



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:57 AM UTC

PDB ID : 9WNQ / pdb_00009wnq
EMDB ID : EMD-66121
Title : Structure of E.coli ribosome in complex with an engineered arrest peptide
Authors : Sriramoju, M.K.; Ko, T.P.; Draczkowski, P.; Hsu, S.T.D.
Deposited on : 2025-09-05
Resolution : 2.59 Å (reported)
Based on initial model : 3JBU

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:

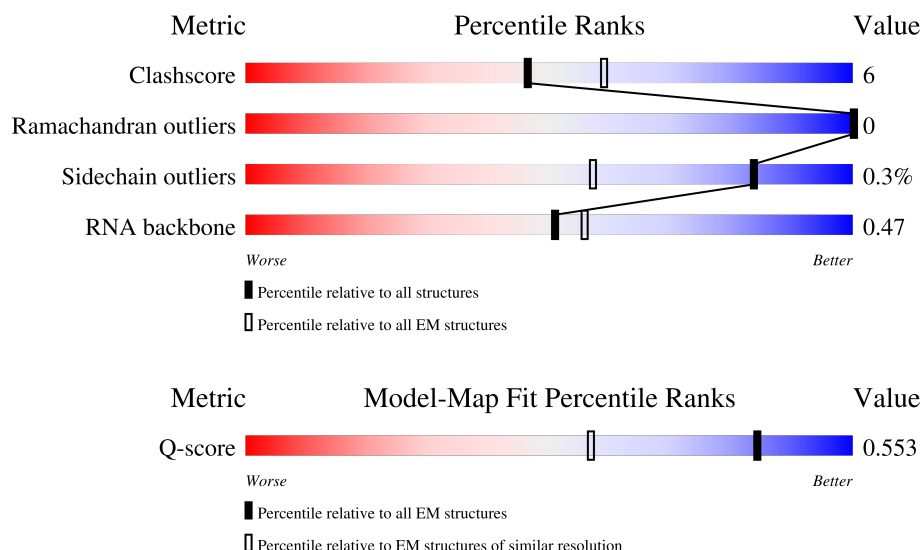
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.59 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.



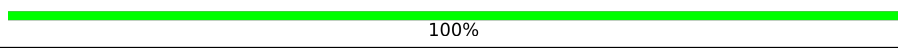
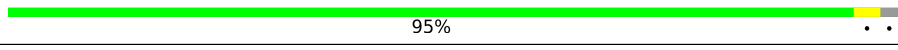
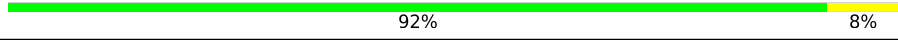
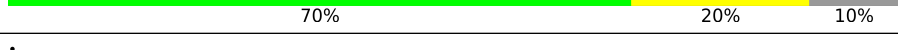
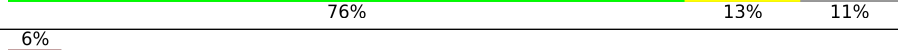
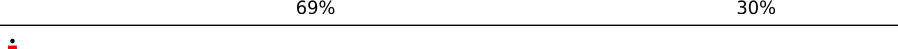
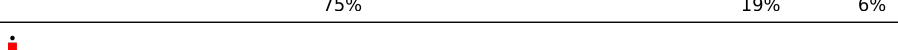
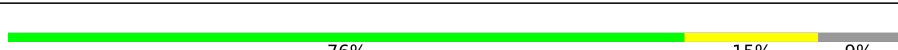
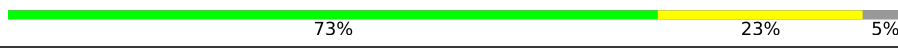
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7741 (2.09 - 3.09)

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	0	78	
2	1	63	
3	2	59	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	4	57	
5	5	55	
6	6	46	
7	7	65	
8	8	38	
9	A	1533	
10	B	241	
11	C	233	
12	D	206	
13	E	167	
14	F	135	
15	G	179	
16	H	130	
17	I	130	
18	J	103	
19	K	129	
20	L	124	
21	M	118	
22	N	101	
23	O	89	
24	P	82	
25	Q	84	
26	R	75	
27	S	92	
28	T	87	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	U	71	
30	X	76	
31	Y	77	
31	Z	77	
32	a	120	
33	b	2904	
34	c	273	
35	d	209	
36	e	201	
37	f	179	
38	g	177	
39	h	149	
40	k	142	
41	l	123	
42	m	144	
43	n	136	
44	o	127	
45	p	117	
46	q	115	
47	r	118	
48	s	103	
49	t	110	
50	u	100	
51	v	104	
52	w	94	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	x	14	7% 71% 14% 14%
54	y	85	93% 6%
55	z	26	15% 58% 35% 8%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 147439 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 protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 3 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 5 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 7 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 9 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1533	Total	C	N	O	P	0	0
			32895	14671	6036	10655	1533		

- Molecule 10 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 11 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	207	Total	C	N	O	S	0	0
			1632	1034	306	289	3		

- Molecule 12 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 14 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 15 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 16 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 17 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 18 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	122	Total	C	N	O	S	0	0
			949	587	195	163	4		

- Molecule 21 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 22 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 23 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 24 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 25 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 26 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 27 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 28 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 29 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	64	Total	C	N	O	S	0	0
			529	329	110	89	1		

- Molecule 30 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	76	Total	C	N	O	P	0	0
			1621	722	287	536	76		

- Molecule 31 is a RNA chain called A-tRNA(PRO),P-tRNA(PRO).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		
31	Z	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

- Molecule 32 is a RNA chain called 5S rRNA.

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

- Molecule 33 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	2902	Total	C	N	O	P	0	0
			62297	27791	11462	20142	2902		

- Molecule 34 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 35 is a protein called 50S ribosomal protein L3.

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

- Molecule 36 is a protein called 50S ribosomal protein L4.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	178	Total	C	N	O	S	0	0
			1419	905	251	257	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 39 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	149	Total	C	N	O	S	0	0
			1108	699	197	211	1		

- Molecule 40 is a protein called 50S ribosomal protein L13.

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

- Molecule 41 is a protein called 50S ribosomal protein L14.

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

- Molecule 42 is a protein called 50S ribosomal protein L15.

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

- Molecule 43 is a protein called 50S ribosomal protein L16.

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

- Molecule 44 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 45 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 46 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 48 is a protein called 50S ribosomal protein L21.

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

- Molecule 49 is a protein called 50S ribosomal protein L22.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	100	Total	C	N	O	S	0	0
			786	496	146	142	2		

- Molecule 51 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	103	Total	C	N	O		0	0
			784	496	147	141			

- Molecule 52 is a protein called 50S ribosomal protein L25.

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	14	Total	C	N	O	P	0	0
			299	133	55	97	14		

- Molecule 54 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

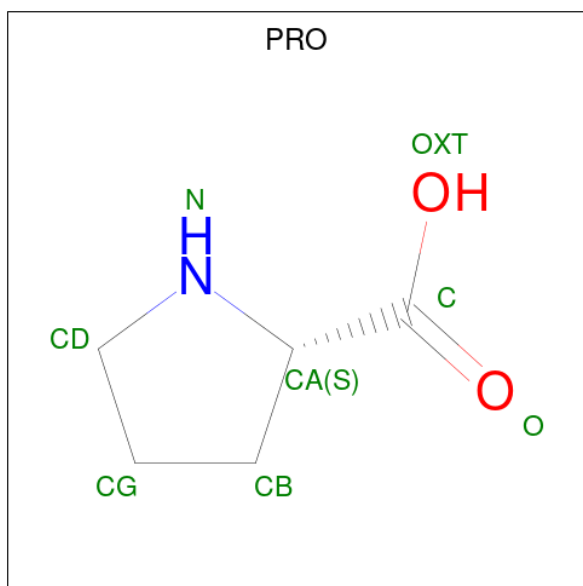
- Molecule 55 is a protein called eRAP-NC.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	z	26	Total	C	N	O	8	0
			303	207	53	43		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	8	1	Total	Zn	0
			1	1	

- Molecule 57 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).

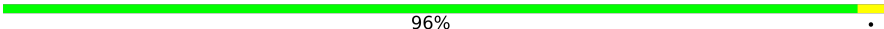


Mol	Chain	Residues	Atoms				AltConf
57	Z	1	Total	C	N	O	0
			7	5	1	1	

3 Residue-property plots [i](#)

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

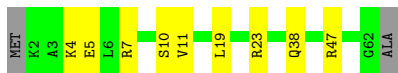
- Molecule 1: Large ribosomal subunit protein bL28

Chain 0:  96%

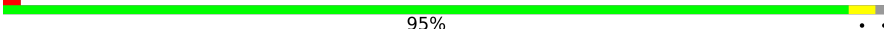


- Molecule 2: Large ribosomal subunit protein uL29

Chain 1:  83% 14%



- Molecule 3: Large ribosomal subunit protein uL30

Chain 2:  95%



- Molecule 4: Large ribosomal subunit protein bL32

Chain 4:  84% 14%



- Molecule 5: Large ribosomal subunit protein bL33

Chain 5:  76% 18% 5%

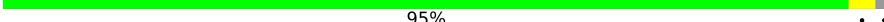


- Molecule 6: 50S ribosomal protein L34

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Large ribosomal subunit protein bL35

