:A:H8	1.84	0.43
20:A:1088:A:N7	20:A:1151:A:N6	2.67	0.43
20:A:1452:G:N2	20:A:1454:U:O2	2.52	0.43
20:A:2042:U:H2'	20:A:2043:G:C8	2.53	0.43
20:A:2085:A:H2'	20:A:2086:G:C8	2.53	0.43
29:M:123:VAL:HB	29:M:143:ILE:HG22	2.01	0.43
1:a:182:C:H2'	1:a:183:G:C8	2.53	0.43
1:a:227:C:H3'	1:a:228:G:C8	2.53	0.43
1:a:722:U:H2'	1:a:723:A:C8	2.53	0.43
1:a:1096:A:H5'	4:e:21:VAL:HG11	2.01	0.43
6:g:87:VAL:HG23	6:g:152:ALA:HB1	2.00	0.43
20:A:1835:A:H2'	20:A:1836:G:C8	2.52	0.43
20:A:2856:A:H62	20:A:2882:G:H21	1.67	0.43
21:B:27:A:H2'	21:B:28:C:C6	2.53	0.43
22:C:180:GLU:OE2	22:C:274:ARG:N	2.52	0.43
23:D:120:GLN:H	23:D:125:ARG:NH2	2.12	0.43
1:a:43:G:O2'	1:a:380:U:O2	2.32	0.43
11:l:67:ARG:HG3	11:l:77:THR:HG22	2.00	0.43
20:A:213:U:H2'	20:A:214:G:C8	2.54	0.43
20:A:702:A:H2'	20:A:703:G:H8	1.84	0.43
20:A:739:A:H62	20:A:773:G:H21	1.67	0.43
20:A:771:C:H2'	20:A:772:C:H6	1.84	0.43
20:A:1441:C:H2'	20:A:1442:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:2236:G:OP1	22:C:170:LYS:NZ	2.51	0.43
20:A:2697:C:O2	28:L:70:ARG:NH2	2.52	0.43
22:C:8:PRO:HB3	22:C:14:ARG:HD3	2.01	0.43
30:N:1:MET:SD	30:N:45:ARG:NH2	2.91	0.43
34:R:31:LEU:O	34:R:35:ALA:N	2.51	0.43
1:a:1386:G:H5''	8:i:70:GLY:HA2	1.99	0.43
19:t:74:ASP:O	19:t:78:LEU:HB2	2.19	0.43
20:A:1035:C:O2'	27:K:2:ARG:NH1	2.51	0.43
20:A:1130:U:N3	20:A:1142:C:O5'	2.47	0.43
20:A:2300:A:H2'	46:3:26:ASN:HD21	1.84	0.43
23:D:89:GLY:O	23:D:91:TYR:N	2.52	0.43
35:S:67:LYS:HA	35:S:91:PRO:HA	2.01	0.43
40:X:37:GLY:HA2	40:X:75:VAL:HG13	2.00	0.43
1:a:1039:U:O2'	1:a:1040:U:O2	2.30	0.42
1:a:1370:G:H2'	1:a:1371:G:C8	2.54	0.42
20:A:792:A:OP2	47:4:3:ARG:NH2	2.51	0.42
20:A:952:A:N7	30:N:11:ARG:NH1	2.67	0.42
20:A:2006:G:H5'	20:A:2008:C:H41	1.84	0.42
40:X:40:VAL:HG21	40:X:76:VAL:HG23	2.00	0.42
1:a:689:G:H21	10:k:118:HIS:HD2	1.67	0.42
1:a:728:G:H2'	1:a:729:G:C8	2.54	0.42
1:a:796:A:H62	1:a:816:U:H3	1.63	0.42
1:a:958:G:O6	1:a:1356:U:O4	2.36	0.42
1:a:1452:C:H2'	1:a:1453:G:H8	1.84	0.42
6:g:68:ASN:ND2	6:g:130:ASN:OD1	2.51	0.42
7:h:79:ARG:NH2	7:h:81:SER:O	2.45	0.42
11:l:97:GLY:HA2	11:l:108:TYR:HD1	1.85	0.42
18:s:16:MET:HA	18:s:19:VAL:HG12	2.01	0.42
20:A:1112:C:H3'	20:A:1136:A:H4'	2.02	0.42
20:A:2154:G:N2	20:A:2165:U:O2	2.48	0.42
20:A:2211:U:H3	20:A:2239:A:H62	1.66	0.42
20:A:2522:G:O2'	20:A:2568:U:O2'	2.33	0.42
30:N:57:TYR:HD1	30:N:57:TYR:HA	1.72	0.42
1:a:1008:U:H3	1:a:1060:A:N6	2.17	0.42
5:f:10:MET:HE1	17:r:28:LYS:HD3	2.01	0.42
5:f:14:ARG:HB2	5:f:17:ILE:HG23	2.01	0.42
8:i:119:LYS:HE3	8:i:125:SER:HA	2.01	0.42
18:s:66:MET:HG3	18:s:69:HIS:CE1	2.54	0.42
20:A:481:U:H2'	20:A:482:G:C8	2.54	0.42
20:A:663:C:H2'	20:A:664:G:C8	2.54	0.42
20:A:1753:G:H2'	20:A:1754:A:H8	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1793:U:O2	20:A:1797:A:N7	2.51	0.42
20:A:1822:U:O2'	20:A:1823:A:O4'	2.37	0.42
24:E:34:TYR:HB2	29:M:1:MET:HE1	2.02	0.42
26:G:25:THR:HG22	26:G:34:THR:HG22	2.01	0.42
39:W:63:MET:HB2	39:W:70:ILE:HB	2.02	0.42
1:a:616:G:H2'	1:a:617:A:C8	2.53	0.42
1:a:1399:C:H2'	1:a:1400:G:C8	2.55	0.42
6:g:93:PRO:HA	6:g:96:ARG:HB3	2.01	0.42
20:A:478:U:H2'	20:A:479:A:H8	1.84	0.42
20:A:682:A:N1	20:A:2383:A:O2'	2.44	0.42
20:A:697:U:H2'	20:A:698:A:C8	2.54	0.42
20:A:1007:U:H2'	20:A:1008:A:H8	1.84	0.42
21:B:1:U:H2'	21:B:2:G:H8	1.83	0.42
1:a:546:U:H4'	1:a:547:A:H3'	2.02	0.42
1:a:1074:G:O6	1:a:1214:U:O4	2.36	0.42
4:e:45:HIS:ND1	4:e:72:VAL:O	2.35	0.42
11:l:20:ASP:OD1	11:l:20:ASP:N	2.52	0.42
15:p:55:LEU:O	15:p:59:TRP:CB	2.67	0.42
16:q:65:MET:HB2	16:q:79:LEU:HD11	2.00	0.42
20:A:1314:C:H2'	20:A:1315:A:C8	2.55	0.42
20:A:2116:U:H2'	20:A:2117:A:C8	2.54	0.42
20:A:2287:A:H2'	20:A:2288:A:C8	2.54	0.42
20:A:2528:U:H2'	20:A:2529:C:C6	2.55	0.42
22:C:69:ARG:HD2	22:C:129:ALA:HB2	2.01	0.42
23:D:119:PHE:HD1	23:D:119:PHE:HA	1.73	0.42
31:O:22:THR:HG21	31:O:67:ARG:H	1.83	0.42
1:a:130:U:H2'	1:a:131:G:H8	1.83	0.42
1:a:854:G:H2'	1:a:855:G:H8	1.84	0.42
1:a:958:G:H2'	1:a:959:U:H6	1.85	0.42
1:a:964:C:OP1	12:m:108:THR:OG1	2.35	0.42
1:a:1378:A:O2'	1:a:1380:G:N7	2.42	0.42
4:e:52:LYS:O	4:e:62:LYS:NZ	2.35	0.42
20:A:1752:U:H2'	20:A:1753:G:H8	1.84	0.42
22:C:141:ILE:HG23	22:C:190:ALA:HB1	2.02	0.42
28:L:22:ILE:HD11	28:L:42:THR:HG23	2.01	0.42
37:U:57:ASN:ND2	37:U:76:ARG:HH21	2.15	0.42
39:W:72:THR:HG22	39:W:93:SER:HB3	2.00	0.42
1:a:1033:U:O4	1:a:1034:A:N6	2.52	0.42
1:a:1285:G:H2'	1:a:1286:G:C8	2.55	0.42
20:A:160:U:H2'	20:A:161:G:O4'	2.20	0.42
20:A:199:A:N6	20:A:871:G:H21	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:887:G:O2'	20:A:888:A:O4'	2.36	0.42
20:A:1050:A:N3	20:A:1193:C:H1'	2.35	0.42
20:A:2050:C:H2'	20:A:2051:A:H8	1.85	0.42
22:C:147:LYS:CA	22:C:148:PRO:CD	2.97	0.42
24:E:66:ARG:HH22	24:E:69:GLY:HA3	1.84	0.42
1:a:419:G:N2	1:a:513:A:N3	2.66	0.42
1:a:1430:G:H2'	1:a:1431:A:C8	2.54	0.42
1:a:1504:G:H2'	1:a:1505:G:C8	2.55	0.42
6:g:111:ARG:HG2	6:g:113:GLU:HG3	2.01	0.42
10:k:84:VAL:HG21	10:k:107:VAL:HG13	2.02	0.42
17:r:54:LYS:HB3	17:r:57:ARG:HH21	1.84	0.42
20:A:369:A:O2'	20:A:371:C:OP2	2.25	0.42
20:A:873:C:H2'	20:A:874:U:C6	2.55	0.42
20:A:2330:U:H2'	20:A:2331:C:H6	1.84	0.42
21:B:36:C:H4'	32:P:101:HIS:CE1	2.54	0.42
21:B:37:A:H2'	21:B:38:U:C6	2.55	0.42
26:G:7:LYS:O	26:G:69:ARG:NH1	2.48	0.42
27:K:5:TYR:H	34:R:64:ARG:HH12	1.67	0.42
1:a:33:C:H5''	11:l:133:LYS:HG2	2.01	0.42
1:a:163:U:H2'	1:a:164:G:H8	1.84	0.42
1:a:980:A:H4'	9:j:57:LYS:HD2	2.01	0.42
6:g:2:PRO:HB2	6:g:3:ARG:H	1.68	0.42
6:g:16:PRO:HG3	8:i:46:GLU:HB2	2.01	0.42
20:A:785:G:H21	20:A:790:A:N6	2.16	0.42
20:A:793:G:N2	20:A:794:U:O2	2.53	0.42
20:A:1498:G:H2'	20:A:1499:G:H8	1.84	0.42
25:F:35:VAL:HB	25:F:155:VAL:HB	2.01	0.42
31:O:24:LEU:HG	31:O:30:ILE:HD12	2.02	0.42
37:U:27:PHE:O	37:U:78:ALA:N	2.52	0.42
46:3:11:SER:OG	46:3:39:GLU:OE2	2.33	0.42
6:g:14:PRO:HA	6:g:21:LYS:HA	2.01	0.42
6:g:36:ARG:HH12	8:i:44:LEU:HD11	1.84	0.42
6:g:42:ILE:HA	6:g:45:ASN:HD22	1.84	0.42
9:j:11:LYS:HE2	9:j:71:LYS:HD3	2.02	0.42
20:A:1377:U:OP2	20:A:1430:U:O2'	2.35	0.42
20:A:2314:A:H2'	20:A:2315:A:C8	2.55	0.42
20:A:2671:A:H62	20:A:2678:G:H21	1.66	0.42
29:M:94:VAL:O	29:M:96:LEU:N	2.53	0.42
49:6:30:ASN:HB3	49:6:32:LYS:H	1.85	0.42
1:a:536:G:OP2	11:l:64:LYS:NZ	2.51	0.41
1:a:551:C:H2'	1:a:552:G:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1450:G:H2'	1:a:1451:U:C6	2.55	0.41
2:c:75:VAL:HG13	2:c:102:ILE:HD13	2.01	0.41
4:e:32:ARG:HH21	4:e:52:LYS:HD2	1.85	0.41
18:s:40:ILE:HG23	18:s:44:PHE:HD2	1.85	0.41
20:A:65:A:H2'	20:A:66:A:C8	2.54	0.41
20:A:2260:G:H2'	20:A:2261:A:C8	2.54	0.41
28:L:88:ARG:HH21	28:L:94:ARG:HA	1.85	0.41
29:M:20:GLY:HA2	29:M:28:GLY:HA2	2.02	0.41
1:a:151:G:N2	1:a:184:C:N3	2.67	0.41
1:a:599:G:H2'	1:a:600:G:C8	2.55	0.41
1:a:1049:G:H2'	1:a:1050:G:C8	2.55	0.41
1:a:1165:U:O4	1:a:1166:A:N6	2.53	0.41
8:i:114:LYS:HA	8:i:121:ALA:HA	2.01	0.41
15:p:38:GLY:HA3	15:p:51:LEU:HD23	2.03	0.41