Chain 7:  95%



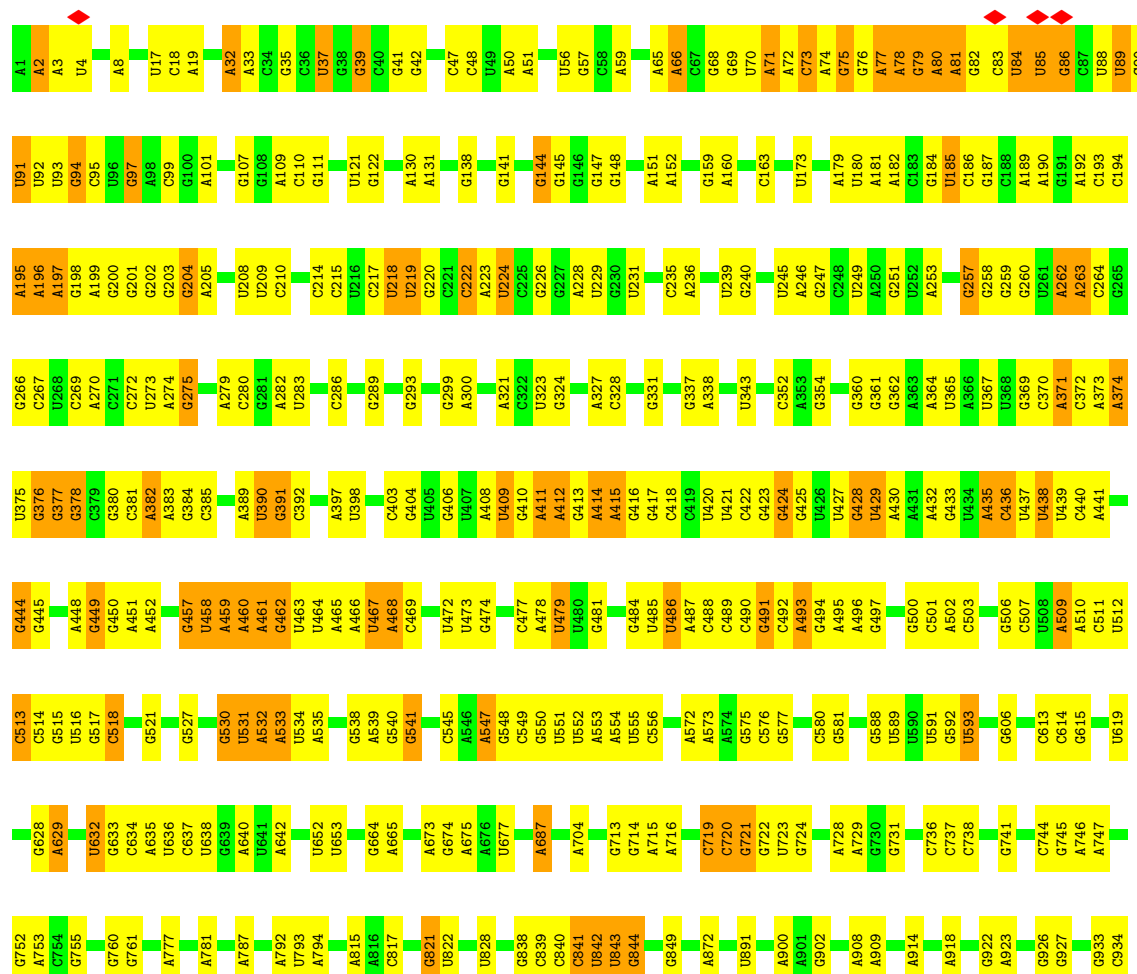
- Molecule 8: 50S ribosomal protein L36

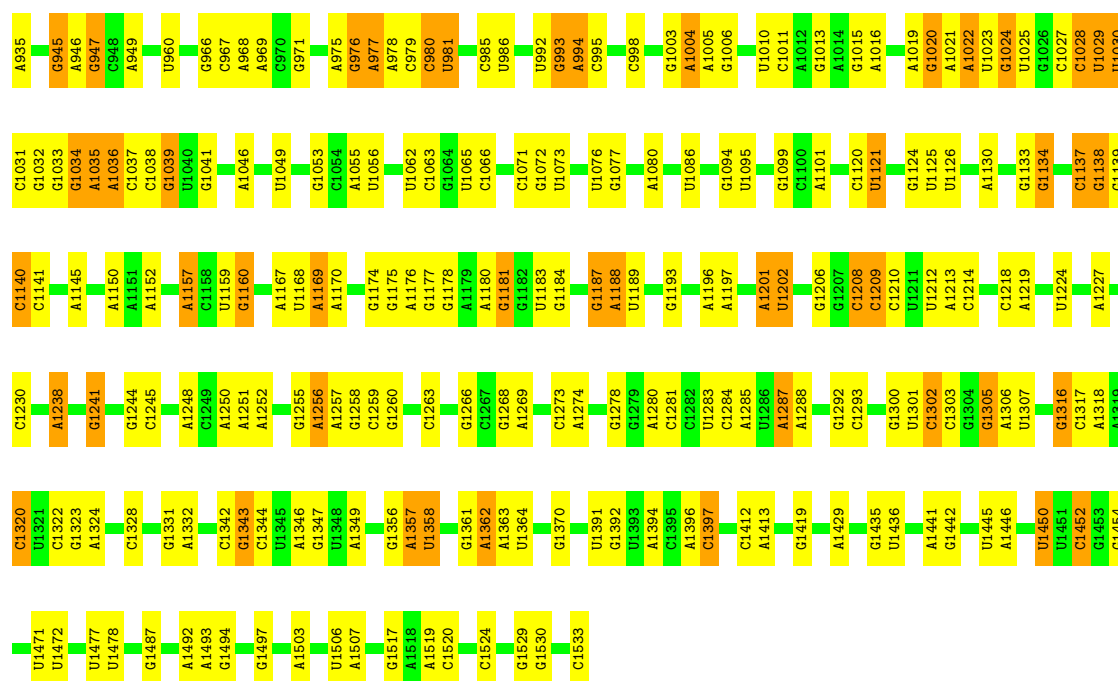
Chain 8:  92%



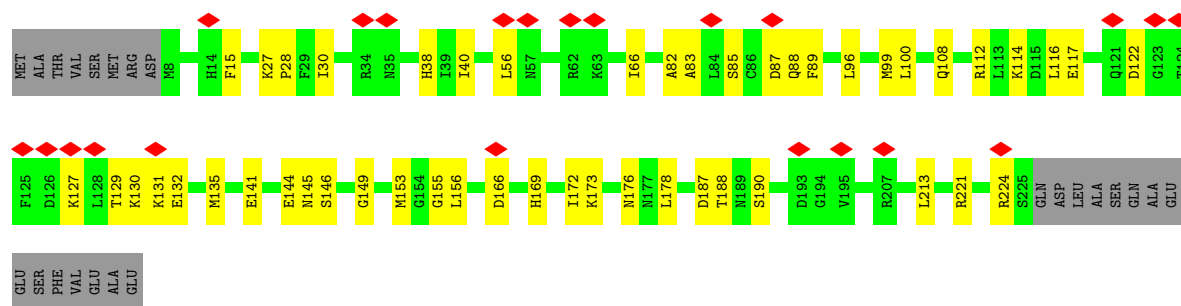
- Molecule 9: 16S ribosomal RNA

Chain A:  59%

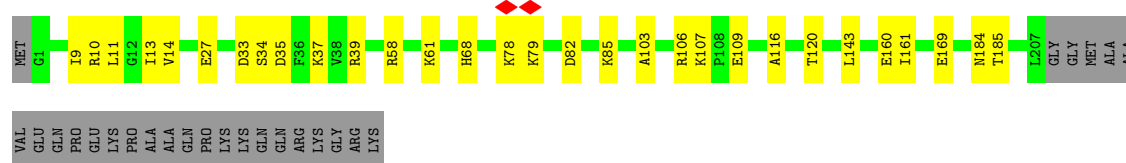
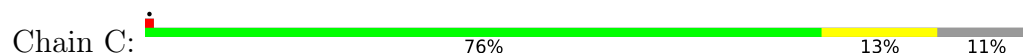




• Molecule 10: 30S ribosomal protein S2

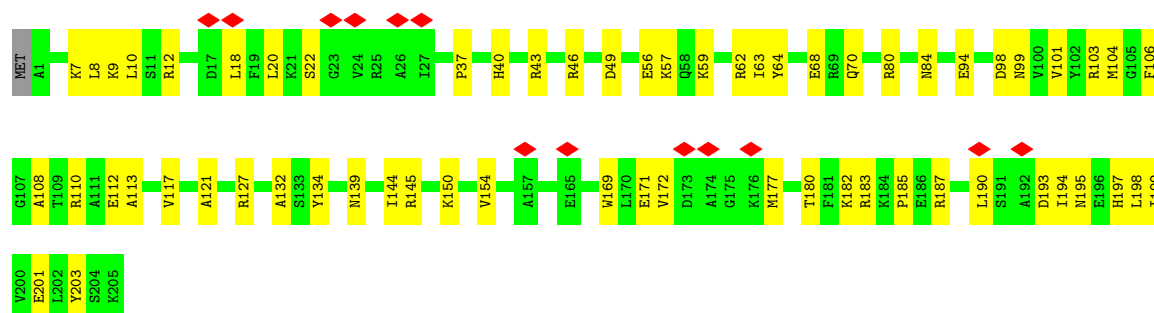


• Molecule 11: 30S ribosomal protein S3

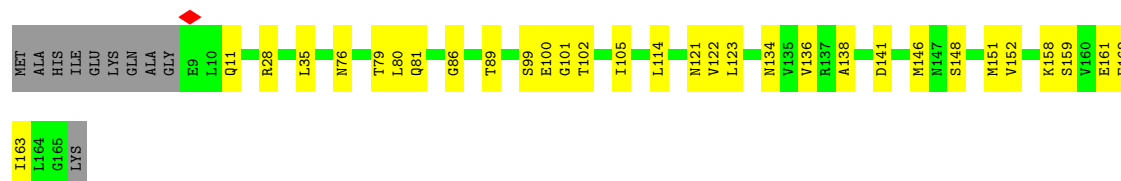
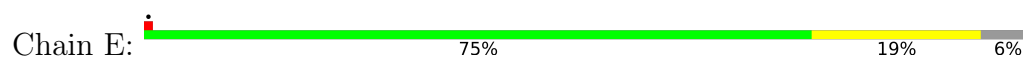


• Molecule 12: 30S ribosomal protein S4

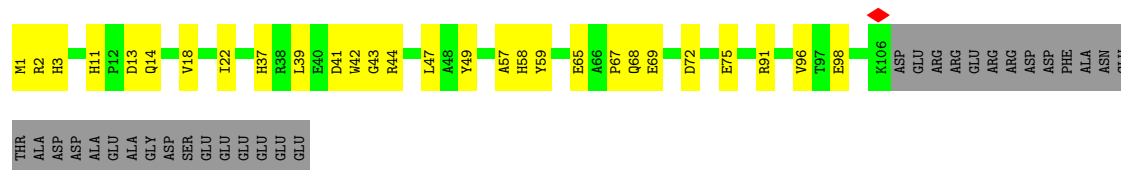




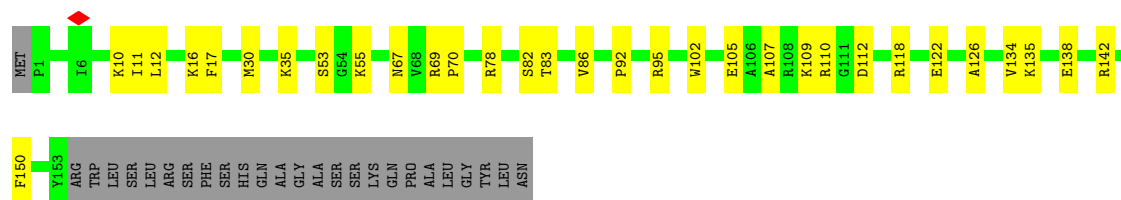
- Molecule 13: 30S ribosomal protein S5



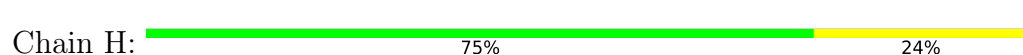
- Molecule 14: 30S ribosomal protein S6, fully modified isoform



- Molecule 15: 30S ribosomal protein S7

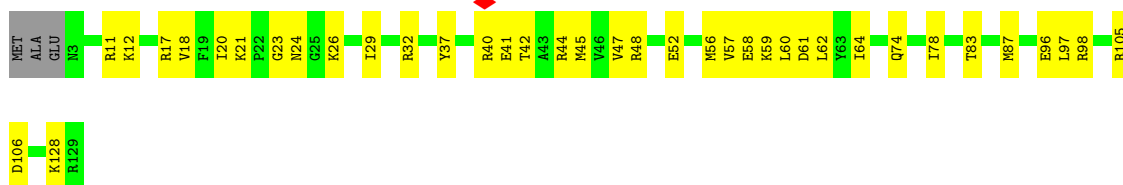


- Molecule 16: 30S ribosomal protein S8



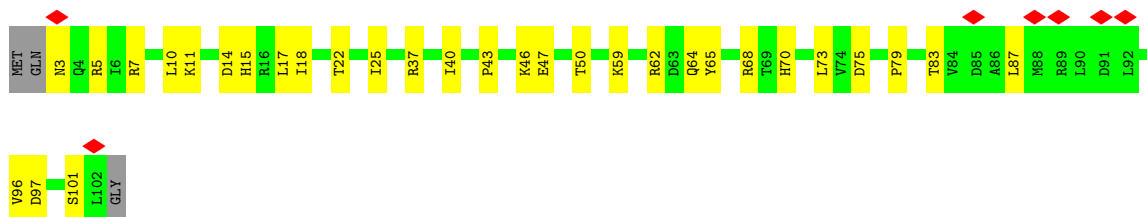
- Molecule 17: 30S ribosomal protein S9

Chain I:  68% 29% .



- Molecule 18: 30S ribosomal protein S10

Chain J:  7% 67% 30% .



- Molecule 19: Small ribosomal subunit protein uS11

Chain K:  76% 15% 9%



- Molecule 20: Small ribosomal subunit protein uS12

Chain L:  70% 28% .



- Molecule 21: 30S ribosomal protein S13

Chain M:  78% 20% .



- Molecule 22: 30S ribosomal protein S14

Chain N:  82% 17% .



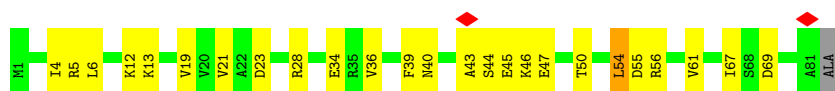
- Molecule 23: 30S ribosomal protein S15

Chain O: 83% 16%



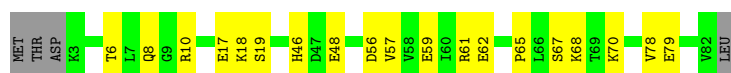
- Molecule 24: 30S ribosomal protein S16

Chain P: 68% 29%



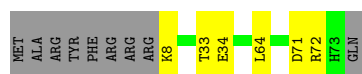
- Molecule 25: 30S ribosomal protein S17

Chain Q: 73% 23% 5%



- Molecule 26: 30S ribosomal protein S18

Chain R: 80% 8% 12%



- Molecule 27: 30S ribosomal protein S19

Chain S: 61% 29% 10%



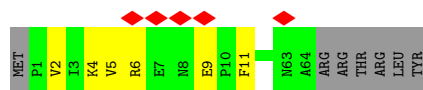
- Molecule 28: 30S ribosomal protein S20

Chain T: 78% 21%



- Molecule 29: 30S ribosomal protein S21

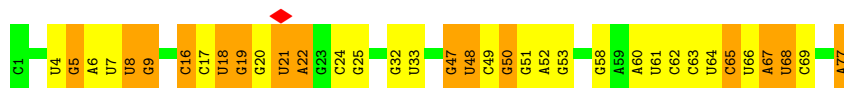
Chain U: 7% 82% 8% 10%



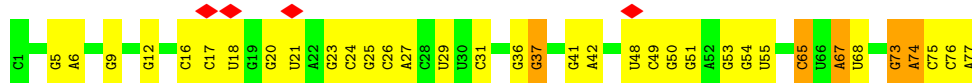
- Molecule 30: E-site tRNA



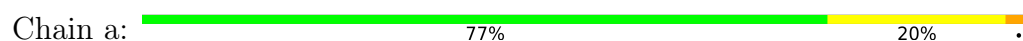
- Molecule 31: A-tRNA(PRO),P-tRNA(PRO)



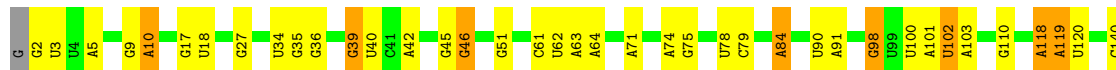
- Molecule 31: A-tRNA(PRO),P-tRNA(PRO)



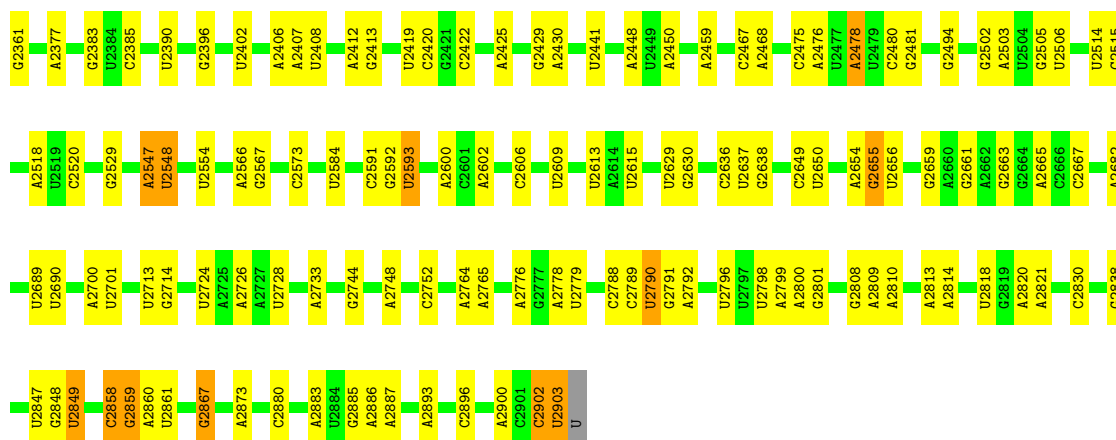
- Molecule 32: 5S rRNA



- Molecule 33: 23S ribosomal RNA







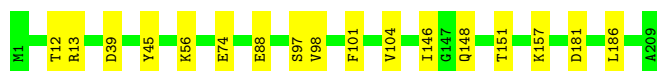
• Molecule 34: Large ribosomal subunit protein uL2

Chain c: 94% 5% .



• Molecule 35: 50S ribosomal protein L3

Chain d: 92% 8%



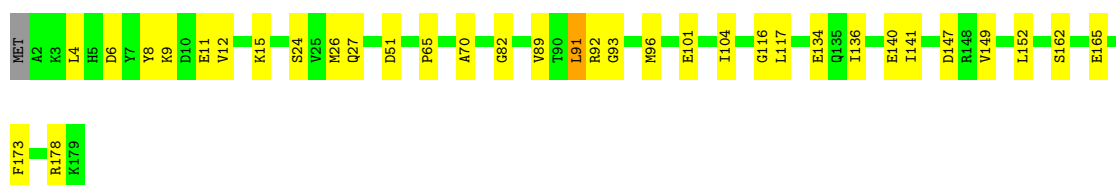
• Molecule 36: 50S ribosomal protein L4

Chain e: 88% 12%



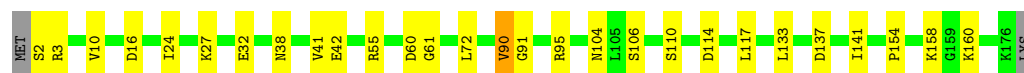
• Molecule 37: Large ribosomal subunit protein uL5

Chain f: 80% 18% ..

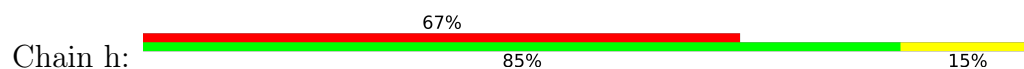


• Molecule 38: Large ribosomal subunit protein uL6

Chain g: 83% 15% ..



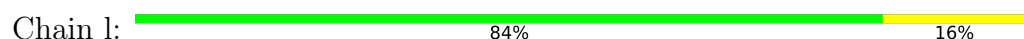
- Molecule 39: 50S ribosomal protein L9



- Molecule 40: 50S ribosomal protein L13



- Molecule 41: 50S ribosomal protein L14



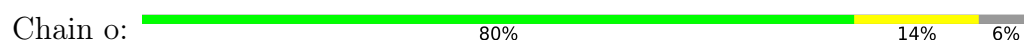
- Molecule 42: 50S ribosomal protein L15



- Molecule 43: 50S ribosomal protein L16

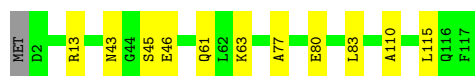


- Molecule 44: Large ribosomal subunit protein bL17



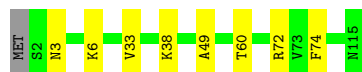
- Molecule 45: Large ribosomal subunit protein uL18

Chain p:  90% 9%

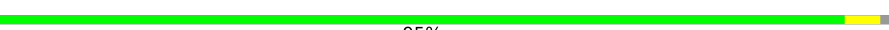


- Molecule 46: Large ribosomal subunit protein bL19

Chain q:  92% 7%



- Molecule 47: Large ribosomal subunit protein bL20

Chain r:  95%



- Molecule 48: 50S ribosomal protein L21

Chain s:  83% 17%



- Molecule 49: 50S ribosomal protein L22

Chain t:  92% 8%



- Molecule 50: Large ribosomal subunit protein uL23

Chain u:  86% 14%



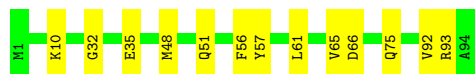
- Molecule 51: 50S ribosomal protein L24

Chain v:  84% 15%



- Molecule 52: 50S ribosomal protein L25

Chain w:  86% 14%



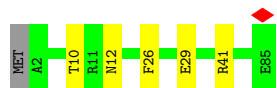
- Molecule 53: mRNA

Chain x:  7% 71% 14% 14%



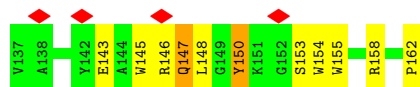
- Molecule 54: Large ribosomal subunit protein bL27

Chain y:  93% 6%



- Molecule 55: eRAP-NC

Chain z:  15% 58% 35% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107133	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.917	Depositor
Minimum map value	-0.648	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	682.0, 682.0, 682.0	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0	0.29	0/635	0.26	0/848
2	1	0.24	0/496	0.28	0/660
3	2	0.27	0/453	0.28	0/605
4	4	0.31	0/450	0.35	0/599
5	5	0.22	0/433	0.29	0/576
6	6	0.32	0/380	0.45	0/498
7	7	0.31	0/513	0.36	0/676
8	8	0.31	0/303	0.27	0/397
9	A	0.27	0/36834	0.31	0/57462
10	B	0.16	0/1735	0.32	0/2338
11	C	0.20	0/1659	0.31	0/2236
12	D	0.16	0/1665	0.34	0/2227
13	E	0.23	0/1169	0.36	0/1573
14	F	0.21	0/881	0.35	0/1189
15	G	0.19	0/1219	0.30	0/1635
16	H	0.26	0/989	0.32	0/1326
17	I	0.20	0/1034	0.35	0/1375
18	J	0.19	0/813	0.38	0/1100
19	K	0.23	0/893	0.30	0/1205
20	L	0.19	0/963	0.33	0/1293
21	M	0.19	0/909	0.30	0/1215
22	N	0.20	0/817	0.31	0/1088
23	O	0.22	0/722	0.29	0/964
24	P	0.21	0/653	0.31	0/877
25	Q	0.20	0/657	0.30	0/881
26	R	0.23	0/553	0.30	0/742
27	S	0.18	0/680	0.32	0/915
28	T	0.21	0/676	0.31	0/895
29	U	0.15	0/536	0.30	0/711
30	X	0.18	0/1810	0.30	0/2820
31	Y	0.27	0/1839	0.36	0/2866
31	Z	0.18	0/1839	0.29	0/2866

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	a	0.29	0/2872	0.30	0/4478
33	b	0.36	0/69773	0.35	0/108851
34	c	0.31	0/2121	0.33	0/2852
35	d	0.31	0/1586	0.36	0/2134
36	e	0.29	0/1571	0.30	0/2113
37	f	0.23	0/1443	0.31	0/1937
38	g	0.21	0/1333	0.28	0/1805
39	h	0.14	0/1119	0.28	0/1512
40	k	0.31	0/1152	0.31	0/1551
41	l	0.29	0/955	0.37	0/1279
42	m	0.29	0/1062	0.36	0/1413
43	n	0.27	0/1093	0.33	0/1460
44	o	0.31	0/973	0.38	0/1301
45	p	0.24	0/902	0.31	0/1209
46	q	0.29	0/929	0.28	0/1242
47	r	0.35	0/960	0.37	0/1278
48	s	0.30	0/829	0.38	0/1107
49	t	0.30	0/864	0.32	0/1156
50	u	0.28	0/793	0.34	0/1060
51	v	0.27	0/792	0.33	0/1057
52	w	0.25	0/766	0.29	0/1025
53	x	0.23	0/333	0.28	0/517
54	y	0.30	0/642	0.30	0/848
55	z	0.20	0/321	0.43	0/442
All	All	0.31	0/160392	0.33	0/240285