20:A:655:G:O2'	24:E:106:ARG:NH2	2.47	0.41
20:A:893:G:H2'	20:A:894:A:H8	1.85	0.41
20:A:1346:G:N2	20:A:1349:U:O4	2.54	0.41
20:A:1502:G:N2	20:A:1504:G:N7	2.68	0.41
20:A:2236:G:H2'	20:A:2237:A:C8	2.56	0.41
20:A:2431:C:H2'	20:A:2432:A:C8	2.55	0.41
20:A:2501:G:H2'	20:A:2502:A:C8	2.55	0.41
22:C:183:MET:HB2	22:C:269:LEU:HB3	2.02	0.41
1:a:681:G:H5'	1:a:741:C:H1'	2.02	0.41
1:a:730:A:H2'	1:a:731:A:C8	2.55	0.41
1:a:1528:U:H2'	1:a:1529:A:C8	2.55	0.41
2:c:150:THR:HB	2:c:166:GLY:HA3	2.03	0.41
3:d:94:ARG:HG2	3:d:96:ASP:H	1.85	0.41
5:f:83:LEU:HD23	5:f:86:ILE:HD11	2.02	0.41
7:h:41:LYS:HA	7:h:46:ILE:HB	2.02	0.41
12:m:19:LEU:HD21	12:m:60:ILE:HG12	2.03	0.41
20:A:65:A:C8	37:U:65:MET:HG3	2.55	0.41
20:A:173:G:H2'	20:A:174:A:C8	2.55	0.41
20:A:454:C:H2'	20:A:455:A:H8	1.86	0.41
20:A:905:G:H5''	20:A:906:C:N3	2.35	0.41
20:A:1550:U:H4'	20:A:1552:A:C4	2.56	0.41
20:A:2148:A:H1'	20:A:2172:A:H1'	2.03	0.41
20:A:2536:U:C6	20:A:2536:U:O4'	2.72	0.41
25:F:106:VAL:HG11	25:F:139:PRO:HD3	2.01	0.41
34:R:98:LEU:HD23	34:R:98:LEU:HA	1.92	0.41
45:2:30:CYS:HB2	45:2:34:GLY:H	1.84	0.41
1:a:944:G:H2'	1:a:945:G:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:995:C:O2	13:n:19:GLN:NE2	2.32	0.41
1:a:1237:G:OP2	1:a:1337:C:N4	2.52	0.41
1:a:1430:G:N2	1:a:1501:U:O2	2.51	0.41
3:d:60:MET:O	3:d:108:ARG:NH1	2.54	0.41
6:g:46:SER:HB2	6:g:121:ALA:HA	2.03	0.41
20:A:21:C:H2'	20:A:22:A:H8	1.85	0.41
20:A:904:A:N6	20:A:905:G:N3	2.68	0.41
20:A:2238:G:OP1	22:C:268:LYS:NZ	2.46	0.41
21:B:74:G:H1'	39:W:30:ILE:HD11	2.01	0.41
22:C:110:LEU:HD23	22:C:110:LEU:HA	1.86	0.41
22:C:142:HIS:HE2	22:C:161:SER:HA	1.85	0.41
1:a:153:G:H2'	1:a:154:G:C8	2.56	0.41
1:a:1313:C:N4	6:g:114:HIS:O	2.53	0.41
1:a:1493:U:H2'	1:a:1494:A:C8	2.55	0.41
2:c:160:ASP:HB3	2:c:161:ILE:H	1.69	0.41
4:e:57:PRO:HA	4:e:60:ILE:HG12	2.02	0.41
20:A:783:A:H2'	20:A:784:C:H6	1.85	0.41
20:A:2763:A:H1'	26:G:63:THR:HG22	2.03	0.41
25:F:38:MET:HE1	25:F:151:GLY:H	1.86	0.41
25:F:56:GLU:OE1	25:F:135:GLN:NE2	2.43	0.41
29:M:33:ARG:NH1	29:M:41:ARG:O	2.53	0.41
44:1:11:PRO:O	44:1:42:THR:OG1	2.38	0.41
1:a:422:A:H2'	1:a:423:G:H8	1.85	0.41
1:a:704:C:O2'	1:a:720:U:O2'	2.32	0.41
1:a:1242:A:OP1	18:s:80:TYR:OH	2.38	0.41
1:a:1367:C:H2'	1:a:1368:G:H8	1.86	0.41
12:m:2:ALA:HA	12:m:3:ARG:HA	1.79	0.41
20:A:648:U:H2'	20:A:649:C:C6	2.56	0.41
20:A:1502:G:C5	20:A:1504:G:H5'	2.56	0.41
27:K:86:LYS:HB3	27:K:88:VAL:HG23	2.02	0.41
30:N:44:ASN:HD21	30:N:93:TRP:HB2	1.86	0.41
37:U:11:VAL:O	37:U:26:THR:OG1	2.39	0.41
1:a:67:U:H2'	1:a:68:U:C6	2.55	0.41
1:a:904:G:H3'	1:a:905:A:H8	1.86	0.41
20:A:192:G:O6	20:A:208:G:O2'	2.39	0.41
20:A:701:U:H2'	20:A:702:A:C8	2.56	0.41
29:M:73:ASP:OD1	29:M:73:ASP:N	2.52	0.41
32:P:68:LYS:O	32:P:71:THR:OG1	2.33	0.41
1:a:188:A:N1	1:a:214:U:N3	2.69	0.41
1:a:462:G:H21	1:a:502:A:H62	1.69	0.41
12:m:86:TYR:OH	12:m:90:ARG:NH2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:39:THR:HG1	15:p:40:TYR:H	1.68	0.41
20:A:539:G:N2	20:A:541:A:H3'	2.36	0.41
20:A:2043:G:N1	20:A:2047:A:OP2	2.43	0.41
20:A:2340:U:H3	20:A:2403:G:H1	1.68	0.41
20:A:2453:A:H4'	20:A:2454:C:H3'	2.03	0.41
26:G:105:LEU:HB2	26:G:113:VAL:HB	2.03	0.41
39:W:6:GLU:OE1	39:W:44:GLU:N	2.53	0.41
1:a:53:U:H2'	1:a:54:G:H8	1.86	0.41
1:a:860:C:N3	17:r:21:HIS:NE2	2.66	0.41
8:i:8:GLY:HA2	8:i:85:ARG:HD2	2.03	0.41
8:i:48:ILE:HG23	8:i:79:ILE:HG21	2.02	0.41
9:j:47:SER:HB2	9:j:67:MET:HB2	2.03	0.41
11:l:102:ASP:OD1	11:l:103:LEU:N	2.52	0.41
20:A:402:A:H2'	20:A:403:G:H8	1.84	0.41
20:A:454:C:H2'	20:A:455:A:C8	2.56	0.41
20:A:669:G:H1	29:M:71:ARG:HH12	1.68	0.41
20:A:1001:G:O6	20:A:2469:G:O2'	2.39	0.41
20:A:1208:C:H2'	20:A:1209:A:H8	1.86	0.41
20:A:1322:A:O2'	20:A:1324:U:OP2	2.37	0.41
20:A:1724:G:O2'	20:A:1776:A:O2'	2.27	0.41
20:A:2154:G:N1	20:A:2165:U:N3	2.49	0.41
20:A:2611:G:H2'	20:A:2612:A:C8	2.56	0.41
20:A:2870:G:H2'	20:A:2871:A:C8	2.55	0.41
22:C:132:LEU:HD12	22:C:188:CYS:HB2	2.03	0.41
24:E:6:LEU:HB2	24:E:14:ASN:HB2	2.02	0.41
24:E:75:GLN:HE22	24:E:82:GLN:HE21	1.69	0.41
26:G:84:GLN:HE21	26:G:134:LYS:HE2	1.84	0.41
33:Q:29:HIS:CD2	33:Q:83:GLN:HB2	2.56	0.41
37:U:10:PRO:HD3	42:Z:30:PHE:CD1	2.56	0.41
1:a:100:A:H2'	1:a:101:A:H8	1.86	0.41
1:a:1044:C:H2'	1:a:1045:U:O4'	2.22	0.41
1:a:1284:A:H1'	1:a:1327:G:H21	1.86	0.41
1:a:1354:A:H8	1:a:1355:A:C8	2.39	0.41
1:a:1363:U:H2'	1:a:1364:A:C8	2.51	0.41
1:a:1427:C:H2'	1:a:1428:A:C8	2.56	0.41
3:d:13:ARG:HB3	3:d:33:PRO:HG3	2.02	0.41
7:h:19:MET:HA	7:h:72:ARG:HH11	1.86	0.41
20:A:1613:A:H5''	22:C:85:PRO:HB3	2.03	0.41
20:A:2799:U:O2'	23:D:37:GLN:NE2	2.54	0.41
28:L:39:ILE:HD13	28:L:39:ILE:HG21	1.91	0.41
1:a:105:G:H2'	1:a:106:A:C8	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:458:U:H2'	1:a:459:A:C8	2.57	0.40
1:a:1366:U:O2	1:a:1386:G:N2	2.37	0.40
3:d:112:ARG:HA	3:d:115:VAL:HG12	2.03	0.40
7:h:108:THR:OG1	7:h:111:GLY:O	2.34	0.40
17:r:20:ASN:OD1	17:r:20:ASN:N	2.53	0.40
20:A:6:A:H2'	20:A:7:A:C8	2.56	0.40
20:A:2108:A:H2'	20:A:2109:G:C8	2.55	0.40
20:A:2514:U:O2	20:A:2518:U:N3	2.54	0.40
22:C:24:ILE:HG23	22:C:82:GLU:HA	2.03	0.40
28:L:118:ALA:HA	28:L:119:PRO:HD3	1.94	0.40
1:a:529:C:H2'	1:a:530:G:H8	1.86	0.40
1:a:569:U:H2'	1:a:570:C:C6	2.57	0.40
1:a:1055:A:H2'	1:a:1056:A:C4	2.56	0.40
1:a:1080:G:O2'	1:a:1205:G:N2	2.54	0.40
1:a:1293:A:H4'	1:a:1294:A:C4	2.56	0.40
9:j:12:ALA:HB2	9:j:96:VAL:HG23	2.03	0.40
20:A:441:A:H2'	20:A:442:A:C8	2.56	0.40
20:A:679:C:H2'	20:A:680:U:C6	2.56	0.40
20:A:938:C:H3'	20:A:939:C:H4'	2.04	0.40
20:A:1009:G:H2'	20:A:1010:U:C6	2.57	0.40
20:A:1131:G:H1	20:A:1138:A:H5'	1.87	0.40
20:A:1145:U:H3'	20:A:1146:A:H4'	2.02	0.40
20:A:1406:C:H2'	20:A:1407:G:C8	2.56	0.40
22:C:142:HIS:CD2	22:C:194:SER:HA	2.56	0.40
1:a:578:A:H3'	11:l:12:ARG:HH21	1.84	0.40
1:a:1175:G:N7	1:a:1197:G:C2	2.89	0.40
1:a:1299:C:OP2	1:a:1300:U:O2'	2.38	0.40
6:g:153:HIS:HB3	10:k:98:ARG:HH12	1.87	0.40
20:A:1843:A:H3'	20:A:1844:C:H6	1.86	0.40
20:A:1937:U:H2'	20:A:1938:C:C6	2.56	0.40
26:G:54:ARG:NH1	26:G:64:ILE:HB	2.36	0.40
35:S:5:ILE:HD11	35:S:58:VAL:HG21	2.03	0.40
1:a:25:G:H2'	1:a:26:A:H8	1.87	0.40
1:a:529:C:H2'	1:a:530:G:C8	2.57	0.40
1:a:729:G:H2'	1:a:730:A:H8	1.87	0.40
1:a:962:A:H2'	1:a:963:G:C8	2.56	0.40
1:a:1199:G:H2'	1:a:1200:G:H8	1.85	0.40
2:c:62:ARG:HB3	2:c:99:HIS:HD2	1.86	0.40
20:A:173:G:H2'	20:A:174:A:H8	1.87	0.40
20:A:1826:A:H2'	20:A:1827:U:C6	2.57	0.40
20:A:2575:A:N3	28:L:23:LYS:HD2	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:2634:C:H1'	23:D:160:LEU:HB2	2.03	0.40
29:M:72:LYS:HE3	29:M:72:LYS:HB3	1.94	0.40
30:N:23:GLY:HA2	39:W:81:THR:HG23	2.04	0.40
42:Z:39:ASN:HB3	42:Z:42:ARG:HG3	2.04	0.40
49:6:30:ASN:HB2	49:6:33:HIS:CD2	2.57	0.40
1:a:702:A:N7	1:a:716:U:N3	2.69	0.40
1:a:751:U:H2'	1:a:752:C:C6	2.57	0.40
1:a:1390:A:HO2'	6:g:102:ARG:HH22	1.68	0.40
1:a:1392:A:C5	6:g:7:VAL:HG11	2.56	0.40