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	0	625	0	652	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	495	0	526	8	0
3	2	449	0	488	1	0
4	4	444	0	458	6	0
5	5	426	0	464	6	0
6	6	377	0	418	0	0
7	7	504	0	572	2	0
8	8	302	0	340	2	0
9	A	32895	0	16552	367	0
10	B	1704	0	1732	31	0
11	C	1632	0	1710	22	0
12	D	1643	0	1708	59	0
13	E	1156	0	1199	22	0
14	F	862	0	864	18	0
15	G	1203	0	1256	19	0
16	H	979	0	1034	22	0
17	I	1022	0	1070	30	0
18	J	803	0	842	24	0
19	K	877	0	887	15	0
20	L	949	0	1014	29	0
21	M	900	0	968	18	0
22	N	805	0	847	15	0
23	O	714	0	737	12	0
24	P	643	0	661	19	0
25	Q	648	0	691	15	0
26	R	544	0	565	6	0
27	S	663	0	690	18	0
28	T	670	0	722	15	0
29	U	529	0	565	6	0
30	X	1621	0	820	41	0
31	Y	1646	0	832	30	0
31	Z	1646	0	832	22	0
32	a	2569	0	1301	10	0
33	b	62297	0	31333	426	0
34	c	2082	0	2154	9	0
35	d	1565	0	1616	15	0
36	e	1552	0	1619	19	0
37	f	1419	0	1457	21	0
38	g	1313	0	1358	18	0
39	h	1108	0	1148	12	0
40	k	1129	0	1162	6	0
41	l	946	0	1023	14	0
42	m	1053	0	1129	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	n	1074	0	1157	9	0
44	o	960	0	1000	12	0
45	p	892	0	923	7	0
46	q	917	0	962	6	0
47	r	947	0	1019	4	0
48	s	816	0	839	13	0
49	t	857	0	922	5	0
50	u	786	0	846	11	0
51	v	784	0	838	11	0
52	w	753	0	780	8	0
53	x	299	0	154	3	0
54	y	634	0	653	3	0
55	z	303	0	280	11	0
56	8	1	0	0	0	0
57	Z	7	0	7	3	0
All	All	147439	0	98396	1461	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 (1461) 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)
31:Z:77:A:HO3'	57:Z:101:PRO:C	1.53	1.15
31:Z:77:A:O3'	57:Z:101:PRO:C	1.89	1.15
31:Y:77:A:O3'	55:z:162:PRO:C	1.90	1.13
12:D:187:ARG:HH22	12:D:190:LEU:HD13	1.35	0.92
33:b:1352:U:HO2'	33:b:1570:A:H8	1.13	0.91
33:b:2141:G:N2	33:b:2150:C:O2	2.05	0.90
33:b:2189:U:H2'	33:b:2190:G:H8	1.36	0.89
33:b:674:G:H1'	36:e:69:ARG:HH12	1.38	0.87
33:b:2185:U:H2'	33:b:2186:G:H8	1.41	0.85
33:b:2141:G:N1	33:b:2150:C:N3	2.25	0.85
38:g:42:GLU:HB3	38:g:55:ARG:HE	1.42	0.83
33:b:1482:G:N1	33:b:1507:C:O2	2.11	0.83
33:b:1428:C:H42	33:b:1570:A:H2	1.28	0.81
9:A:1397:C:OP2	13:E:28:ARG:NH2	2.14	0.80
33:b:2345:G:H4'	33:b:2346:A:H5'	1.64	0.80
9:A:415:A:N6	9:A:428:G:O6	2.15	0.80
9:A:110:C:H3'	9:A:111:G:H21	1.46	0.79
9:A:263:A:OP2	28:T:73:ARG:NH1	2.17	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:1439:A:H62	33:b:1552:A:H8	1.32	0.77
9:A:464:U:O2	9:A:466:A:N7	2.18	0.77
16:H:17:GLN:HE21	16:H:71:VAL:HG12	1.50	0.76
21:M:65:GLU:HG2	21:M:67:ASP:H	1.49	0.76
33:b:27:G:N2	33:b:512:G:O2'	2.18	0.76
9:A:199:A:H61	9:A:217:C:H42	1.32	0.76
9:A:76:G:H22	9:A:92:U:H3	1.34	0.75
31:Y:77:A:O3'	55:z:162:PRO:O	2.04	0.75
33:b:713:G:H21	33:b:718:A:H2	1.33	0.75
9:A:673:A:H2'	9:A:674:G:C8	2.22	0.75
9:A:460:A:N7	9:A:474:G:N2	2.33	0.74
17:I:45:MET:SD	17:I:45:MET:N	2.60	0.74
11:C:78:LYS:HD2	11:C:79:LYS:HG2	1.70	0.74
33:b:1315:C:HO2'	33:b:1392:A:H8	1.33	0.74
24:P:12:LYS:HG2	24:P:13:LYS:HG2	1.71	0.73
33:b:1060:U:H3	33:b:1088:A:H8	1.34	0.73
9:A:458:U:O2	9:A:459:A:N6	2.21	0.73
33:b:878:A:H3'	33:b:879:G:H8	1.54	0.73
10:B:96:LEU:H	10:B:99:MET:HE3	1.54	0.73
13:E:76:ASN:N	13:E:79:THR:O	2.22	0.73
31:Y:9:G:OP1	31:Y:47:G:N2	2.19	0.73
33:b:1854:A:H62	33:b:1888:G:H8	1.37	0.72
11:C:13:ILE:HG22	11:C:14:VAL:HG13	1.70	0.72
41:l:77:ILE:HG13	46:q:72:ARG:HG3	1.71	0.72
23:O:88:ARG:NE	33:b:713:G:OP2	2.22	0.72
33:b:1056:G:O2'	33:b:1086:A:O2'	2.07	0.71
27:S:31:ARG:HH22	27:S:51:HIS:HB2	1.56	0.71
28:T:65:LEU:HD12	28:T:66:ILE:HG12	1.73	0.71
16:H:95:MET:HE3	16:H:129:ALA:HB1	1.73	0.71
31:Y:8:U:O2'	31:Y:22:A:N1	2.20	0.71
30:X:19:G:N3	30:X:57:G:N2	2.39	0.71
9:A:107:G:N7	28:T:9:ARG:NH2	2.37	0.70
9:A:1126:U:OP1	18:J:5:ARG:NH1	2.25	0.70
9:A:376:G:O6	9:A:390:U:C4	2.44	0.70
9:A:438:U:O2'	9:A:493:A:N6	2.25	0.70
33:b:1453:A:N6	44:o:74:GLU:OE2	2.23	0.70
33:b:952:G:H21	33:b:2267:A:H2	1.40	0.70
9:A:1178:G:N2	9:A:1181:G:OP2	2.25	0.69
35:d:12:THR:HG22	35:d:13:ARG:H	1.57	0.69
17:I:105:ARG:NH1	17:I:106:ASP:O	2.24	0.69
37:f:11:GLU:O	37:f:15:LYS:NZ	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:376:G:C6	9:A:390:U:N3	2.60	0.69
32:a:44:G:H21	32:a:47:C:H5	1.41	0.69
28:T:14:GLU:HA	28:T:17:ARG:HG2	1.73	0.69
28:T:43:LYS:HB3	28:T:86:ALA:HA	1.75	0.69
33:b:877:A:O2'	33:b:900:A:N6	2.26	0.69
33:b:1106:G:H2'	33:b:1107:G:C8	2.29	0.68
9:A:1021:A:H2'	9:A:1022:A:C8	2.28	0.68
33:b:284:U:H3	33:b:356:G:H1	1.41	0.68
9:A:501:C:H2'	9:A:502:A:H8	1.59	0.68
33:b:2136:G:N7	33:b:2153:C:N4	2.42	0.68
22:N:53:ASP:OD1	22:N:58:ARG:NH1	2.27	0.68
9:A:412:A:N6	9:A:414:A:O3'	2.26	0.68
22:N:85:GLU:OE1	22:N:89:ARG:NH2	2.26	0.68
27:S:28:LYS:NZ	27:S:29:PRO:O	2.27	0.68
33:b:1509:A:O2'	33:b:1510:G:O4'	2.11	0.68
33:b:2202:U:O2'	33:b:2204:G:OP1	2.11	0.68
16:H:40:LYS:NZ	16:H:46:GLU:O	2.26	0.68
17:I:87:MET:HE3	17:I:97:LEU:HD12	1.76	0.67
33:b:1071:G:N1	33:b:1091:G:OP2	2.27	0.67
30:X:30:C:H42	30:X:39:G:H1	1.43	0.67
12:D:139:ASN:H	12:D:182:LYS:HA	1.59	0.67
32:a:51:G:OP1	45:p:63:LYS:NZ	2.27	0.67
33:b:1858:A:N6	33:b:1884:G:O2'	2.28	0.67
31:Y:77:A:C3'	55:z:162:PRO:O	2.42	0.67
9:A:187:G:N2	9:A:190:A:OP2	2.28	0.67
13:E:80:LEU:HG	13:E:81:GLN:H	1.60	0.67
9:A:416:G:H1	9:A:427:U:H3	1.42	0.67
30:X:36:C:H5	53:x:12:G:H1	1.43	0.67
9:A:71:A:N6	9:A:99:C:O2'	2.28	0.67
33:b:79:C:HO2'	33:b:346:A:H8	1.43	0.67
37:f:6:ASP:HA	37:f:9:LYS:HG2	1.76	0.66
33:b:247:G:N2	33:b:250:G:O2'	2.28	0.66
29:U:5:VAL:HG13	29:U:9:GLU:HB2	1.76	0.66
33:b:884:U:O4	33:b:886:A:N6	2.27	0.66
34:c:133:ARG:NH2	34:c:187:ASP:OD1	2.29	0.66
27:S:31:ARG:NH1	27:S:32:THR:O	2.28	0.66
13:E:105:ILE:HD11	13:E:123:LEU:HD23	1.77	0.66
33:b:1753:G:N2	33:b:1756:G:OP2	2.24	0.66
33:b:2183:A:H2'	33:b:2184:A:C4	2.31	0.66
9:A:1035:A:H5''	9:A:1036:A:C8	2.31	0.66
33:b:2055:C:O2'	33:b:2056:G:OP2	2.14	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:380:G:N2	9:A:383:A:OP2	2.25	0.65
9:A:262:A:O2'	9:A:263:A:OP1	2.15	0.65
22:N:35:ALA:HB3	22:N:40:ARG:HH21	1.61	0.65
9:A:477:C:N3	9:A:478:A:N6	2.45	0.65
20:L:106:VAL:HG21	20:L:116:TYR:HD2	1.62	0.65
33:b:2189:U:H2'	33:b:2190:G:C8	2.26	0.65
12:D:121:ALA:HA	12:D:145:ARG:HD3	1.78	0.65
31:Y:47:G:H4'	31:Y:48:U:H5	1.60	0.65
33:b:1870:C:O2'	33:b:1871:A:O4'	2.15	0.65
9:A:500:G:H2'	9:A:501:C:C6	2.32	0.65
12:D:194:ILE:HG22	12:D:197:HIS:HE1	1.62	0.65
31:Y:66:U:O2	31:Y:67:A:N6	2.30	0.65
19:K:92:ARG:NH2	19:K:111:ASP:OD2	2.29	0.65
24:P:45:GLU:OE1	24:P:46:LYS:NZ	2.30	0.65
33:b:1315:C:O2'	33:b:1392:A:H8	1.79	0.65
33:b:2127:G:O2'	33:b:2128:G:O4'	2.11	0.65
9:A:501:C:OP1	20:L:113:ARG:NH2	2.29	0.64
9:A:41:G:H2'	9:A:42:G:H8	1.62	0.64
9:A:477:C:H2'	9:A:478:A:C8	2.32	0.64
15:G:10:LYS:NZ	15:G:11:ILE:O	2.29	0.64
16:H:76:ARG:HE	16:H:79:ARG:HA	1.62	0.64
33:b:2114:A:N6	33:b:2119:A:N7	2.45	0.64
5:5:30:LYS:NZ	33:b:2287:A:OP1	2.30	0.64
23:O:73:ASP:OD2	23:O:76:ARG:NE	2.30	0.64
10:B:127:LYS:HZ3	10:B:129:THR:HB	1.61	0.64
12:D:94:GLU:HG2	12:D:185:PRO:HG3	1.79	0.64
35:d:88:GLU:OE1	35:d:88:GLU:N	2.29	0.64
9:A:380:G:O2'	9:A:382:A:N6	2.25	0.64
24:P:5:ARG:NH2	24:P:23:ASP:O	2.31	0.64
32:a:1:U:H2'	32:a:2:G:H8	1.63	0.64
33:b:845:A:H62	33:b:932:U:H3	1.45	0.64
43:n:58:LYS:O	43:n:60:GLN:NE2	2.29	0.64
9:A:376:G:C6	9:A:390:U:C4	2.86	0.64
9:A:384:G:H2'	9:A:385:C:C6	2.32	0.64
33:b:1095:A:OP2	33:b:1098:A:N6	2.31	0.64
34:c:146:MET:HE3	34:c:154:LEU:HD21	1.79	0.64
9:A:449:G:H2'	9:A:450:G:C8	2.34	0.63
9:A:628:G:H2'	9:A:629:A:C8	2.33	0.63
9:A:1125:U:OP1	18:J:37:ARG:NH1	2.31	0.63
30:X:15:G:H22	30:X:48:C:H42	1.46	0.63
31:Y:5:G:O6	31:Y:68:U:O4	2.15	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:142:ARG:NH2	30:X:41:U:O5'	2.32	0.63
33:b:1417:C:HO2'	33:b:1587:G:HO2'	1.44	0.63
33:b:1509:A:O2'	33:b:1510:G:O5'	2.13	0.63
33:b:483:A:O2'	51:v:56:GLY:O	2.17	0.63
16:H:21:LYS:O	16:H:64:TYR:OH	2.16	0.63
16:H:52:GLY:HA2	16:H:56:PRO:HA	1.80	0.63
33:b:2790:U:H2'	33:b:2893:A:N7	2.14	0.63
17:I:20:ILE:HD11	17:I:60:LEU:HD12	1.80	0.63
20:L:72:ASN:HD21	20:L:104:SER:HB2	1.63	0.63
9:A:371:A:N1	9:A:389:A:N6	2.45	0.62
9:A:753:A:OP1	23:O:72:LYS:NZ	2.32	0.62
33:b:886:A:N1	33:b:892:A:N6	2.46	0.62
19:K:80:ASN:OD1	19:K:105:ARG:NH1	2.31	0.62
9:A:449:G:O6	9:A:486:U:O4	2.16	0.62
14:F:37:HIS:ND1	14:F:98:GLU:OE2	2.31	0.62
28:T:27:MET:HE1	28:T:66:ILE:HG13	1.79	0.62
9:A:70:U:O2'	9:A:94:G:N2	2.32	0.62
44:o:119:SER:OG	44:o:120:GLU:OE1	2.17	0.62
9:A:445:G:H22	9:A:489:C:H42	1.45	0.62
9:A:509:A:OP2	12:D:46:ARG:NH2	2.20	0.62
13:E:86:GLY:HA3	13:E:141:ASP:HB3	1.82	0.62
18:J:10:LEU:HB3	18:J:18:ILE:HD11	1.82	0.62
33:b:345:A:H1'	33:b:346:A:H2	1.63	0.62
15:G:30:MET:HE2	15:G:35:LYS:HG3	1.82	0.62
33:b:1713:A:H61	33:b:1745:A:N6	1.97	0.62
20:L:34:THR:HG22	20:L:35:ARG:HG3	1.81	0.62
33:b:370:G:O2'	33:b:424:G:OP1	2.18	0.62
12:D:187:ARG:NH2	12:D:190:LEU:HD13	2.12	0.62
5:5:25:LYS:NZ	5:5:32:GLU:O	2.25	0.62
9:A:714:G:H2'	9:A:715:A:C8	2.35	0.62
39:h:132:PHE:HB2	39:h:140:ALA:HB3	1.80	0.62
12:D:99:ASN:OD1	12:D:110:ARG:NH2	2.32	0.62
31:Z:5:G:H2'	31:Z:6:A:H8	1.65	0.61
11:C:109:GLU:HB2	11:C:143:LEU:HD22	1.82	0.61
33:b:1064:C:N4	33:b:1072:C:OP1	2.33	0.61
33:b:2135:A:H5''	33:b:2136:G:C5	2.35	0.61
33:b:974:G:H8	33:b:990:A:H62	1.48	0.61
33:b:1060:U:H4'	33:b:1061:U:H5'	1.80	0.61
33:b:2174:C:H2'	33:b:2175:C:C6	2.34	0.61
30:X:46:G:O2'	30:X:47:U:O4'	2.18	0.61
33:b:1538:G:O2'	33:b:1539:U:O4'	2.14	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:106:VAL:HB	20:L:116:TYR:HB3	1.83	0.61
9:A:976:G:N2	9:A:1362:A:HO2'	1.98	0.61
31:Y:5:G:H1	31:Y:68:U:H3	1.49	0.61
9:A:249:U:O2	9:A:275:G:O6	2.19	0.61
34:c:145:GLU:HB2	34:c:188:CYS:HB3	1.82	0.61
50:u:54:GLU:N	50:u:54:GLU:OE1	2.34	0.60
9:A:429:U:OP1	12:D:8:LEU:HD22	2.01	0.60
33:b:1152:C:H5'	47:r:80:ILE:HD11	1.83	0.60
9:A:35:G:N3	20:L:114:SER:OG	2.33	0.60
12:D:144:ILE:HG21	12:D:177:MET:HE2	1.82	0.60
30:X:42:C:N4	30:X:43:G:O6	2.35	0.60
33:b:1062:G:O2'	33:b:1063:G:O4'	2.16	0.60
9:A:1077:G:N2	9:A:1080:A:OP2	2.31	0.60
23:O:25:GLU:OE2	23:O:76:ARG:NH1	2.34	0.60
33:b:1057:A:N6	33:b:1087:G:O2'	2.28	0.60
4:4:54:VAL:HG12	4:4:55:ILE:H	1.66	0.60
9:A:2:A:O2'	9:A:3:A:O4'	2.10	0.60
33:b:1352:U:O2'	33:b:1570:A:H8	1.80	0.60
38:g:16:ASP:HB3	38:g:27:LYS:HB2	1.83	0.60
9:A:1306:A:N6	9:A:1331:G:O2'	2.34	0.60
36:e:143:LEU:HD13	36:e:146:VAL:HG11	1.82	0.60
13:E:114:LEU:HD13	13:E:122:VAL:HG11	1.83	0.60
9:A:1357:A:O2'	9:A:1358:U:OP1	2.19	0.60
27:S:28:LYS:HD2	27:S:29:PRO:HD2	1.83	0.60
33:b:2164:C:H4'	33:b:2165:C:H5'	1.84	0.60
9:A:677:U:H3	9:A:713:G:H22	1.50	0.60
9:A:1028:C:N4	9:A:1029:U:O2	2.34	0.60
33:b:2180:U:H2'	33:b:2181:U:C6	2.37	0.60
37:f:134:GLU:N	37:f:134:GLU:OE1	2.35	0.60
11:C:68:HIS:HA	11:C:103:ALA:HB3	1.83	0.60
30:X:63:C:H2'	30:X:64:G:H8	1.66	0.60
33:b:1483:G:H1	33:b:1506:U:H3	1.49	0.60
33:b:2177:C:H2'	33:b:2178:C:C6	2.37	0.60
9:A:478:A:H2'	9:A:479:U:H4'	1.82	0.59
9:A:512:U:OP1	12:D:43:ARG:NH1	2.35	0.59
17:I:62:LEU:O	17:I:64:ILE:HG12	2.02	0.59
33:b:627:A:OP1	42:m:78:ARG:NH1	2.32	0.59
9:A:337:G:H2'	9:A:338:A:C8	2.36	0.59
9:A:628:G:H2'	9:A:629:A:H8	1.66	0.59
9:A:640:A:O2'	16:H:107:LYS:NZ	2.34	0.59
30:X:49:G:H1	30:X:65:U:H3	1.49	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:1055:G:N2	33:b:1105:U:O2	2.35	0.59
54:y:26:PHE:N	54:y:29:GLU:OE1	2.28	0.59
9:A:501:C:H2'	9:A:502:A:C8	2.37	0.59
14:F:1:MET:HE3	14:F:2:ARG:H	1.67	0.59
14:F:22:ILE:HD13	14:F:39:LEU:HD21	1.84	0.59
33:b:597:G:O2'	42:m:11:GLY:O	2.15	0.59
44:o:32:GLU:HG2	44:o:115:LEU:HD12	1.84	0.59
8:8:2:LYS:NZ	33:b:2478:A:OP2	2.32	0.59
33:b:284:U:O2	33:b:356:G:N2	2.27	0.59
9:A:1150:A:H4'	18:J:43:PRO:HG3	1.83	0.59
11:C:106:ARG:HB3	11:C:107:LYS:HD2	1.85	0.59
9:A:201:G:H3'	9:A:202:G:C8	2.37	0.59
31:Y:24:C:H2'	31:Y:25:G:C8	2.38	0.59
33:b:2126:A:N6	33:b:2162:G:O4'	2.35	0.59
9:A:198:G:O6	9:A:219:U:O2	2.20	0.59
30:X:29:A:H2	30:X:42:C:C4	2.21	0.59
33:b:1080:A:H3'	33:b:1081:U:H4'	1.84	0.59
12:D:182:LYS:HG3	12:D:183:ARG:HG3	1.84	0.58
33:b:2100:G:H2'	33:b:2101:A:C8	2.38	0.58
9:A:946:A:H2'	9:A:947:G:H8	1.67	0.58
29:U:6:ARG:O	29:U:9:GLU:HG2	2.02	0.58
31:Y:77:A:H3'	55:z:162:PRO:O	2.04	0.58
33:b:546:U:H2'	33:b:547:A:C2	2.39	0.58
33:b:1021:A:H62	33:b:1141:U:H3	1.48	0.58
9:A:457:G:H22	9:A:474:G:H2'	1.69	0.58
9:A:1086:U:H3	9:A:1099:G:H22	1.51	0.58
12:D:187:ARG:O	12:D:187:ARG:NH1	2.37	0.58
9:A:202:G:O2'	9:A:468:A:OP1	2.21	0.58
9:A:370:C:H2'	9:A:371:A:H8	1.67	0.58
9:A:840:C:N4	9:A:842:U:O2	2.37	0.58
9:A:980:C:O2'	22:N:12:ARG:NH1	2.36	0.58
15:G:105:GLU:OE1	15:G:109:LYS:NZ	2.36	0.58
36:e:125:SER:HA	36:e:157:LEU:HD11	1.84	0.58
48:s:40:MET:HG3	48:s:48:LYS:HG2	1.85	0.58
9:A:946:A:H2'	9:A:947:G:C8	2.39	0.58
20:L:74:GLN:NE2	20:L:75:GLU:OE2	2.36	0.58
24:P:40:ASN:CG	24:P:43:ALA:HB2	2.28	0.58
33:b:2135:A:N6	33:b:2158:A:H4'	2.18	0.58
12:D:40:HIS:CE1	12:D:43:ARG:HH21	2.22	0.58
16:H:10:LEU:HG	16:H:74:ILE:HD11	1.85	0.58
33:b:2848:G:O2'	33:b:2849:U:O5'	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:459:A:H62	9:A:474:G:N2	2.01	0.58
12:D:94:GLU:CD	12:D:99:ASN:HD21	2.12	0.58
33:b:740:C:H5	33:b:757:G:H1	1.52	0.58
9:A:437:U:OP1	12:D:150:LYS:NZ	2.36	0.58
27:S:62:THR:OG1	27:S:64:GLU:OE2	2.22	0.58
33:b:1080:A:N7	33:b:1081:U:O2'	2.35	0.57
33:b:1802:A:H2'	33:b:1803:A:C8	2.39	0.57
2:1:19:LEU:HD12	2:1:23:ARG:HH21	1.68	0.57
16:H:87:ARG:N	16:H:90:GLU:OE2	2.38	0.57
30:X:15:G:N2	30:X:48:C:H42	2.01	0.57
33:b:286:U:H2'	33:b:287:G:H8	1.68	0.57
33:b:2147:A:H2'	33:b:2148:G:O4'	2.04	0.57
33:b:2858:C:O2'	33:b:2859:G:O5'	2.21	0.57
9:A:606:G:N2	9:A:632:U:OP1	2.36	0.57
11:C:160:GLU:HG2	11:C:161:ILE:H	1.68	0.57
13:E:102:THR:O	13:E:121:ASN:ND2	2.36	0.57
17:I:23:GLY:O	17:I:60:LEU:N	2.38	0.57
48:s:49:ILE:HD12	48:s:54:VAL:HA	1.86	0.57
52:w:32:GLY:O	52:w:93:ARG:NH1	2.38	0.57
14:F:11:HIS:ND1	14:F:13:ASP:OD1	2.36	0.57
28:T:73:ARG:O	28:T:77:ASN:ND2	2.22	0.57
13:E:80:LEU:HD23	13:E:146:MET:HG2	1.85	0.57
9:A:967:C:H5''	17:I:128:LYS:HD3	1.86	0.57
12:D:169:TRP:CE2	12:D:185:PRO:HB3	2.38	0.57
17:I:74:GLN:O	17:I:78:ILE:HG12	2.04	0.57
25:Q:17:GLU:CD	25:Q:17:GLU:H	2.13	0.57
36:e:122:GLU:OE1	36:e:122:GLU:N	2.30	0.57
1:0:65:ASP:OD1	1:0:65:ASP:N	2.36	0.57
9:A:337:G:H2'	9:A:338:A:H8	1.70	0.57
19:K:16:SER:HA	19:K:78:ILE:HA	1.86	0.57
31:Z:51:G:H22	31:Z:65:C:H5	1.53	0.57
33:b:1505:A:H2'	33:b:1506:U:C6	2.40	0.57
9:A:41:G:H2'	9:A:42:G:C8	2.39	0.57
33:b:886:A:O4'	33:b:890:C:N4	2.38	0.57
33:b:1051:G:H4'	33:b:1052:C:OP1	2.05	0.57
9:A:85:U:O4'	9:A:86:G:N2	2.38	0.57
18:J:47:GLU:N	18:J:47:GLU:OE1	2.38	0.57
42:m:10:GLU:OE1	42:m:10:GLU:N	2.35	0.57
42:m:123:ARG:NE	42:m:143:GLU:OE2	2.38	0.57
48:s:6:GLN:HB3	48:s:11:GLN:HG2	1.86	0.57
9:A:389:A:N3	9:A:390:U:H5''	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:30:ILE:HD11	10:B:38:HIS:HB3	1.86	0.56
33:b:2115:G:O2'	33:b:2166:U:O2	2.23	0.56
33:b:2328:A:H2'	33:b:2329:U:C6	2.40	0.56
37:f:136:ILE:HA	37:f:141:ILE:HD11	1.86	0.56
33:b:1649:G:O2'	44:o:106:ASP:OD2	2.21	0.56
33:b:2141:G:O6	33:b:2150:C:N4	2.38	0.56
9:A:664:G:H22	9:A:741:G:H1	1.53	0.56
9:A:746:A:H2'	9:A:747:A:C8	2.40	0.56
9:A:1356:G:H2'	9:A:1357:A:C8	2.40	0.56
24:P:19:VAL:HG23	24:P:36:VAL:HG23	1.86	0.56
24:P:61:VAL:HG22	24:P:67:ILE:HD11	1.88	0.56
30:X:14:A:H3'	30:X:15:G:H8	1.70	0.56
46:q:72:ARG:HD2	46:q:74:PHE:CZ	2.40	0.56
9:A:1301:U:O2'	9:A:1302:C:H5'	2.05	0.56
29:U:6:ARG:H	29:U:9:GLU:HG3	1.70	0.56
33:b:890:C:H2'	33:b:891:G:H4'	1.88	0.56
3:2:40:ASP:OD2	3:2:45:ARG:NH2	2.38	0.56
31:Z:73:G:H2'	31:Z:74:A:C8	2.40	0.56
33:b:287:G:H2'	33:b:288:U:C6	2.40	0.56
9:A:89:U:H2'	9:A:90:C:C6	2.39	0.56
9:A:1037:C:H2'	9:A:1038:C:C6	2.41	0.56
30:X:28:G:N1	30:X:29:A:N3	2.53	0.56
33:b:1871:A:H2'	33:b:1872:A:C8	2.41	0.56
33:b:1936:A:H2	33:b:1943:U:H5	1.54	0.56
37:f:65:PRO:HB3	37:f:89:VAL:HG23	1.87	0.56
38:g:104:ASN:ND2	38:g:114:ASP:OD1	2.37	0.56
9:A:1020:G:O6	9:A:1021:A:N6	2.39	0.56
32:a:45:A:O4'	37:f:92:ARG:NH1	2.38	0.56
33:b:285:G:N2	33:b:355:U:O2	2.39	0.56
33:b:286:U:H2'	33:b:287:G:C8	2.41	0.56
17:I:11:ARG:HG3	17:I:12:LYS:H	1.70	0.56
23:O:79:GLN:HE22	23:O:83:ARG:HD2	1.70	0.56
33:b:1086:A:H3'	33:b:1087:G:H2'	1.86	0.56
4:4:46:ASP:OD1	4:4:46:ASP:N	2.38	0.56
9:A:184:G:H4'	9:A:224:U:H4'	1.88	0.56
13:E:138:ALA:HA	13:E:141:ASP:HB2	1.88	0.56
52:w:51:GLN:OE1	52:w:57:TYR:OH	2.22	0.56
33:b:1486:U:H2'	33:b:1487:U:O2	2.05	0.56
31:Y:50:G:N2	31:Y:67:A:N7	2.54	0.55
32:a:1:U:H2'	32:a:2:G:C8	2.40	0.55
37:f:116:GLY:HA3	37:f:178:ARG:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1450:U:H3'	9:A:1452:C:H41	1.69	0.55
30:X:6:A:H62	30:X:66:U:H3	1.54	0.55
31:Y:67:A:C2	31:Y:68:U:H1'	2.40	0.55
33:b:705:A:N6	33:b:726:G:H1'	2.21	0.55
33:b:2135:A:H2'	33:b:2156:G:N2	2.21	0.55
33:b:2155:U:H2'	33:b:2156:G:C4	2.41	0.55
34:c:185:GLU:HG3	34:c:187:ASP:H	1.70	0.55
43:n:57:VAL:O	43:n:59:ARG:N	2.38	0.55
9:A:195:A:O2'	9:A:196:A:O5'	2.23	0.55
14:F:44:ARG:HA	14:F:57:ALA:O	2.06	0.55
9:A:1015:G:H2'	9:A:1016:A:C8	2.41	0.55
9:A:193:C:H2'	9:A:194:C:C6	2.41	0.55
9:A:203:G:N2	9:A:465:A:H61	2.04	0.55
16:H:25:THR:OG1	16:H:57:GLU:OE2	2.22	0.55
25:Q:8:GLN:HE22	25:Q:78:VAL:HG21	1.72	0.55
37:f:24:SER:HB2	37:f:27:GLN:HB2	1.88	0.55