20:A:252:C:OP2	20:A:2408:C:O2'	2.32	0.40
20:A:1292:U:N3	24:E:71:GLY:O	2.54	0.40
20:A:1465:A:H2'	20:A:1466:G:C8	2.57	0.40
20:A:2328:A:H2'	20:A:2329:U:C6	2.57	0.40
20:A:2702:G:N1	20:A:2734:U:OP2	2.41	0.40
21:B:83:G:N1	21:B:84:G:C6	2.90	0.40
22:C:195:VAL:HG12	22:C:196:GLY:H	1.87	0.40
22:C:209:GLY:O	22:C:213:TRP:N	2.54	0.40
30:N:5:LYS:HD3	30:N:69:PHE:HD1	1.86	0.40
36:T:44:THR:HG23	45:2:24:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	c	202/204 (99%)	177 (88%)	25 (12%)	0	100	100
3	d	199/201 (99%)	175 (88%)	24 (12%)	0	100	100
4	e	161/163 (99%)	146 (91%)	15 (9%)	0	100	100
5	f	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
6	g	152/154 (99%)	138 (91%)	14 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	129/131 (98%)	119 (92%)	10 (8%)	0	100	100
8	i	126/128 (98%)	107 (85%)	19 (15%)	0	100	100
9	j	97/99 (98%)	85 (88%)	12 (12%)	0	100	100
10	k	115/117 (98%)	93 (81%)	22 (19%)	0	100	100
11	l	134/136 (98%)	107 (80%)	27 (20%)	0	100	100
12	m	110/112 (98%)	90 (82%)	20 (18%)	0	100	100
13	n	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
14	o	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
15	p	87/89 (98%)	78 (90%)	9 (10%)	0	100	100
16	q	81/83 (98%)	69 (85%)	12 (15%)	0	100	100
17	r	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
18	s	76/78 (97%)	69 (91%)	7 (9%)	0	100	100
19	t	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
22	C	271/275 (98%)	228 (84%)	43 (16%)	0	100	100
23	D	205/207 (99%)	177 (86%)	27 (13%)	1 (0%)	24	56
24	E	204/206 (99%)	170 (83%)	34 (17%)	0	100	100
25	F	174/177 (98%)	153 (88%)	21 (12%)	0	100	100
26	G	172/176 (98%)	147 (86%)	23 (13%)	2 (1%)	10	39
27	K	141/145 (97%)	123 (87%)	18 (13%)	0	100	100
28	L	120/122 (98%)	102 (85%)	18 (15%)	0	100	100
29	M	144/146 (99%)	109 (76%)	33 (23%)	2 (1%)	9	36
30	N	139/141 (99%)	121 (87%)	18 (13%)	0	100	100
31	O	119/123 (97%)	94 (79%)	25 (21%)	0	100	100
32	P	115/117 (98%)	98 (85%)	17 (15%)	0	100	100
33	Q	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
34	R	110/118 (93%)	104 (94%)	6 (6%)	0	100	100
35	S	98/102 (96%)	88 (90%)	10 (10%)	0	100	100
36	T	110/112 (98%)	94 (86%)	16 (14%)	0	100	100
37	U	86/89 (97%)	71 (83%)	13 (15%)	2 (2%)	5	29
38	V	99/101 (98%)	75 (76%)	21 (21%)	3 (3%)	3	25
39	W	92/94 (98%)	71 (77%)	20 (22%)	1 (1%)	11	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	X	74/76 (97%)	62 (84%)	12 (16%)	0	100	100
41	Y	52/54 (96%)	41 (79%)	11 (21%)	0	100	100
42	Z	59/61 (97%)	54 (92%)	5 (8%)	0	100	100
43	0	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
44	1	58/60 (97%)	39 (67%)	19 (33%)	0	100	100
45	2	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
46	3	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
47	4	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
48	5	62/64 (97%)	53 (86%)	9 (14%)	0	100	100
49	6	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
All	All	5102/5212 (98%)	4375 (86%)	716 (14%)	11 (0%)	44	71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	G	48	ASN
26	G	47	GLY
29	M	95	VAL
38	V	73	PRO
39	W	16	SER
23	D	90	GLU
37	U	52	ASN
29	M	16	ARG
38	V	72	ASP
37	U	50	VAL
38	V	88	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	c	162/162 (100%)	162 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	d	175/175 (100%)	175 (100%)	0	100	100
4	e	126/126 (100%)	126 (100%)	0	100	100
5	f	86/86 (100%)	86 (100%)	0	100	100
6	g	131/131 (100%)	131 (100%)	0	100	100
7	h	112/112 (100%)	112 (100%)	0	100	100
8	i	101/101 (100%)	101 (100%)	0	100	100
9	j	90/90 (100%)	90 (100%)	0	100	100
10	k	91/91 (100%)	91 (100%)	0	100	100
11	l	118/118 (100%)	118 (100%)	0	100	100
12	m	95/95 (100%)	95 (100%)	0	100	100
13	n	51/51 (100%)	51 (100%)	0	100	100
14	o	78/78 (100%)	78 (100%)	0	100	100
15	p	79/79 (100%)	78 (99%)	1 (1%)	61	70
16	q	76/76 (100%)	76 (100%)	0	100	100
17	r	57/57 (100%)	56 (98%)	1 (2%)	51	66
18	s	68/68 (100%)	68 (100%)	0	100	100
19	t	62/62 (100%)	61 (98%)	1 (2%)	55	67
22	C	225/225 (100%)	224 (100%)	1 (0%)	84	81
23	D	169/170 (99%)	167 (99%)	2 (1%)	63	71
24	E	172/172 (100%)	171 (99%)	1 (1%)	78	79
25	F	153/154 (99%)	153 (100%)	0	100	100
26	G	146/146 (100%)	146 (100%)	0	100	100
27	K	122/122 (100%)	121 (99%)	1 (1%)	73	76
28	L	98/98 (100%)	97 (99%)	1 (1%)	68	74
29	M	111/112 (99%)	110 (99%)	1 (1%)	70	75
30	N	111/112 (99%)	110 (99%)	1 (1%)	70	75
31	O	104/105 (99%)	104 (100%)	0	100	100
32	P	91/91 (100%)	91 (100%)	0	100	100
33	Q	97/97 (100%)	97 (100%)	0	100	100
34	R	88/94 (94%)	88 (100%)	0	100	100
35	S	83/83 (100%)	82 (99%)	1 (1%)	63	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	T	95/95 (100%)	95 (100%)	0	100	100
37	U	80/80 (100%)	78 (98%)	2 (2%)	42	60
38	V	85/85 (100%)	84 (99%)	1 (1%)	63	71
39	W	84/85 (99%)	84 (100%)	0	100	100
40	X	61/61 (100%)	61 (100%)	0	100	100
41	Y	46/47 (98%)	46 (100%)	0	100	100
42	Z	55/55 (100%)	55 (100%)	0	100	100
43	0	49/49 (100%)	49 (100%)	0	100	100
44	1	54/55 (98%)	54 (100%)	0	100	100
45	2	46/46 (100%)	46 (100%)	0	100	100
46	3	49/49 (100%)	49 (100%)	0	100	100
47	4	38/39 (97%)	38 (100%)	0	100	100
48	5	51/51 (100%)	51 (100%)	0	100	100
49	6	35/35 (100%)	35 (100%)	0	100	100
All	All	4356/4371 (100%)	4341 (100%)	15 (0%)	84	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	p	22	VAL
17	r	25	ILE
19	t	49	LEU
22	C	257	TYR
23	D	53	TYR
23	D	119	PHE
24	E	74	ARG
27	K	45	PHE
28	L	24	VAL
29	M	143	ILE
30	N	7	VAL
35	S	22	VAL
37	U	48	VAL
37	U	50	VAL
38	V	63	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
2	c	33	HIS
2	c	68	HIS
2	c	125	ASN
3	d	97	ASN
3	d	133	HIS
4	e	8	HIS
4	e	43	ASN
6	g	19	ASN
6	g	41	ASN
6	g	45	ASN
6	g	68	ASN
6	g	148	ASN
7	h	99	ASN
8	i	14	ASN
8	i	81	HIS
8	i	89	GLN
9	j	97	ASN
10	k	101	GLN
11	l	6	GLN
11	l	39	ASN
11	l	90	HIS
12	m	27	ASN
12	m	91	HIS
14	o	9	ASN
14	o	38	GLN
15	p	65	GLN
16	q	6	ASN
16	q	50	HIS
17	r	56	GLN
18	s	23	GLN
18	s	57	HIS
19	t	67	HIS
19	t	69	ASN
22	C	128	ASN
22	C	153	GLN
22	C	177	ASN
22	C	232	HIS
23	D	126	HIS
23	D	135	HIS
24	E	75	GLN
24	E	141	GLN
24	E	169	ASN
25	F	2	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	G	44	ASN
26	G	84	GLN
27	K	48	HIS
27	K	131	HIS
28	L	82	ASN
29	M	83	ASN
30	N	9	HIS
30	N	123	HIS
32	P	39	ASN
32	P	101	HIS
33	Q	29	HIS
34	R	38	GLN
34	R	81	HIS
35	S	81	HIS
35	S	90	GLN
36	T	65	ASN
36	T	66	ASN
38	V	45	GLN
40	X	38	GLN
41	Y	17	ASN
41	Y	32	ASN
41	Y	34	GLN
43	0	52	HIS
44	1	3	GLN
45	2	32	ASN
45	2	40	HIS
45	2	48	HIS
46	3	16	ASN
46	3	26	ASN
47	4	8	ASN
47	4	13	GLN
48	5	4	GLN
48	5	7	HIS
48	5	34	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1526/1528 (99%)	392 (25%)	0
20	A	2889/2903 (99%)	708 (24%)	24 (0%)
21	B	113/116 (97%)	30 (26%)	1 (0%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4528/4547 (99%)	1130 (24%)	25 (0%)