38:g:2:SER:OG	38:g:3:ARG:N	2.38	0.55
9:A:1412:C:H2'	9:A:1413:A:C8	2.42	0.55
17:I:96:GLU:N	17:I:96:GLU:OE1	2.39	0.55
31:Y:47:G:H4'	31:Y:48:U:C5	2.42	0.55
33:b:715:A:O2'	33:b:716:A:O4'	2.25	0.55
33:b:2187:U:H2'	33:b:2188:U:C4	2.41	0.55
9:A:417:G:N2	9:A:541:G:OP1	2.39	0.55
45:p:43:ASN:ND2	45:p:46:GLU:OE1	2.39	0.55
9:A:432:A:H2'	9:A:433:G:O4'	2.07	0.55
12:D:101:VAL:HG13	12:D:113:ALA:HB1	1.89	0.55
21:M:51:GLN:N	21:M:51:GLN:OE1	2.40	0.55
33:b:2178:C:H2'	33:b:2179:C:C6	2.41	0.55
41:l:17:ARG:HB2	41:l:45:GLU:HG3	1.89	0.54
9:A:370:C:H2'	9:A:371:A:C8	2.42	0.54
15:G:78:ARG:HG3	15:G:82:SER:O	2.07	0.54
9:A:1030:U:OP2	9:A:1031:C:N4	2.41	0.54
11:C:34:SER:OG	11:C:58:ARG:NH2	2.40	0.54
27:S:49:ALA:HA	27:S:58:PRO:HA	1.89	0.54
31:Y:19:G:O2'	31:Y:58:G:N2	2.39	0.54
33:b:1115:G:H2'	33:b:1116:G:H8	1.71	0.54
33:b:2902:C:N4	33:b:2903:U:O4	2.41	0.54
55:z:145:TRP:CZ2	55:z:147:GLN:HG2	2.43	0.54
9:A:949:A:OP2	21:M:104:ASN:ND2	2.39	0.54
9:A:1006:G:H1	9:A:1023:U:H2'	1.73	0.54
51:v:103:ILE:HG22	51:v:104:LYS:HG3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:2109:U:N3	33:b:2110:G:O6	2.39	0.54
38:g:38:ASN:O	38:g:41:VAL:HG12	2.07	0.54
10:B:127:LYS:HG2	10:B:129:THR:H	1.71	0.54
20:L:75:GLU:O	20:L:76:HIS:ND1	2.41	0.54
33:b:1057:A:H62	33:b:1087:G:HO2'	1.54	0.54
33:b:1058:U:H5'	33:b:1060:U:H5''	1.90	0.54
33:b:1172:C:P	33:b:1174:U:H3	2.30	0.54
33:b:1483:G:N2	33:b:1506:U:O2	2.40	0.54
9:A:462:G:H1	9:A:469:C:N4	2.04	0.54
9:A:1187:G:O2'	9:A:1188:A:OP1	2.25	0.54
26:R:33:THR:OG1	26:R:34:GLU:OE1	2.25	0.54
43:n:50:ARG:HG3	43:n:65:ILE:HD11	1.90	0.54
9:A:219:U:H2'	9:A:220:G:H8	1.73	0.54
9:A:222:C:H2'	9:A:223:A:H8	1.73	0.54
10:B:187:ASP:OD1	10:B:188:THR:N	2.32	0.54
15:G:112:ASP:O	15:G:118:ARG:NE	2.38	0.54
33:b:1381:G:H2'	33:b:1382:G:H5''	1.90	0.54
33:b:2130:U:H5'	33:b:2131:U:H5''	1.89	0.54
33:b:1055:G:N1	33:b:1105:U:C2	2.67	0.54
33:b:1085:A:O2'	33:b:1086:A:N3	2.41	0.54
50:u:54:GLU:HG3	50:u:88:LYS:HD2	1.88	0.54
9:A:35:G:O2'	20:L:114:SER:O	2.24	0.54
9:A:375:U:H4'	24:P:6:LEU:HD11	1.91	0.54
9:A:977:A:N6	9:A:1224:U:OP1	2.41	0.54
12:D:56:GLU:HG2	12:D:198:LEU:HD22	1.90	0.54
33:b:284:U:H2'	33:b:285:G:C8	2.43	0.54
9:A:449:G:O6	9:A:486:U:C4	2.61	0.53
33:b:310:A:O2'	33:b:311:A:H2'	2.07	0.53
41:l:65:THR:HG23	41:l:68:GLY:H	1.73	0.53
9:A:65:A:N7	9:A:381:C:N4	2.53	0.53
9:A:1187:G:N3	22:N:99:SER:OG	2.38	0.53
33:b:1103:A:H2'	33:b:1104:C:H5'	1.90	0.53
42:m:91:ASP:OD1	42:m:92:LEU:N	2.41	0.53
9:A:981:U:OP2	22:N:8:ARG:NH2	2.42	0.53
9:A:1201:A:H4'	9:A:1202:U:H5'	1.90	0.53
33:b:608:A:H2'	33:b:609:A:C8	2.44	0.53
33:b:2185:U:H2'	33:b:2186:G:C8	2.32	0.53
43:n:47:GLU:OE2	43:n:50:ARG:NH2	2.39	0.53
5:5:44:ARG:HD3	33:b:643:A:C6	2.43	0.53
9:A:459:A:H2'	9:A:460:A:O4'	2.09	0.53
15:G:86:VAL:HG12	15:G:150:PHE:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:13:GLU:OE2	23:O:83:ARG:NH2	2.34	0.53
31:Y:5:G:O6	31:Y:68:U:C4	2.62	0.53
39:h:68:ARG:HA	39:h:71:LYS:HE2	1.89	0.53
9:A:1323:G:H2'	9:A:1324:A:C8	2.44	0.53
15:G:107:ALA:HA	15:G:122:GLU:CD	2.34	0.53
19:K:112:VAL:HG12	26:R:72:ARG:HE	1.73	0.53
20:L:109:ARG:HH22	20:L:112:ALA:HB3	1.73	0.53
9:A:3:A:N3	9:A:613:C:H1'	2.24	0.53
33:b:1506:U:H2'	33:b:1507:C:C6	2.43	0.53
9:A:417:G:H2'	9:A:418:C:C6	2.43	0.53
9:A:1035:A:H5''	9:A:1036:A:H8	1.72	0.53
33:b:415:A:N1	33:b:2408:U:H5	2.06	0.53
33:b:2637:U:H2'	33:b:2638:G:O4'	2.08	0.53
9:A:197:A:N1	9:A:220:G:O2'	2.41	0.53
9:A:613:C:P	12:D:80:ARG:HH21	2.32	0.53
31:Y:22:A:N6	31:Y:47:G:H2'	2.23	0.53
33:b:79:C:O2'	33:b:346:A:H8	1.91	0.53
33:b:1064:C:O2'	33:b:1069:A:N7	2.41	0.53
33:b:2191:A:H2'	33:b:2192:U:C6	2.44	0.53
7:7:35:LYS:NZ	33:b:2390:U:OP2	2.42	0.53
31:Z:48:U:H4'	31:Z:49:C:H5'	1.91	0.53
33:b:1062:G:H22	33:b:1088:A:N6	2.06	0.53
9:A:1152:A:OP1	18:J:70:HIS:ND1	2.41	0.53
33:b:2160:C:H2'	33:b:2161:C:C6	2.44	0.53
9:A:553:A:H2'	9:A:554:A:H8	1.74	0.52
9:A:1071:C:H2'	9:A:1072:G:H8	1.73	0.52
9:A:1124:G:H4'	18:J:40:ILE:HD11	1.91	0.52
9:A:1305:G:N2	9:A:1332:A:OP2	2.41	0.52
19:K:36:ARG:NH1	19:K:82:GLU:OE2	2.43	0.52
9:A:1169:A:H3'	9:A:1170:A:H8	1.74	0.52
27:S:18:VAL:HG21	27:S:43:MET:HG3	1.91	0.52
33:b:639:U:H2'	33:b:640:C:C6	2.44	0.52
33:b:1068:G:H2'	33:b:1070:A:H62	1.74	0.52
9:A:68:G:H1	9:A:101:A:H61	1.57	0.52
33:b:1084:A:N3	33:b:1105:U:O2'	2.37	0.52
33:b:1862:G:H1	33:b:1880:U:H5	1.57	0.52
30:X:15:G:H22	30:X:48:C:N4	2.07	0.52
33:b:636:G:N1	42:m:76:GLU:OE2	2.30	0.52
33:b:856:G:H2'	33:b:857:G:C8	2.44	0.52
33:b:1490:A:H5''	33:b:1491:G:OP2	2.09	0.52
33:b:1744:A:H3'	33:b:1745:A:H5''	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:o:58:ASP:OD2	44:o:63:ARG:NH2	2.40	0.52
9:A:1006:G:O6	9:A:1023:U:C2	2.63	0.52
33:b:45:G:H5'	33:b:46:G:OP1	2.09	0.52
33:b:1141:U:H4'	33:b:1142:A:O4'	2.09	0.52
33:b:2591:C:H2'	33:b:2592:G:C8	2.44	0.52
9:A:424:G:H2'	9:A:425:G:H8	1.75	0.52
24:P:39:PHE:HD1	24:P:50:THR:HB	1.74	0.52
33:b:2151:U:N3	33:b:2152:G:O6	2.39	0.52
33:b:2192:U:H2'	33:b:2193:G:H8	1.75	0.52
40:k:31:GLU:HG2	40:k:142:ILE:HG22	1.92	0.52
9:A:81:A:O2'	9:A:82:G:O4'	2.20	0.52
21:M:45:SER:OG	21:M:46:GLU:OE1	2.28	0.52
33:b:1353:A:H2'	33:b:1354:A:C8	2.45	0.52
9:A:713:G:H2'	9:A:714:G:C8	2.44	0.52
12:D:18:LEU:H	12:D:18:LEU:HD23	1.74	0.52
12:D:98:ASP:N	12:D:98:ASP:OD1	2.41	0.52
33:b:887:U:O2	33:b:891:G:N2	2.43	0.52
10:B:156:LEU:HD11	10:B:178:LEU:HD13	1.91	0.52
31:Y:24:C:H2'	31:Y:25:G:H8	1.75	0.52
31:Z:5:G:H2'	31:Z:6:A:C8	2.44	0.52
33:b:2141:G:H2'	33:b:2142:A:C8	2.44	0.52
37:f:162:SER:OG	37:f:165:GLU:OE1	2.22	0.52
48:s:32:THR:HA	48:s:62:GLU:HA	1.92	0.52
9:A:77:A:N6	9:A:78:A:N3	2.58	0.51
21:M:62:PHE:HB3	21:M:64:VAL:HG23	1.92	0.51
30:X:30:C:N4	30:X:39:G:H1	2.08	0.51
44:o:120:GLU:OE1	44:o:120:GLU:N	2.43	0.51
4:4:38:HIS:ND1	4:4:39:LEU:O	2.41	0.51
9:A:253:A:O4'	9:A:275:G:N2	2.28	0.51
25:Q:61:ARG:NE	25:Q:62:GLU:O	2.36	0.51
37:f:91:LEU:HD13	37:f:96:MET:HA	1.92	0.51
41:l:19:VAL:HB	41:l:41:ILE:CG2	2.39	0.51
9:A:464:U:C2	9:A:466:A:N7	2.78	0.51
9:A:1133:G:H2'	9:A:1134:G:C8	2.46	0.51
33:b:877:A:N1	33:b:898:C:N4	2.58	0.51
33:b:2847:U:H2'	33:b:2848:G:O4'	2.10	0.51
9:A:674:G:H2'	9:A:675:A:H8	1.74	0.51
9:A:1038:C:H2'	9:A:1039:G:C8	2.45	0.51
9:A:1251:A:H2'	9:A:1252:A:C8	2.45	0.51
11:C:82:ASP:N	11:C:82:ASP:OD1	2.40	0.51
18:J:15:HIS:O	18:J:18:ILE:HG22	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:2134:A:N6	33:b:2159:G:H4'	2.26	0.51
38:g:95:ARG:HH21	38:g:106:SER:HB3	1.74	0.51
19:K:96:ILE:HG22	29:U:11:PHE:HZ	1.76	0.51
32:a:46:A:H3'	32:a:47:C:O2	2.11	0.51
33:b:9:G:O2'	33:b:10:A:O5'	2.23	0.51
33:b:1537:G:O2'	33:b:1538:G:O4'	2.28	0.51
9:A:462:G:H22	9:A:469:C:N4	2.08	0.51
9:A:488:C:H2'	9:A:489:C:C6	2.45	0.51
32:a:13:G:O2'	32:a:15:A:OP2	2.28	0.51
9:A:377:G:HO2'	9:A:378:G:H8	1.57	0.51
9:A:381:C:O2'	9:A:382:A:O5'	2.29	0.51
9:A:1287:A:H2'	9:A:1288:A:C8	2.46	0.51
33:b:2106:U:O4	33:b:2183:A:N6	2.44	0.51
35:d:74:GLU:OE1	35:d:74:GLU:N	2.34	0.51
48:s:26:ASP:OD1	48:s:26:ASP:N	2.41	0.51
9:A:440:C:C2	9:A:441:A:C8	2.99	0.51
9:A:673:A:H2'	9:A:674:G:H8	1.73	0.51
9:A:219:U:H2'	9:A:220:G:C8	2.46	0.51
9:A:424:G:H2'	9:A:425:G:C8	2.46	0.51
9:A:634:C:H2'	9:A:635:A:H8	1.75	0.51
16:H:53:ASP:OD1	16:H:53:ASP:N	2.41	0.51
20:L:70:GLY:HA3	20:L:98:ARG:HH22	1.74	0.51
33:b:1019:U:H3	33:b:1142:A:H62	1.59	0.51
33:b:1205:A:O2'	33:b:1206:G:OP1	2.26	0.51
51:v:96:PHE:O	51:v:100:SER:HA	2.11	0.51
9:A:229:U:O2'	24:P:23:ASP:OD2	2.21	0.50
21:M:10:ASP:HA	21:M:44:ILE:HB	1.93	0.50
33:b:2243:U:H2'	33:b:2244:U:C6	2.46	0.50
23:O:11:VAL:HG21	23:O:21:THR:HG22	1.92	0.50
33:b:878:A:C2	33:b:879:G:H1'	2.46	0.50
11:C:82:ASP:HA	11:C:85:LYS:HD2	1.93	0.50
33:b:277:G:H5''	33:b:278:A:H5'	1.93	0.50
33:b:1936:A:C2	33:b:1943:U:H5	2.28	0.50
37:f:147:ASP:OD1	37:f:147:ASP:N	2.45	0.50
41:l:112:PHE:HB3	41:l:115:ILE:HD12	1.93	0.50
9:A:459:A:N6	9:A:474:G:C2	2.76	0.50
17:I:21:LYS:O	17:I:61:ASP:N	2.43	0.50
21:M:49:GLU:HA	21:M:52:ILE:HB	1.94	0.50
33:b:286:U:N3	33:b:355:U:O2	2.45	0.50
33:b:1607:C:N4	33:b:1622:G:OP2	2.39	0.50
33:b:1936:A:H2	33:b:1943:U:C5	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:2102:G:N1	33:b:2188:U:N3	2.59	0.50
40:k:43:GLU:OE1	40:k:43:GLU:N	2.44	0.50
9:A:1076:U:OP1	10:B:173:LYS:NZ	2.45	0.50
9:A:502:A:H2'	9:A:503:C:C6	2.46	0.50
14:F:96:VAL:HG23	14:F:98:GLU:HG2	1.94	0.50
46:q:49:ALA:HB3	46:q:60:THR:HG22	1.94	0.50
9:A:1137:C:H1'	9:A:1138:G:N1	2.27	0.50
11:C:109:GLU:OE1	11:C:109:GLU:N	2.45	0.50
12:D:10:LEU:HD23	12:D:62:ARG:HD2	1.92	0.50
13:E:11:GLN:OE1	13:E:11:GLN:N	2.45	0.50