All (1130) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	5	A
1	a	6	G
1	a	7	A
1	a	11	U
1	a	12	G
1	a	19	G
1	a	28	G
1	a	29	A
1	a	35	G
1	a	36	G
1	a	41	G
1	a	44	C
1	a	45	C
1	a	48	A
1	a	55	C
1	a	60	C
1	a	65	G
1	a	72	U
1	a	73	C
1	a	74	C
1	a	75	U
1	a	97	G
1	a	113	G
1	a	114	A
1	a	117	G
1	a	126	C
1	a	127	A
1	a	135	A
1	a	136	A
1	a	137	C
1	a	150	G
1	a	152	G
1	a	169	C
1	a	183	G
1	a	188	A
1	a	189	C
1	a	202	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	211	G
1	a	212	A
1	a	215	G
1	a	218	A
1	a	219	G
1	a	222	G
1	a	223	C
1	a	226	U
1	a	227	C
1	a	229	G
1	a	235	G
1	a	255	U
1	a	256	G
1	a	261	A
1	a	262	G
1	a	266	G
1	a	277	A
1	a	281	G
1	a	282	C
1	a	289	A
1	a	294	A
1	a	296	G
1	a	304	G
1	a	306	C
1	a	308	A
1	a	321	A
1	a	323	C
1	a	330	A
1	a	331	C
1	a	336	A
1	a	342	A
1	a	343	C
1	a	361	G
1	a	362	G
1	a	367	C
1	a	369	G
1	a	381	C
1	a	382	U
1	a	387	C
1	a	388	A
1	a	393	A
1	a	399	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	403	G
1	a	407	G
1	a	412	A
1	a	420	U
1	a	421	G
1	a	422	A
1	a	426	A
1	a	427	A
1	a	428	G
1	a	429	A
1	a	437	C
1	a	439	G
1	a	443	G
1	a	444	U
1	a	454	U
1	a	455	U
1	a	456	G
1	a	457	U
1	a	463	A
1	a	464	A
1	a	469	A
1	a	476	U
1	a	478	A
1	a	479	G
1	a	480	U
1	a	482	A
1	a	483	C
1	a	484	U
1	a	485	G
1	a	487	A
1	a	489	G
1	a	490	U
1	a	493	C
1	a	495	U
1	a	496	G
1	a	499	G
1	a	500	G
1	a	501	U
1	a	510	A
1	a	511	G
1	a	526	C
1	a	528	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	533	C
1	a	534	C
1	a	536	G
1	a	542	G
1	a	546	U
1	a	547	A
1	a	548	A
1	a	560	C
1	a	562	A
1	a	577	U
1	a	578	A
1	a	583	G
1	a	585	G
1	a	587	A
1	a	590	G
1	a	591	C
1	a	592	G
1	a	603	G
1	a	611	A
1	a	634	U
1	a	646	G
1	a	648	U
1	a	649	C
1	a	656	A
1	a	668	U
1	a	671	G
1	a	674	C
1	a	676	G
1	a	680	A
1	a	681	G
1	a	686	G
1	a	701	U
1	a	702	A
1	a	710	A
1	a	719	A
1	a	735	C
1	a	736	A
1	a	738	U
1	a	744	A
1	a	757	G
1	a	763	A
1	a	764	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	770	G
1	a	775	G
1	a	802	A
1	a	808	U
1	a	832	C
1	a	835	U
1	a	836	G
1	a	842	U
1	a	843	A
1	a	847	G
1	a	852	A
1	a	858	U
1	a	859	C
1	a	860	C
1	a	861	G
1	a	862	C
1	a	867	C
1	a	869	G
1	a	886	U
1	a	887	U
1	a	888	A
1	a	889	A
1	a	890	G
1	a	896	C
1	a	901	G
1	a	905	A
1	a	937	U
1	a	938	G
1	a	942	G
1	a	943	G
1	a	945	G
1	a	946	C
1	a	947	C
1	a	948	C
1	a	950	C
1	a	951	A
1	a	954	A
1	a	955	G
1	a	956	C
1	a	962	A
1	a	974	A
1	a	975	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	976	U
1	a	977	U
1	a	981	A
1	a	982	G
1	a	984	A
1	a	985	A
1	a	986	C
1	a	987	G
1	a	988	C
1	a	989	G
1	a	990	A
1	a	991	A
1	a	992	G
1	a	999	A
1	a	1005	U
1	a	1008	U
1	a	1009	G
1	a	1012	A
1	a	1017	U
1	a	1018	U
1	a	1020	A
1	a	1024	C
1	a	1025	U
1	a	1030	A
1	a	1031	G
1	a	1033	U
1	a	1034	A
1	a	1037	G
1	a	1039	U
1	a	1040	U
1	a	1042	C
1	a	1043	C
1	a	1044	C
1	a	1048	G
1	a	1052	A
1	a	1056	A
1	a	1060	A
1	a	1061	C
1	a	1066	G
1	a	1069	G
1	a	1072	U
1	a	1074	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1075	U
1	a	1080	G
1	a	1081	U
1	a	1082	C
1	a	1089	U
1	a	1096	A
1	a	1097	G
1	a	1101	U
1	a	1102	U
1	a	1104	G
1	a	1109	A
1	a	1110	G
1	a	1111	U
1	a	1116	C
1	a	1117	A
1	a	1119	C
1	a	1124	G
1	a	1126	A
1	a	1129	C
1	a	1140	G
1	a	1142	U
1	a	1145	C
1	a	1146	A
1	a	1148	C
1	a	1152	U
1	a	1153	A
1	a	1154	G
1	a	1155	U
1	a	1156	U
1	a	1159	G
1	a	1160	C
1	a	1161	A
1	a	1169	G
1	a	1172	A
1	a	1173	C
1	a	1174	U
1	a	1176	C
1	a	1182	A
1	a	1183	C
1	a	1184	A
1	a	1190	G
1	a	1196	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1197	G
1	a	1199	G
1	a	1205	G
1	a	1211	A
1	a	1212	A
1	a	1227	U
1	a	1228	A
1	a	1229	U
1	a	1230	G
1	a	1236	G
1	a	1237	G
1	a	1239	U
1	a	1240	A
1	a	1241	C
1	a	1242	A
1	a	1251	A
1	a	1254	A
1	a	1255	U
1	a	1256	G
1	a	1259	A
1	a	1265	A
1	a	1268	G
1	a	1272	C
1	a	1273	G
1	a	1276	A
1	a	1282	C
1	a	1283	G
1	a	1284	A
1	a	1293	A
1	a	1295	A
1	a	1296	U
1	a	1297	C
1	a	1298	U
1	a	1300	U
1	a	1302	A
1	a	1303	A
1	a	1305	G
1	a	1309	C
1	a	1312	U
1	a	1314	A
1	a	1315	G
1	a	1317	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1320	G
1	a	1324	G
1	a	1327	G
1	a	1332	C
1	a	1333	A
1	a	1335	C
1	a	1336	U
1	a	1337	C
1	a	1346	G
1	a	1350	C
1	a	1351	C
1	a	1352	G
1	a	1353	G
1	a	1356	U
1	a	1360	U
1	a	1362	G
1	a	1364	A
1	a	1378	A
1	a	1379	C
1	a	1383	G
1	a	1385	G
1	a	1393	C
1	a	1394	G
1	a	1400	G
1	a	1404	C
1	a	1405	U
1	a	1406	U
1	a	1409	A
1	a	1411	A
1	a	1412	C
1	a	1413	A
1	a	1414	C
1	a	1415	C
1	a	1416	G
1	a	1417	C
1	a	1433	A
1	a	1434	G
1	a	1438	G
1	a	1441	A
1	a	1457	A
1	a	1458	G
1	a	1461	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1465	U
1	a	1466	U
1	a	1467	U
1	a	1468	U
1	a	1500	U
1	a	1507	G
1	a	1509	A
1	a	1510	G
1	a	1511	U
1	a	1515	A
1	a	1516	A
1	a	1518	A
1	a	1519	A
1	a	1521	G
1	a	1522	U
1	a	1545	G
1	a	1546	G
1	a	1549	C
1	a	1550	A
20	A	14	A
20	A	15	A
20	A	16	G
20	A	29	A
20	A	49	G
20	A	50	A
20	A	52	G
20	A	64	U
20	A	72	A
20	A	75	U
20	A	76	G
20	A	86	G
20	A	89	G
20	A	90	U
20	A	97	G
20	A	102	G
20	A	103	A
20	A	110	G
20	A	118	A
20	A	119	A
20	A	120	U
20	A	131	A
20	A	151	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	155	U
20	A	156	U
20	A	159	G
20	A	162	A
20	A	163	A
20	A	165	A
20	A	166	C
20	A	169	A
20	A	180	G
20	A	182	U
20	A	184	G
20	A	185	A
20	A	189	A
20	A	199	A
20	A	202	A
20	A	207	A
20	A	218	G
20	A	219	A
20	A	224	A
20	A	225	A
20	A	229	A
20	A	231	A
20	A	232	U
20	A	233	U
20	A	235	G
20	A	236	A
20	A	244	A
20	A	251	G
20	A	254	A
20	A	255	G
20	A	268	A
20	A	270	C
20	A	278	A
20	A	284	C
20	A	285	U
20	A	286	U
20	A	288	C
20	A	298	U
20	A	300	G
20	A	302	A
20	A	312	U
20	A	313	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	318	A
20	A	321	C
20	A	322	U
20	A	324	U
20	A	327	G
20	A	332	G
20	A	339	G
20	A	344	G
20	A	367	A
20	A	383	A
20	A	386	G
20	A	391	C
20	A	396	C
20	A	399	A
20	A	400	G
20	A	404	G
20	A	410	G
20	A	411	A
20	A	412	G
20	A	421	A
20	A	424	A
20	A	426	G
20	A	427	A
20	A	445	C
20	A	446	G
20	A	451	G
20	A	452	A
20	A	487	A
20	A	488	U
20	A	494	A
20	A	495	C
20	A	496	C
20	A	497	A
20	A	506	A
20	A	507	G
20	A	513	G
20	A	517	A
20	A	518	A
20	A	521	G
20	A	543	U
20	A	544	A
20	A	547	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	548	C
20	A	549	C
20	A	561	G
20	A	566	C
20	A	569	C
20	A	570	A
20	A	571	A
20	A	572	G
20	A	580	U
20	A	585	A
20	A	586	A
20	A	587	U
20	A	588	G
20	A	599	U
20	A	600	G
20	A	610	G
20	A	612	A
20	A	613	U
20	A	623	A
20	A	624	G
20	A	640	A
20	A	651	A
20	A	652	A
20	A	653	G
20	A	654	A
20	A	655	G
20	A	660	A
20	A	661	G
20	A	670	A
20	A	673	G
20	A	676	A
20	A	677	G
20	A	682	A
20	A	684	U
20	A	693	U
20	A	694	G
20	A	696	G
20	A	708	A
20	A	710	A
20	A	711	C
20	A	722	G
20	A	726	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	727	C
20	A	741	G
20	A	756	A
20	A	758	A
20	A	759	C
20	A	766	G
20	A	769	G
20	A	770	A
20	A	786	U
20	A	787	U
20	A	788	G
20	A	792	A
20	A	804	A
20	A	805	G
20	A	808	G
20	A	815	G
20	A	816	C
20	A	817	G
20	A	822	A
20	A	823	A
20	A	824	U
20	A	825	U
20	A	828	A
20	A	832	G
20	A	833	A
20	A	840	A
20	A	845	G
20	A	846	C
20	A	849	G
20	A	851	U
20	A	852	C
20	A	859	A
20	A	861	A
20	A	867	U
20	A	885	U
20	A	886	U
20	A	888	A
20	A	891	A
20	A	897	G
20	A	900	G
20	A	901	U
20	A	904	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	905	G
20	A	906	C
20	A	907	A
20	A	914	G
20	A	919	A
20	A	922	G
20	A	923	G
20	A	925	C
20	A	926	C
20	A	927	A
20	A	928	U
20	A	932	G
20	A	934	G
20	A	935	U
20	A	939	C
20	A	942	A
20	A	943	U
20	A	946	A
20	A	949	U
20	A	950	A
20	A	951	A
20	A	953	C
20	A	960	U
20	A	961	G
20	A	964	A
20	A	966	U
20	A	978	G
20	A	985	A
20	A	986	G
20	A	993	A
20	A	997	A
20	A	999	A
20	A	1001	G
20	A	1006	G
20	A	1013	A
20	A	1014	A
20	A	1015	A
20	A	1016	G
20	A	1029	G
20	A	1036	A
20	A	1042	G
20	A	1047	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	1048	A
20	A	1049	A
20	A	1051	A
20	A	1052	U
20	A	1053	A
20	A	1061	A
20	A	1062	G
20	A	1065	G
20	A	1066	A
20	A	1073	U
20	A	1085	C
20	A	1086	A
20	A	1087	G
20	A	1089	C
20	A	1094	A
20	A	1095	G
20	A	1096	G
20	A	1097	A
20	A	1100	U
20	A	1101	U
20	A	1103	G
20	A	1104	C
20	A	1105	U
20	A	1107	A
20	A	1108	G
20	A	1109	A
20	A	1110	A
20	A	1111	G
20	A	1112	C
20	A	1113	A
20	A	1115	C
20	A	1116	C
20	A	1117	A
20	A	1118	C
20	A	1119	C
20	A	1120	A
20	A	1122	U
20	A	1124	A
20	A	1125	A
20	A	1128	A
20	A	1129	G
20	A	1131	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	1132	C
20	A	1133	G
20	A	1134	U
20	A	1135	A
20	A	1137	U
20	A	1138	A
20	A	1139	G
20	A	1140	C
20	A	1141	U
20	A	1142	C
20	A	1143	A
20	A	1144	C
20	A	1145	U
20	A	1146	A
20	A	1147	G
20	A	1148	U
20	A	1151	A
20	A	1152	G
20	A	1156	C
20	A	1162	G
20	A	1167	A
20	A	1168	A
20	A	1171	G
20	A	1172	U
20	A	1174	C
20	A	1175	C
20	A	1179	G
20	A	1181	U
20	A	1182	A
20	A	1183	A
20	A	1188	A
20	A	1196	A
20	A	1210	C
20	A	1213	U
20	A	1215	A
20	A	1216	G
20	A	1217	G
20	A	1218	U
20	A	1219	G
20	A	1249	G
20	A	1257	A
20	A	1258	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	1272	G
20	A	1273	G
20	A	1274	A
20	A	1275	G
20	A	1277	G
20	A	1284	A
20	A	1285	G
20	A	1290	A
20	A	1292	U
20	A	1293	G
20	A	1294	C
20	A	1302	A
20	A	1308	G
20	A	1309	A
20	A	1310	A
20	A	1311	A
20	A	1320	A
20	A	1323	A
20	A	1336	U
20	A	1337	A
20	A	1338	U
20	A	1349	U
20	A	1350	C
20	A	1357	A
20	A	1365	U
20	A	1366	C
20	A	1375	G
20	A	1376	U
20	A	1377	U
20	A	1388	U
20	A	1394	G
20	A	1396	G
20	A	1397	G
20	A	1400	G
20	A	1401	A
20	A	1404	G
20	A	1414	A
20	A	1415	U
20	A	1420	A
20	A	1421	A
20	A	1422	C
20	A	1428	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	1431	A
20	A	1432	U
20	A	1436	U
20	A	1443	G
20	A	1445	U
20	A	1448	U
20	A	1449	U
20	A	1450	U
20	A	1451	U
20	A	1452	G
20	A	1453	U
20	A	1455	U
20	A	1457	A
20	A	1461	A
20	A	1462	U
20	A	1463	G
20	A	1469	A
20	A	1470	C
20	A	1471	G
20	A	1475	U
20	A	1488	G
20	A	1489	C
20	A	1492	G
20	A	1494	G
20	A	1495	A
20	A	1496	U
20	A	1497	U
20	A	1500	A
20	A	1501	A
20	A	1502	G
20	A	1503	U
20	A	1504	G
20	A	1505	C
20	A	1509	U
20	A	1510	C
20	A	1516	A
20	A	1519	G
20	A	1521	G
20	A	1525	U
20	A	1531	G
20	A	1532	A
20	A	1536	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	1539	U
20	A	1545	A
20	A	1548	C
20	A	1551	U
20	A	1552	A
20	A	1559	A
20	A	1560	G
20	A	1566	A
20	A	1568	G
20	A	1573	G
20	A	1576	A
20	A	1577	A
20	A	1579	U
20	A	1584	G
20	A	1585	U
20	A	1586	A
20	A	1588	C
20	A	1589	G
20	A	1590	A
20	A	1600	C
20	A	1601	G
20	A	1602	U
20	A	1604	A
20	A	1605	C
20	A	1606	A
20	A	1612	A
20	A	1613	A
20	A	1615	A
20	A	1623	C
20	A	1629	A
20	A	1630	G
20	A	1631	A
20	A	1632	A
20	A	1633	A
20	A	1634	A
20	A	1635	C
20	A	1640	G
20	A	1645	U
20	A	1646	A
20	A	1650	U
20	A	1651	A
20	A	1653	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	1677	U
20	A	1689	A
20	A	1690	G
20	A	1691	C
20	A	1717	G
20	A	1737	C
20	A	1738	G
20	A	1741	A
20	A	1756	U
20	A	1757	U
20	A	1767	G
20	A	1770	G
20	A	1774	A
20	A	1776	A
20	A	1777	G
20	A	1778	G
20	A	1782	A
20	A	1787	A
20	A	1790	G
20	A	1795	U
20	A	1798	A
20	A	1814	C
20	A	1815	A
20	A	1817	A
20	A	1821	G
20	A	1822	U
20	A	1823	A
20	A	1829	A
20	A	1830	A
20	A	1833	A
20	A	1834	U
20	A	1841	U
20	A	1842	G
20	A	1843	A
20	A	1862	A
20	A	1872	G
20	A	1881	G
20	A	1882	C
20	A	1886	G
20	A	1896	A
20	A	1913	A
20	A	1917	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	1933	A
20	A	1940	U
20	A	1941	A
20	A	1943	G
20	A	1944	G
20	A	1952	A
20	A	1957	U
20	A	1958	U
20	A	1969	U
20	A	1970	U
20	A	1976	C
20	A	1978	G
20	A	1979	C
20	A	1981	C
20	A	1984	A
20	A	1985	A
20	A	1986	G
20	A	1989	G
20	A	1996	U
20	A	2006	G
20	A	2007	U
20	A	2034	A
20	A	2037	A
20	A	2039	C
20	A	2044	A
20	A	2045	A
20	A	2046	G
20	A	2047	A
20	A	2048	U
20	A	2056	A
20	A	2057	C
20	A	2066	G
20	A	2069	C
20	A	2070	G
20	A	2074	A
20	A	2075	G
20	A	2082	U
20	A	2083	G
20	A	2107	G
20	A	2114	U
20	A	2122	A
20	A	2124	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	2125	U
20	A	2126	A
20	A	2128	A
20	A	2129	G
20	A	2130	G
20	A	2131	A
20	A	2132	U
20	A	2133	A
20	A	2134	G
20	A	2139	G
20	A	2140	A
20	A	2143	C
20	A	2144	G
20	A	2145	A
20	A	2146	U
20	A	2148	A
20	A	2149	G
20	A	2150	A
20	A	2153	G
20	A	2154	G
20	A	2158	G
20	A	2159	C
20	A	2160	U
20	A	2162	G
20	A	2170	G
20	A	2172	A
20	A	2173	G
20	A	2174	G
20	A	2176	G
20	A	2179	G
20	A	2180	G
20	A	2182	G
20	A	2183	G
20	A	2184	G
20	A	2185	A
20	A	2186	U
20	A	2187	A
20	A	2190	A
20	A	2200	U
20	A	2201	A
20	A	2206	C
20	A	2212	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	2213	A
20	A	2217	G
20	A	2218	C
20	A	2225	A
20	A	2227	U
20	A	2239	A
20	A	2252	G
20	A	2253	G
20	A	2273	G
20	A	2280	A
20	A	2282	A
20	A	2292	A
20	A	2297	C
20	A	2301	A
20	A	2302	A
20	A	2318	G
20	A	2319	U
20	A	2323	A
20	A	2325	A
20	A	2327	C
20	A	2333	A
20	A	2334	A
20	A	2336	A
20	A	2337	G
20	A	2339	G
20	A	2341	A
20	A	2348	G
20	A	2349	A
20	A	2350	A
20	A	2359	G
20	A	2364	C
20	A	2379	G
20	A	2390	A
20	A	2391	A
20	A	2393	G
20	A	2397	G
20	A	2398	G
20	A	2399	C
20	A	2402	A
20	A	2404	U
20	A	2405	G
20	A	2406	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	2407	U
20	A	2416	U
20	A	2417	C
20	A	2419	G
20	A	2420	C
20	A	2436	C
20	A	2437	U
20	A	2439	A
20	A	2443	G
20	A	2445	U
20	A	2455	C
20	A	2459	G
20	A	2461	G
20	A	2462	A
20	A	2469	G
20	A	2473	A
20	A	2489	C
20	A	2492	A
20	A	2498	G
20	A	2504	G
20	A	2505	U
20	A	2512	C
20	A	2516	G
20	A	2517	A
20	A	2518	U
20	A	2519	G
20	A	2521	C
20	A	2532	A
20	A	2534	C
20	A	2548	C
20	A	2549	G
20	A	2557	G
20	A	2558	G
20	A	2566	U
20	A	2567	G
20	A	2568	U
20	A	2570	C
20	A	2580	A
20	A	2581	G
20	A	2586	A
20	A	2587	C
20	A	2588	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	2592	G
20	A	2595	G
20	A	2596	G
20	A	2598	U
20	A	2599	U
20	A	2600	C
20	A	2616	A
20	A	2623	U
20	A	2627	U
20	A	2643	U
20	A	2650	U
20	A	2660	C
20	A	2661	U
20	A	2677	G
20	A	2682	G
20	A	2696	G
20	A	2703	U
20	A	2728	G
20	A	2746	G
20	A	2747	A
20	A	2753	U
20	A	2755	A
20	A	2764	A
20	A	2766	C
20	A	2770	U
20	A	2778	A
20	A	2779	A
20	A	2780	G
20	A	2792	A
20	A	2793	U
20	A	2804	A
20	A	2805	U
20	A	2806	U
20	A	2808	C
20	A	2810	U
20	A	2812	A
20	A	2813	A
20	A	2814	G
20	A	2819	U
20	A	2829	G
20	A	2831	G
20	A	2835	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	A	2836	G
20	A	2844	A
20	A	2845	G
20	A	2846	A
20	A	2847	U
20	A	2848	A
20	A	2868	G
20	A	2870	G
20	A	2878	G
20	A	2883	G
20	A	2891	C
20	A	2897	G
20	A	2904	G
21	B	8	G
21	B	10	G
21	B	11	A
21	B	13	A
21	B	22	G
21	B	23	A
21	B	29	C
21	B	31	G
21	B	36	C
21	B	40	C
21	B	42	G
21	B	43	A
21	B	50	A
21	B	54	U
21	B	55	A
21	B	70	G
21	B	71	A
21	B	73	U
21	B	74	G
21	B	82	G
21	B	85	U
21	B	86	U
21	B	87	U
21	B	88	C
21	B	94	G
21	B	97	A
21	B	99	A
21	B	102	A
21	B	107	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	B	115	G