14:F:43:GLY:HA2	14:F:58:HIS:CE1	2.47	0.50
33:b:90:U:H2'	33:b:91:A:C2	2.46	0.50
12:D:190:LEU:HD12	12:D:193:ASP:CG	2.36	0.50
33:b:287:G:H2'	33:b:288:U:H6	1.77	0.50
33:b:2135:A:H5''	33:b:2136:G:C6	2.47	0.50
52:w:48:MET:O	52:w:51:GLN:HG3	2.12	0.50
9:A:1004:A:H2'	9:A:1005:A:O4'	2.12	0.50
28:T:19:HIS:O	28:T:23:ARG:HG2	2.12	0.50
33:b:2593:U:H5	33:b:2600:A:N1	2.10	0.50
9:A:745:G:H2'	9:A:746:A:H8	1.77	0.49
11:C:39:ARG:NH1	22:N:91:GLU:OE1	2.45	0.49
15:G:134:VAL:O	15:G:138:GLU:HG2	2.12	0.49
32:a:66:A:OP2	32:a:108:A:N6	2.44	0.49
33:b:1076:C:H2'	33:b:1088:A:H61	1.77	0.49
33:b:1086:A:H8	33:b:1104:C:C4	2.30	0.49
33:b:1535:A:C2	33:b:1537:G:H1'	2.47	0.49
40:k:90:GLU:OE1	40:k:90:GLU:N	2.39	0.49
9:A:449:G:H1	9:A:486:U:H3	1.59	0.49
9:A:462:G:H2'	9:A:463:U:C6	2.47	0.49
9:A:1036:A:H2'	9:A:1037:C:C2	2.47	0.49
21:M:53:ASP:OD1	21:M:54:THR:N	2.45	0.49
24:P:4:ILE:HG12	24:P:21:VAL:HG22	1.94	0.49
33:b:414:C:H2'	33:b:415:A:C8	2.47	0.49
33:b:895:U:O2'	33:b:896:A:O5'	2.27	0.49
33:b:1796:U:H2'	33:b:1797:G:H8	1.76	0.49
38:g:42:GLU:HB3	38:g:55:ARG:NE	2.20	0.49
9:A:652:U:O4	9:A:752:G:O2'	2.24	0.49
16:H:78:SER:HB2	16:H:84:ILE:HG22	1.94	0.49
33:b:181:A:H2'	33:b:182:A:C8	2.47	0.49
33:b:288:U:H2'	33:b:289:G:C8	2.46	0.49
33:b:887:U:H4'	33:b:888:C:H5'	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:1059:G:H8	33:b:1062:G:OP2	1.96	0.49
9:A:59:A:H3'	9:A:331:G:H22	1.77	0.49
9:A:376:G:N2	9:A:377:G:C5	2.79	0.49
9:A:1250:A:H2'	9:A:1251:A:C8	2.47	0.49
12:D:195:ASN:HA	12:D:198:LEU:HD13	1.94	0.49
15:G:67:ASN:ND2	15:G:126:ALA:O	2.45	0.49
33:b:279:A:H2'	33:b:280:U:O4'	2.12	0.49
33:b:849:A:H2'	33:b:850:U:C6	2.46	0.49
33:b:1779:U:H5	33:b:1784:A:N7	2.11	0.49
33:b:2139:U:H2'	33:b:2152:G:C6	2.47	0.49
38:g:60:ASP:OD1	38:g:61:GLY:N	2.41	0.49
9:A:249:U:C2	9:A:275:G:O6	2.64	0.49
9:A:410:G:H2'	9:A:429:U:C5	2.47	0.49
9:A:429:U:H5'	12:D:8:LEU:HD13	1.94	0.49
9:A:1021:A:H2'	9:A:1022:A:H8	1.77	0.49
17:I:59:LYS:O	17:I:60:LEU:HD13	2.13	0.49
18:J:25:ILE:HD11	18:J:87:LEU:HD22	1.94	0.49
33:b:1064:C:H41	33:b:1072:C:P	2.34	0.49
33:b:1084:A:H2'	33:b:1085:A:C5	2.47	0.49
42:m:141:LYS:HZ3	42:m:143:GLU:HG2	1.77	0.49
9:A:77:A:C6	9:A:78:A:H1'	2.47	0.49
9:A:445:G:H22	9:A:489:C:N4	2.11	0.49
13:E:148:SER:O	13:E:151:MET:HG2	2.12	0.49
16:H:26:MET:N	16:H:57:GLU:OE2	2.43	0.49
33:b:1083:U:C2	33:b:1085:A:H5''	2.48	0.49
33:b:1173:U:O2'	33:b:1175:A:N6	2.45	0.49
33:b:2134:A:H62	33:b:2159:G:H4'	1.77	0.49
9:A:259:G:H2'	9:A:260:G:H8	1.77	0.49
9:A:530:G:N7	31:Z:36:G:O2'	2.44	0.49
14:F:42:TRP:HB2	14:F:59:TYR:HB2	1.94	0.49
33:b:1469:A:H2'	33:b:1470:A:C8	2.48	0.49
35:d:97:SER:OG	35:d:98:VAL:N	2.45	0.49
41:l:70:ARG:HD2	41:l:76:VAL:HG12	1.94	0.49
50:u:18:GLU:CD	50:u:18:GLU:H	2.19	0.49
18:J:3:ASN:ND2	18:J:79:PRO:HG2	2.28	0.49
27:S:17:LYS:HA	27:S:20:LYS:HG2	1.95	0.49
33:b:1062:G:O6	33:b:1088:A:H2'	2.13	0.49
33:b:1105:U:N3	33:b:1106:G:N7	2.61	0.49
9:A:75:G:C2	9:A:76:G:H1'	2.48	0.49
9:A:728:A:H2'	9:A:729:A:C8	2.47	0.49
15:G:12:LEU:HD12	15:G:12:LEU:H	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:29:ILE:HG12	17:I:64:ILE:HB	1.95	0.49
31:Y:50:G:O6	31:Y:65:C:N4	2.46	0.49
38:g:133:LEU:CD1	38:g:141:ILE:HG13	2.43	0.49
45:p:77:ALA:O	45:p:80:GLU:HG3	2.13	0.49
9:A:1175:G:H2'	9:A:1176:A:H8	1.78	0.49
13:E:76:ASN:HB3	13:E:80:LEU:HD12	1.95	0.49
27:S:15:LEU:HA	27:S:18:VAL:HG12	1.94	0.49
34:c:21:ASN:ND2	34:c:23:GLU:OE2	2.44	0.49
52:w:35:GLU:N	52:w:35:GLU:OE1	2.46	0.49
9:A:1004:A:H5'	9:A:1025:U:H1'	1.94	0.48
14:F:2:ARG:HG2	14:F:91:ARG:HH21	1.77	0.48
14:F:72:ASP:O	14:F:75:GLU:HG2	2.13	0.48
20:L:72:ASN:OD1	20:L:72:ASN:N	2.46	0.48
30:X:27:C:H2'	30:X:28:G:C8	2.49	0.48
9:A:17:U:H2'	9:A:18:C:C6	2.48	0.48
31:Z:67:A:H2'	31:Z:68:U:O2	2.13	0.48
9:A:1323:G:H2'	9:A:1324:A:H8	1.78	0.48
11:C:9:ILE:HG23	11:C:10:ARG:HG3	1.94	0.48
31:Y:22:A:H62	31:Y:47:G:H2'	1.77	0.48
31:Z:77:A:C3'	57:Z:101:PRO:O	2.58	0.48
33:b:2138:G:O6	33:b:2153:C:N4	2.46	0.48
33:b:2291:U:H2'	33:b:2292:U:C6	2.49	0.48
13:E:152:VAL:HG21	16:H:98:LEU:HD23	1.96	0.48
33:b:2126:A:N3	33:b:2127:G:N1	2.62	0.48
17:I:57:VAL:HA	17:I:60:LEU:HD23	1.93	0.48
25:Q:48:GLU:N	25:Q:48:GLU:OE1	2.46	0.48
28:T:52:GLU:OE1	28:T:52:GLU:N	2.42	0.48
30:X:36:C:H5	53:x:12:G:H22	1.60	0.48
31:Y:32:G:H2'	31:Y:33:U:H6	1.79	0.48
33:b:368:A:O2'	33:b:369:U:OP1	2.28	0.48
33:b:2193:G:H2'	33:b:2194:U:C6	2.48	0.48
9:A:77:A:H2'	9:A:78:A:H4'	1.96	0.48
9:A:90:C:O2'	9:A:91:U:OP2	2.29	0.48
9:A:635:A:H2'	9:A:636:U:H6	1.79	0.48
33:b:1762:A:O2'	33:b:1763:G:OP1	2.26	0.48
38:g:90:VAL:HG12	38:g:91:GLY:H	1.77	0.48
9:A:409:U:H2'	9:A:410:G:C8	2.49	0.48
9:A:478:A:C5	9:A:479:U:H1'	2.49	0.48
33:b:288:U:H2'	33:b:289:G:H8	1.78	0.48
42:m:82:LEU:HD22	42:m:90:VAL:HG21	1.95	0.48
9:A:77:A:C5	9:A:78:A:H1'	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:674:G:O2'	36:e:69:ARG:NH1	2.46	0.48
51:v:48:PRO:HG3	51:v:56:GLY:HA3	1.95	0.48
9:A:202:G:H2'	9:A:203:G:H5'	1.96	0.48
9:A:373:A:N3	9:A:373:A:H2'	2.29	0.48
9:A:1493:A:H2	31:Z:37:G:H21	1.60	0.48
11:C:27:GLU:OE1	11:C:27:GLU:N	2.47	0.48
31:Y:77:A:C3'	55:z:162:PRO:C	2.84	0.48
31:Z:73:G:HO2'	31:Z:74:A:P	2.37	0.48
33:b:1097:U:H5'	33:b:1098:A:C8	2.49	0.48
33:b:1585:C:H2'	33:b:1586:A:O4'	2.14	0.48
41:l:92:GLU:OE1	41:l:92:GLU:N	2.47	0.48
4:4:32:LYS:HG3	4:4:33:THR:HG23	1.96	0.48
9:A:56:U:H2'	9:A:57:G:C8	2.49	0.48
9:A:1450:U:H3'	9:A:1452:C:N4	2.28	0.48
33:b:721:A:H2'	33:b:722:A:C8	2.49	0.48
33:b:886:A:C6	33:b:892:A:N6	2.82	0.48
33:b:1071:G:H22	33:b:1091:G:P	2.37	0.48
9:A:461:A:H2'	9:A:462:G:C8	2.49	0.47
10:B:82:ALA:HB2	10:B:213:LEU:HD13	1.95	0.47
17:I:40:ARG:HD2	17:I:44:ARG:CZ	2.44	0.47
33:b:2100:G:N1	33:b:2189:U:N3	2.61	0.47
9:A:553:A:H2'	9:A:554:A:C8	2.48	0.47
31:Y:9:G:OP2	31:Y:47:G:H1'	2.14	0.47
33:b:593:U:H2'	33:b:594:U:C6	2.49	0.47
33:b:2127:G:O6	33:b:2162:G:N1	2.47	0.47
33:b:2187:U:H2'	33:b:2188:U:C5	2.49	0.47
43:n:111:GLU:O	43:n:115:GLU:HG2	2.14	0.47
2:1:4:LYS:HG2	33:b:102:U:O4	2.14	0.47
4:4:54:VAL:HG11	44:o:98:LEU:HD13	1.96	0.47
9:A:472:U:H2'	9:A:473:U:C2	2.49	0.47
9:A:1176:A:H2'	9:A:1177:G:C8	2.49	0.47
22:N:32:ASP:HB3	22:N:35:ALA:HB2	1.96	0.47
33:b:548:G:H5''	33:b:549:G:OP2	2.14	0.47
33:b:742:A:H2'	33:b:743:A:C8	2.50	0.47
33:b:2281:A:O2'	33:b:2282:G:H5'	2.14	0.47
33:b:2306:C:OP2	33:b:2307:G:O2'	2.26	0.47
9:A:516:U:O2	9:A:533:A:N7	2.46	0.47
9:A:1180:A:OP2	17:I:98:ARG:NH2	2.45	0.47
18:J:59:LYS:HE3	18:J:62:ARG:NH2	2.29	0.47
33:b:2126:A:H61	33:b:2162:G:C4'	2.26	0.47
33:b:2848:G:HO2'	33:b:2849:U:P	2.36	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:54:GLN:N	51:v:55:PRO:HD3	2.30	0.47
9:A:462:G:H2'	9:A:463:U:H6	1.80	0.47
9:A:1524:C:OP2	19:K:124:LYS:NZ	2.36	0.47
18:J:83:THR:O	18:J:87:LEU:HG	2.15	0.47
30:X:49:G:H2'	30:X:50:C:C6	2.50	0.47
33:b:2097:A:H2'	33:b:2098:U:C6	2.49	0.47
33:b:2133:G:H1'	33:b:2157:G:H22	1.80	0.47
36:e:5:LEU:HD11	36:e:12:LEU:CD1	2.44	0.47
33:b:890:C:C4	33:b:891:G:H1'	2.49	0.47
33:b:1538:G:H2'	33:b:1539:U:C6	2.50	0.47
33:b:2062:A:O2'	33:b:2063:C:O5'	2.29	0.47
33:b:2790:U:H2'	33:b:2893:A:C8	2.49	0.47
37:f:4:LEU:HG	37:f:101:GLU:HG2	1.96	0.47
37:f:140:GLU:N	37:f:140:GLU:OE1	2.47	0.47
50:u:96:VAL:HA	50:u:99:ALA:HB3	1.97	0.47
9:A:195:A:H2'	9:A:196:A:C8	2.49	0.47
9:A:269:C:H2'	9:A:270:A:C8	2.50	0.47
9:A:1130:A:OP1	17:I:17:ARG:NH2	2.48	0.47
9:A:1218:C:H2'	9:A:1219:A:C8	2.50	0.47
17:I:44:ARG:HA	17:I:47:VAL:HG12	1.96	0.47
20:L:74:GLN:HG3	20:L:75:GLU:H	1.80	0.47
21:M:54:THR:HA	21:M:57:ASP:OD2	2.15	0.47
31:Z:76:C:H2'	31:Z:77:A:C8	2.49	0.47
33:b:265:A:N6	33:b:428:A:C8	2.82	0.47
33:b:511:U:HO2'	33:b:512:G:P	2.36	0.47
33:b:880:G:H5''	33:b:881:G:OP1	2.14	0.47
33:b:1856:U:H2'	33:b:1857:G:O4'	2.14	0.47
33:b:2138:G:N1	33:b:2153:C:N3	2.61	0.47
37:f:93:GLY:O	37:f:96:MET:HG2	2.15	0.47
9:A:462:G:H1	9:A:469:C:H41	1.61	0.47
13:E:89:THR:OG1	13:E:134:ASN:ND2	2.47	0.47
17:I:83:THR:HG23	17:I:97:LEU:HD13	1.96	0.47
33:b:780:G:H21	33:b:783:A:H62	1.60	0.47
33:b:959:A:H2'	33:b:960:A:C8	2.50	0.47
49:t:4:ILE:HG13	49:t:106:VAL:HG22	1.95	0.47
50:u:94:ASP:OD1	50:u:94:ASP:N	2.44	0.47
9:A:512:U:H2'	9:A:513:C:C6	2.50	0.47
9:A:1038:C:H2'	9:A:1039:G:H8	1.80	0.47
10:B:89:PHE:HB3	10:B:149:GLY:O	2.15	0.47
33:b:191:A:H2'	33:b:192:C:C6	2.50	0.47
33:b:2859:G:H2'	33:b:2860:A:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:203:G:H21	9:A:465:A:H61	1.63	0.47
13:E:159:SER:O	13:E:163:ILE:HG12	2.15	0.47
25:Q:10:ARG:HG2	25:Q:57:VAL:HG22	1.97	0.47
33:b:78:U:H2'	33:b:79:C:C6	2.49	0.47
33:b:1507:C:H2'	33:b:1508:A:C4	2.50	0.47