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	155	U
20	A	179	A
20	A	311	A
20	A	654	A
20	A	693	U
20	A	755	A
20	A	890	A
20	A	960	U
20	A	963	C
20	A	1100	U
20	A	1138	A
20	A	1142	C
20	A	1146	A
20	A	1147	G
20	A	1502	G
20	A	1530	A
20	A	1584	G
20	A	1585	U
20	A	1604	A
20	A	1605	C
20	A	2281	A
20	A	2317	G
20	A	2475	C
20	A	2811	U
21	B	101	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
20	A	2
1	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	928:U	O3'	931:C	P	12.58
1	a	75:U	O3'	96:U	P	12.00
1	A	1579:U	O3'	1583:A	P	10.23

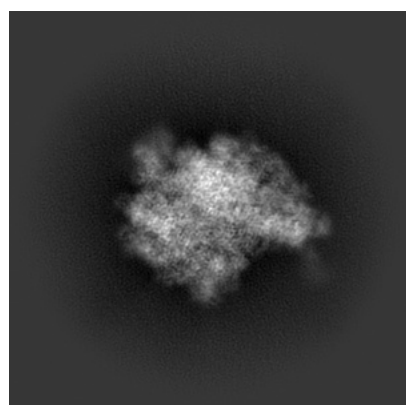
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0657. These allow visual inspection of the internal detail of the map and identification of artifacts.

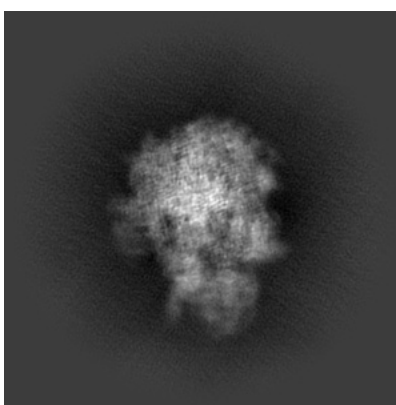
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

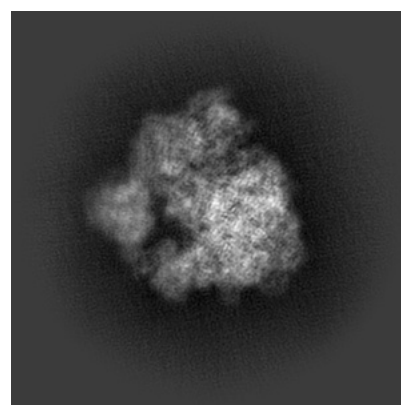
6.1.1 Primary map



X



Y

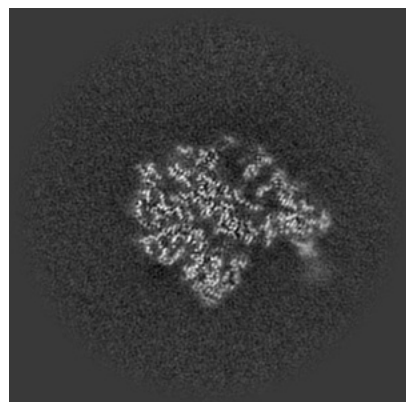


Z

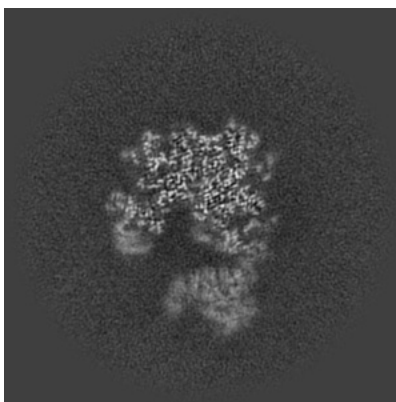
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

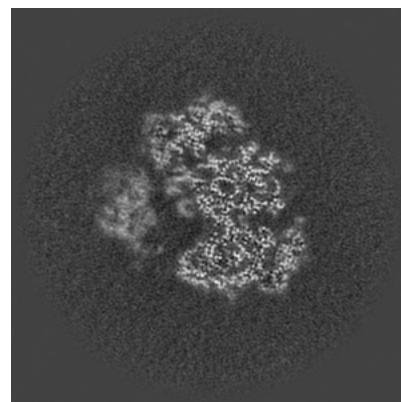
6.2.1 Primary map



X Index: 220



Y Index: 220

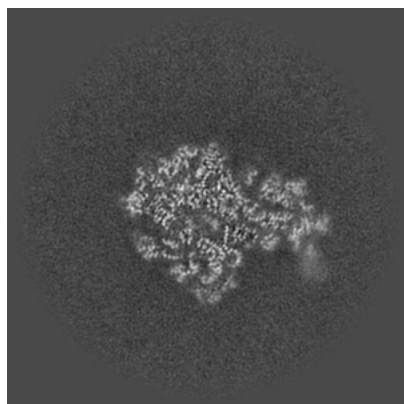


Z Index: 220

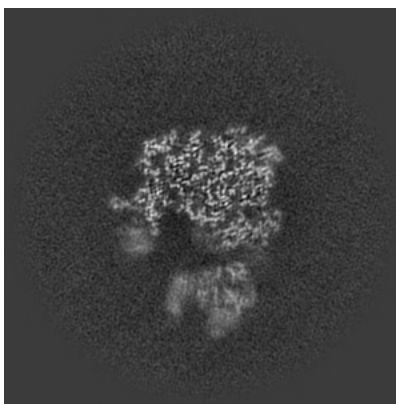
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

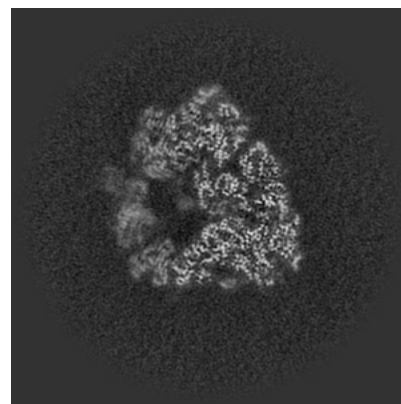
6.3.1 Primary map



X Index: 228



Y Index: 231

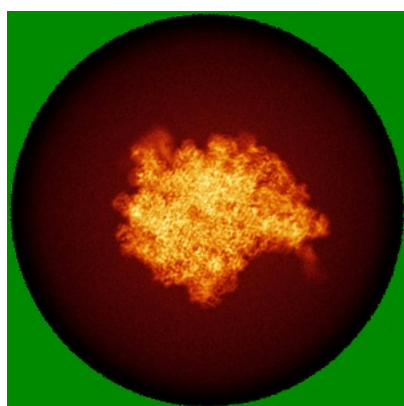


Z Index: 209

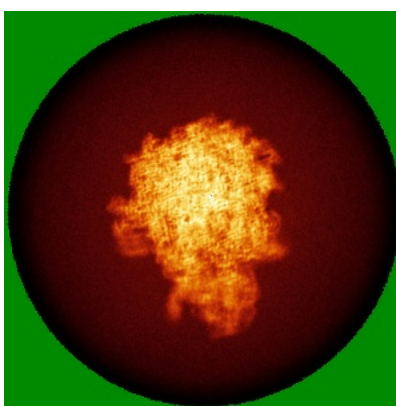
The images above show the largest variance slices of the map in three orthogonal directions.

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

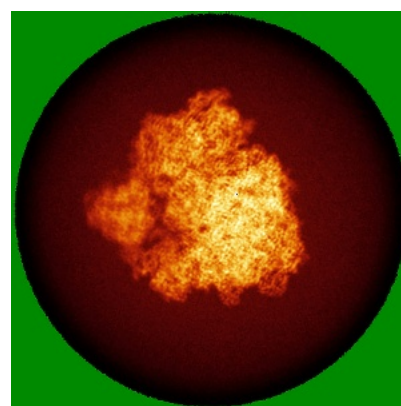
6.4.1 Primary map



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

This section was not generated.

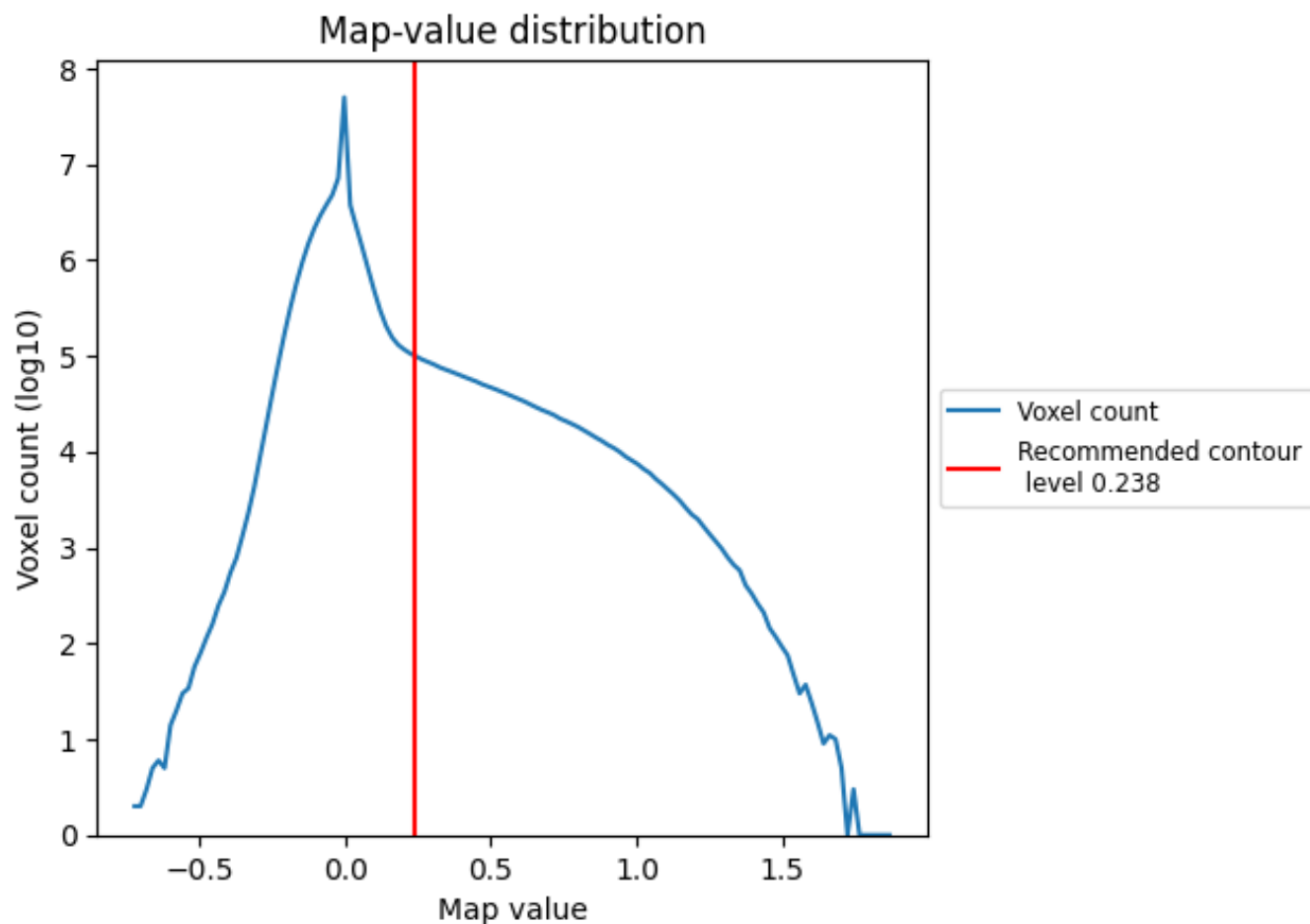
6.6 Mask visualisation

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

7 Map analysis [i](#)

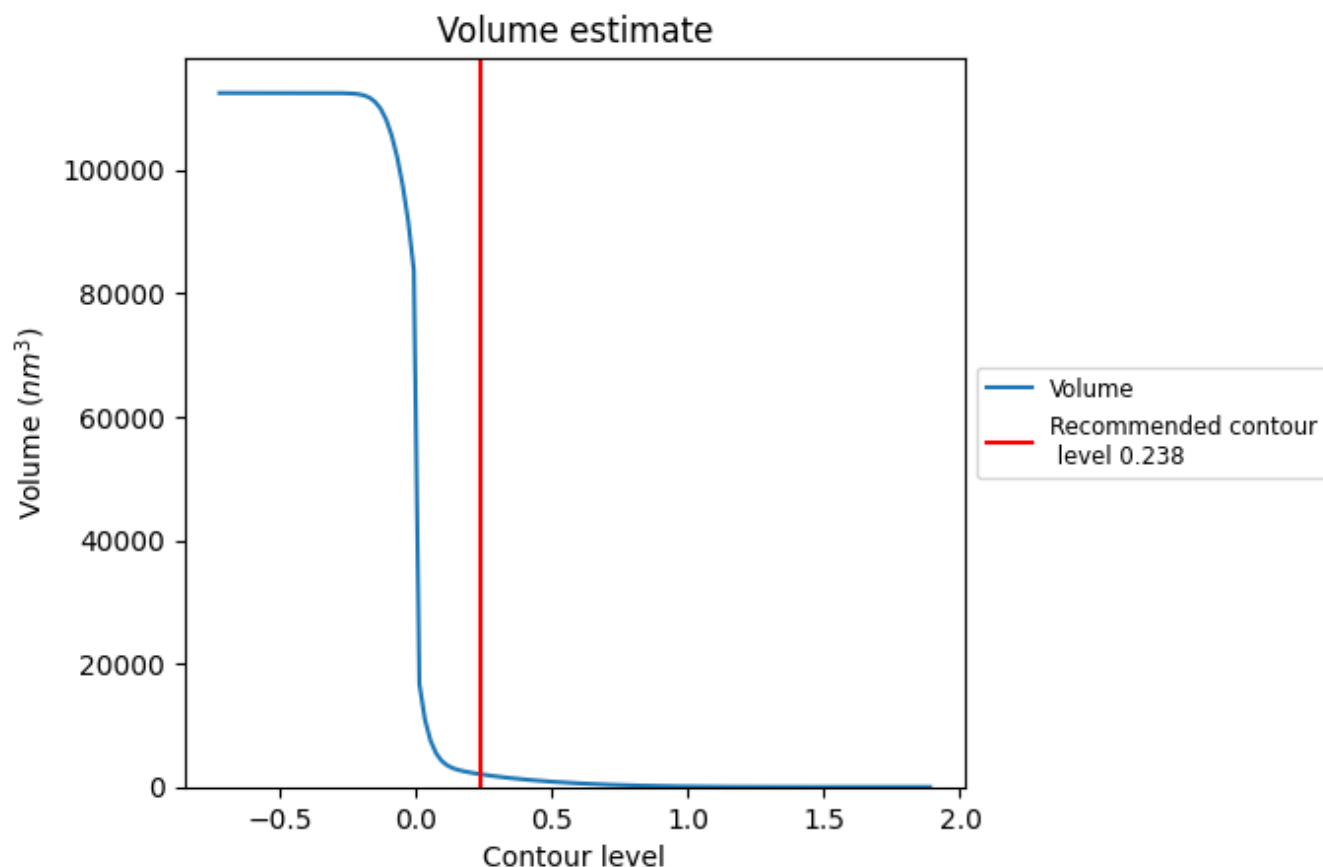
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

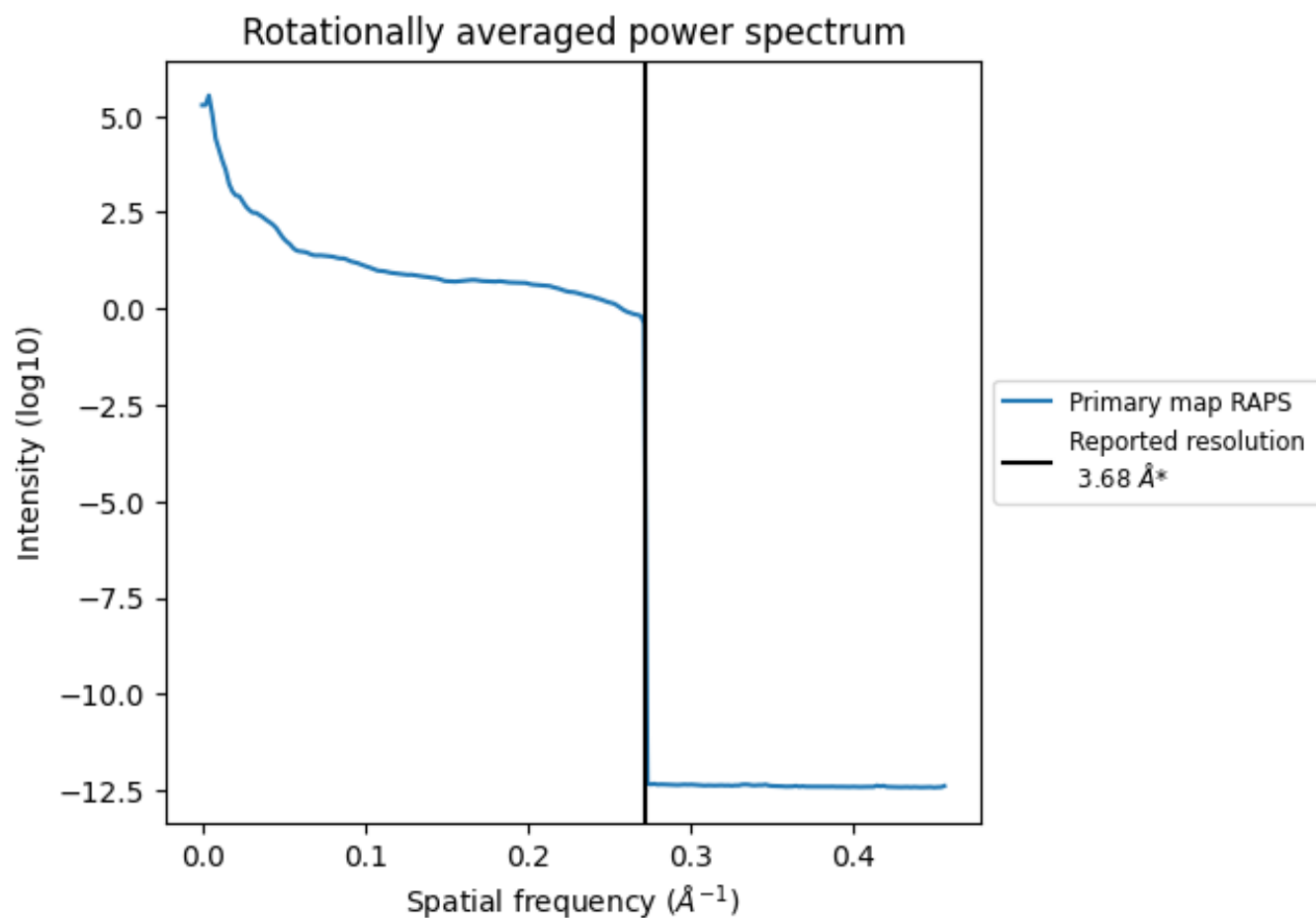
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2048 nm^3 ; this corresponds to an approximate mass of 1850 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

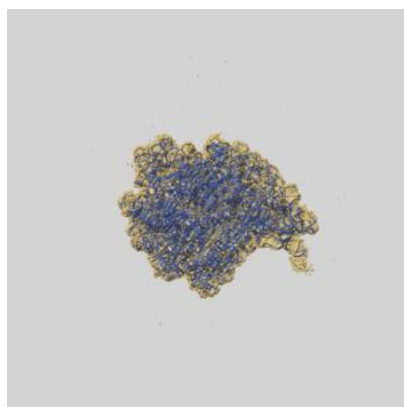
8 Fourier-Shell correlation

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

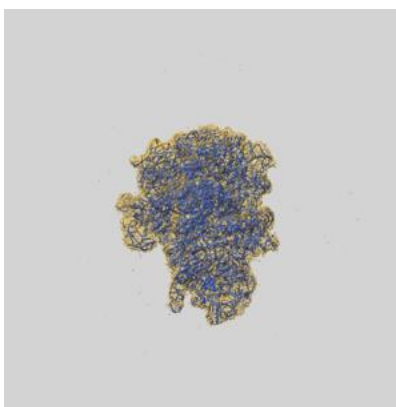
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0657 and PDB model 6O8X. Per-residue inclusion information can be found in section [3](#) on page [13](#).

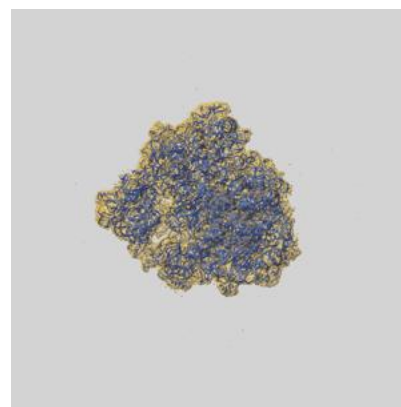
9.1 Map-model overlay [i](#)



X



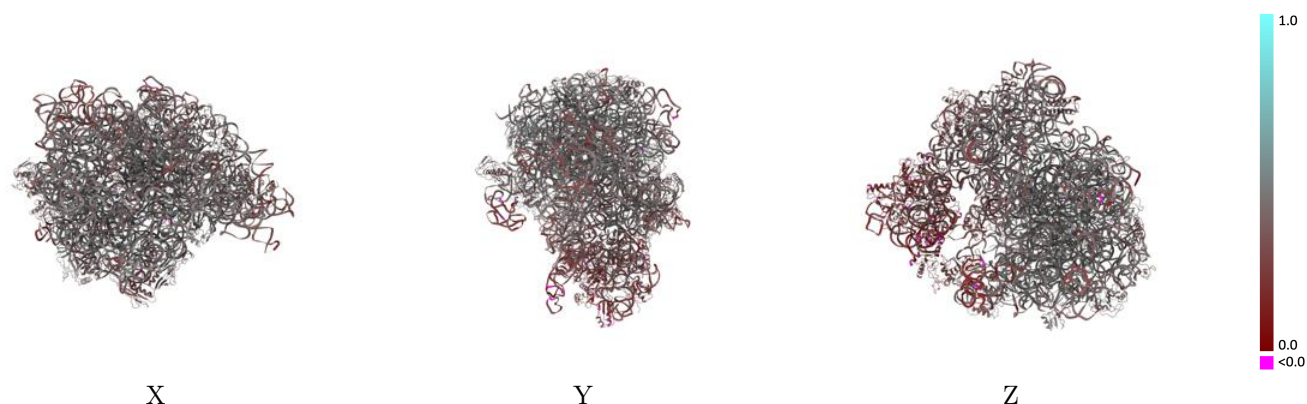
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

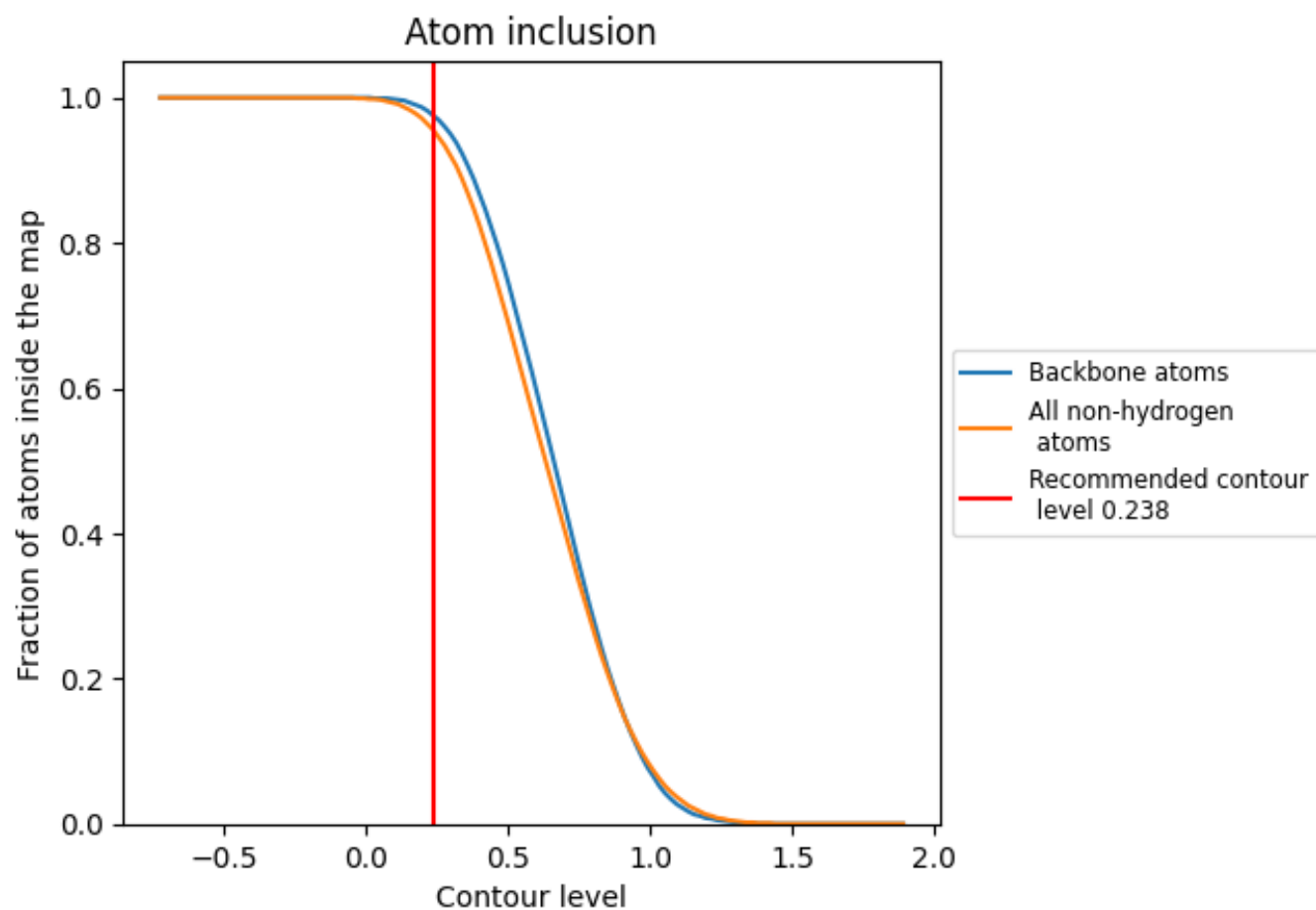


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.4020
0	 0.9090	 0.4630
1	 0.8830	 0.2890
2	 0.9570	 0.4650
3	 0.8760	 0.4560
4	 0.9230	 0.4470
5	 0.9130	 0.4770
6	 0.9560	 0.4600
A	 0.9900	 0.4290
B	 0.9960	 0.4020
C	 0.9260	 0.4520
D	 0.9300	 0.4690
E	 0.9220	 0.4370
F	 0.8600	 0.3250
G	 0.8870	 0.3780
K	 0.9300	 0.4550
L	 0.9040	 0.4720
M	 0.9320	 0.4460
N	 0.8180	 0.4070
O	 0.9180	 0.4350
P	 0.8920	 0.3700
Q	 0.9150	 0.4560
R	 0.9020	 0.4120
S	 0.9240	 0.4500
T	 0.9230	 0.4500
U	 0.9150	 0.4240
V	 0.8650	 0.3960
W	 0.3150	 0.2990
X	 0.9460	 0.4660
Y	 0.8910	 0.4570
Z	 0.9040	 0.3750
a	 0.9880	 0.3700
c	 0.5310	 0.2820
d	 0.8960	 0.3340
e	 0.8850	 0.3640



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.8810	 0.3990
g	 0.8560	 0.2080
h	 0.9150	 0.4090
i	 0.8960	 0.2830
j	 0.8100	 0.2520
k	 0.9090	 0.3700
l	 0.8570	 0.3950
m	 0.7680	 0.2210
n	 0.8930	 0.2790
o	 0.8820	 0.4010
p	 0.9290	 0.3920
q	 0.8760	 0.4040
r	 0.8940	 0.3900
s	 0.8480	 0.2450
t	 0.8860	 0.3680