12:D:154:VAL:HG11	12:D:177:MET:HE3	1.95	0.46
15:G:110:ARG:HD3	15:G:122:GLU:OE2	2.15	0.46
20:L:33:CYS:SG	20:L:79:ILE:HD13	2.55	0.46
28:T:66:ILE:HG23	28:T:70:LYS:HD3	1.97	0.46
30:X:48:C:N4	30:X:59:G:O4'	2.48	0.46
30:X:63:C:H2'	30:X:64:G:C8	2.49	0.46
31:Y:51:G:H2'	31:Y:52:A:H5'	1.96	0.46
33:b:894:U:H2'	33:b:895:U:C6	2.50	0.46
33:b:2192:U:H2'	33:b:2193:G:C8	2.51	0.46
36:e:171:ASP:OD1	36:e:171:ASP:N	2.46	0.46
9:A:274:A:N3	9:A:275:G:H1'	2.29	0.46
9:A:838:G:H2'	9:A:839:C:H6	1.80	0.46
9:A:843:U:H5''	9:A:844:G:C5	2.50	0.46
10:B:87:ASP:HB2	10:B:224:ARG:NH1	2.30	0.46
19:K:79:LYS:HD3	19:K:80:ASN:HD22	1.80	0.46
33:b:358:U:C2	33:b:359:G:C8	3.03	0.46
33:b:2155:U:H2'	33:b:2156:G:C5	2.50	0.46
33:b:2194:U:H2'	33:b:2195:U:H6	1.79	0.46
42:m:20:GLY:HA2	42:m:28:GLY:HA2	1.97	0.46
7:7:34:THR:OG1	33:b:2420:C:OP1	2.28	0.46
9:A:410:G:H2'	9:A:429:U:C4	2.50	0.46
9:A:458:U:H3	9:A:474:G:H22	1.63	0.46
12:D:10:LEU:HG	12:D:62:ARG:NH1	2.31	0.46
17:I:58:GLU:HB2	17:I:59:LYS:HD3	1.97	0.46
18:J:40:ILE:HB	18:J:73:LEU:HB3	1.97	0.46
33:b:845:A:C2	33:b:847:U:H1'	2.50	0.46
33:b:2267:A:H62	33:b:2272:U:H3	1.64	0.46
33:b:2659:G:P	38:g:158:LYS:HZ1	2.38	0.46
9:A:967:C:H2'	9:A:968:A:C2	2.51	0.46
9:A:1024:G:H2'	9:A:1025:U:C6	2.50	0.46
31:Z:24:C:H2'	31:Z:25:G:C8	2.51	0.46
32:a:57:A:C2	37:f:26:MET:HE1	2.50	0.46
33:b:2467:C:H2'	33:b:2468:A:O4'	2.15	0.46
33:b:2809:A:H2'	33:b:2810:A:C8	2.51	0.46
35:d:39:ASP:N	35:d:39:ASP:OD1	2.49	0.46
9:A:539:A:H2'	9:A:540:G:C8	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:35:LEU:HD21	13:E:136:VAL:HG21	1.97	0.46
16:H:112:ASP:OD1	16:H:112:ASP:N	2.49	0.46
33:b:740:C:H5	33:b:757:G:H22	1.62	0.46
33:b:1000:A:H2'	33:b:1001:A:C8	2.50	0.46
33:b:2125:G:H21	33:b:2173:A:H62	1.63	0.46
33:b:2178:C:H2'	33:b:2179:C:H6	1.79	0.46
42:m:132:ARG:HG3	42:m:142:ILE:HD12	1.98	0.46
12:D:40:HIS:CG	12:D:43:ARG:HE	2.33	0.46
12:D:99:ASN:O	12:D:103:ARG:HG2	2.16	0.46
16:H:90:GLU:N	16:H:90:GLU:OE1	2.49	0.46
30:X:19:G:O6	33:b:2112:G:O2'	2.25	0.46
33:b:2858:C:O2'	33:b:2859:G:C8	2.64	0.46
9:A:408:A:C6	9:A:409:U:C4	3.04	0.46
9:A:674:G:H2'	9:A:675:A:C8	2.50	0.46
9:A:1140:C:H2'	9:A:1141:C:C6	2.51	0.46
15:G:92:PRO:HA	15:G:95:ARG:HD3	1.98	0.46
18:J:65:TYR:HB3	22:N:95:LEU:HD22	1.97	0.46
21:M:58:GLU:O	21:M:61:LYS:HG2	2.16	0.46
25:Q:18:LYS:HD3	25:Q:46:HIS:HE1	1.81	0.46
33:b:1796:U:H2'	33:b:1797:G:C8	2.51	0.46
45:p:110:ALA:HB1	45:p:115:LEU:HD12	1.98	0.46
10:B:66:ILE:N	10:B:88:GLN:OE1	2.48	0.46
12:D:59:LYS:O	12:D:63:ILE:HG23	2.16	0.46
30:X:69:C:H2'	30:X:70:C:C6	2.51	0.46
33:b:2159:G:H2'	33:b:2160:C:C6	2.51	0.46
33:b:2181:U:H2'	33:b:2182:U:C6	2.51	0.46
35:d:181:ASP:HB3	35:d:186:LEU:HB2	1.97	0.46
48:s:79:ARG:O	48:s:81:LYS:HG2	2.15	0.46
9:A:262:A:HO2'	9:A:263:A:P	2.37	0.46
21:M:80:MET:HE2	21:M:80:MET:HB2	1.82	0.46
25:Q:6:THR:HB	25:Q:59:GLU:OE2	2.16	0.46
30:X:56:C:O2'	30:X:57:G:OP1	2.31	0.46
36:e:190:ALA:O	36:e:194:LYS:HG3	2.16	0.46
55:z:148:LEU:HD12	55:z:148:LEU:HA	1.71	0.46
9:A:403:C:H2'	9:A:404:G:H8	1.81	0.46
33:b:639:U:H2'	33:b:640:C:H6	1.80	0.46
33:b:1050:A:H3'	33:b:1051:G:H8	1.81	0.46
50:u:56:GLU:HG3	50:u:88:LYS:HA	1.98	0.46
50:u:96:VAL:O	50:u:100:GLU:N	2.48	0.46
9:A:56:U:H2'	9:A:57:G:H8	1.81	0.45
9:A:84:U:H2'	9:A:86:G:H21	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:47:LEU:HD13	14:F:49:TYR:O	2.15	0.45
16:H:46:GLU:OE1	16:H:46:GLU:N	2.49	0.45
28:T:26:MET:O	28:T:29:THR:OG1	2.30	0.45
31:Z:31:C:H41	31:Z:41:G:H1	1.64	0.45
33:b:1078:U:O2'	33:b:1079:C:O5'	2.33	0.45
33:b:1507:C:H2'	33:b:1508:A:N3	2.32	0.45
33:b:2166:U:H2'	33:b:2167:U:C6	2.51	0.45
47:r:105:ALA:HB1	48:s:48:LYS:NZ	2.31	0.45
48:s:55:ASP:OD1	48:s:56:GLY:N	2.47	0.45
9:A:151:A:H3'	9:A:152:A:H8	1.80	0.45
9:A:185:U:H2'	9:A:186:C:C6	2.51	0.45
9:A:324:G:N1	9:A:327:A:OP2	2.49	0.45
9:A:1320:C:N3	27:S:35:ARG:NH1	2.64	0.45
20:L:51:VAL:HG23	20:L:64:SER:O	2.16	0.45
24:P:45:GLU:CD	24:P:45:GLU:H	2.24	0.45
33:b:886:A:N6	33:b:892:A:H61	2.14	0.45
33:b:1082:U:H3	33:b:1086:A:H2	1.63	0.45
33:b:1173:U:H2'	33:b:1175:A:N7	2.31	0.45
33:b:2111:U:H4'	33:b:2119:A:H5'	1.98	0.45
33:b:2121:G:H2'	33:b:2122:U:C6	2.52	0.45
33:b:2133:G:O3'	33:b:2157:G:N2	2.50	0.45
35:d:101:PHE:HD1	35:d:104:VAL:HG21	1.81	0.45
44:o:86:ARG:HH21	44:o:117:ASP:CG	2.24	0.45
9:A:2:A:H1'	9:A:613:C:O2'	2.16	0.45
13:E:159:SER:OG	13:E:161:GLU:OE2	2.24	0.45
30:X:7:A:N6	30:X:49:G:C6	2.84	0.45
33:b:674:G:H1'	36:e:69:ARG:NH1	2.17	0.45
33:b:833:A:H2'	33:b:834:G:C8	2.51	0.45
39:h:53:GLU:O	39:h:57:LYS:HG2	2.17	0.45
9:A:257:G:H2'	9:A:258:G:H8	1.82	0.45
10:B:15:PHE:HB3	10:B:40:ILE:H	1.81	0.45
12:D:57:LYS:HA	12:D:199:ILE:HD11	1.98	0.45
18:J:22:THR:HA	18:J:25:ILE:HG22	1.98	0.45
19:K:44:ALA:HB3	19:K:69:CYS:HB2	1.99	0.45
21:M:46:GLU:OE1	21:M:46:GLU:N	2.48	0.45
30:X:21:A:H62	30:X:46:G:H1'	1.81	0.45
33:b:1050:A:C5	33:b:1051:G:C5	3.04	0.45
33:b:2112:G:OP2	33:b:2112:G:H4'	2.16	0.45
36:e:146:VAL:HG12	36:e:185:LYS:HB2	1.98	0.45
52:w:75:GLN:HB2	52:w:92:VAL:HG23	1.99	0.45
9:A:462:G:H22	9:A:469:C:H42	1.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1273:C:H2'	9:A:1274:A:O4'	2.16	0.45
22:N:64:ARG:HG2	22:N:77:GLY:O	2.16	0.45
27:S:68:HIS:HB3	27:S:72:GLU:HG3	1.98	0.45
33:b:307:G:N2	33:b:310:A:OP2	2.49	0.45
33:b:880:G:H2'	33:b:881:G:C8	2.52	0.45
33:b:1198:U:H2'	33:b:1199:U:C6	2.51	0.45
33:b:2514:U:H2'	33:b:2515:C:C6	2.52	0.45
33:b:2813:A:H2'	33:b:2814:A:C8	2.51	0.45
9:A:993:G:O2'	9:A:994:A:N7	2.49	0.45
9:A:1328:C:OP1	21:M:27:THR:HG21	2.16	0.45
31:Y:18:U:O2'	31:Y:19:G:O5'	2.32	0.45
33:b:878:A:H3'	33:b:879:G:C8	2.41	0.45
33:b:1847:A:O2'	33:b:1848:A:H8	1.99	0.45
33:b:2102:G:N1	33:b:2187:U:O2	2.50	0.45
34:c:132:MET:HG3	34:c:188:CYS:O	2.17	0.45
41:l:114:LYS:HB2	41:l:114:LYS:HE2	1.79	0.45
9:A:1208:C:H2'	9:A:1209:C:H5'	1.99	0.45
11:C:35:ASP:OD1	11:C:58:ARG:NH2	2.39	0.45
21:M:49:GLU:OE1	21:M:49:GLU:N	2.46	0.45
24:P:46:LYS:HE2	24:P:46:LYS:HB2	1.78	0.45
26:R:71:ASP:OD1	26:R:72:ARG:N	2.49	0.45
28:T:53:MET:HE2	28:T:53:MET:HB2	1.90	0.45
30:X:18:G:H5'	30:X:60:U:C4	2.52	0.45
31:Z:51:G:H1	31:Z:65:C:H41	1.65	0.45
33:b:2064:C:H2'	33:b:2065:C:C6	2.51	0.45
33:b:2649:C:H2'	33:b:2650:U:H6	1.81	0.45
33:b:2790:U:H5'	33:b:2791:G:OP1	2.16	0.45
39:h:8:LYS:NZ	39:h:13:GLY:O	2.49	0.45
5:5:47:VAL:HG12	5:5:48:ILE:N	2.32	0.45
9:A:473:U:H2'	9:A:474:G:C4	2.52	0.45
9:A:518:C:N3	9:A:530:G:N2	2.65	0.45
9:A:721:G:H4'	9:A:722:G:O4'	2.16	0.45
9:A:1477:U:H2'	9:A:1478:U:C6	2.52	0.45
9:A:1493:A:O2'	33:b:1913:A:N1	2.48	0.45
33:b:155:A:H2'	33:b:156:A:C8	2.51	0.45
33:b:1053:C:H3'	33:b:1054:A:H2	1.81	0.45
33:b:1542:U:H2'	33:b:1543:G:O4'	2.17	0.45
9:A:1244:G:H2'	9:A:1245:C:C6	2.52	0.45
9:A:1435:G:H2'	9:A:1436:U:C6	2.52	0.45
12:D:187:ARG:HH12	12:D:190:LEU:HB2	1.82	0.45
20:L:79:ILE:HG21	20:L:96:THR:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:19:HIS:CD2	28:T:23:ARG:HD3	2.51	0.45
33:b:784:G:H5'	33:b:785:G:OP1	2.17	0.45
38:g:27:LYS:HD3	38:g:32:GLU:HB3	1.99	0.45
38:g:137:ASP:O	38:g:141:ILE:HG22	2.17	0.45
9:A:440:C:H2'	9:A:441:A:H8	1.82	0.45
9:A:473:U:H2'	9:A:474:G:N9	2.32	0.45
9:A:636:U:H2'	9:A:637:C:C6	2.52	0.45
11:C:78:LYS:HB3	11:C:78:LYS:HE3	1.65	0.45
18:J:11:LYS:HG3	18:J:97:ASP:HB3	1.98	0.45
31:Z:6:A:N1	31:Z:68:U:H5	2.15	0.45
33:b:39:G:H2'	33:b:40:U:O2	2.16	0.45
33:b:1682:G:H2'	33:b:1683:U:C6	2.52	0.45
33:b:1720:U:H2'	33:b:1721:G:O4'	2.17	0.45
33:b:2159:G:H2'	33:b:2160:C:H6	1.82	0.45
37:f:70:ALA:HB3	37:f:82:GLY:H	1.82	0.45
9:A:514:C:C2	9:A:515:G:C8	3.05	0.44
9:A:575:G:O2'	9:A:821:G:OP2	2.30	0.44
10:B:172:ILE:HG22	10:B:176:ASN:HD21	1.81	0.44
12:D:101:VAL:HG22	12:D:106:PHE:HB2	1.99	0.44
17:I:18:VAL:HG22	17:I:64:ILE:HD12	1.99	0.44
22:N:95:LEU:HD23	22:N:95:LEU:HA	1.78	0.44
23:O:13:GLU:CD	23:O:83:ARG:HH22	2.24	0.44
26:R:34:GLU:OE1	26:R:34:GLU:N	2.47	0.44
43:n:119:LEU:HD12	43:n:119:LEU:HA	1.85	0.44
9:A:264:C:O2'	25:Q:65:PRO:O	2.36	0.44
13:E:161:GLU:H	13:E:161:GLU:HG3	1.63	0.44
24:P:44:SER:HB2	24:P:47:GLU:OE1	2.17	0.44
27:S:11:ASP:OD2	27:S:34:SER:OG	2.28	0.44
30:X:35:C:H2'	30:X:36:C:O2	2.17	0.44
33:b:1064:C:O2'	33:b:1065:U:OP2	2.35	0.44
33:b:2655:G:N2	33:b:2665:A:OP2	2.47	0.44
53:x:22:A:O2'	53:x:23:A:H5'	2.17	0.44
9:A:436:C:H2'	9:A:437:U:H6	1.83	0.44
9:A:1342:C:HO2'	9:A:1343:G:H8	1.64	0.44
12:D:108:ALA:HB3	12:D:112:GLU:HG3	1.99	0.44
30:X:51:G:C4	30:X:52:A:C8	3.04	0.44
33:b:279:A:H61	33:b:361:G:H1'	1.82	0.44
33:b:547:A:H3'	33:b:548:G:C8	2.52	0.44
33:b:848:C:H2'	33:b:849:A:H8	1.82	0.44
9:A:73:C:H5	9:A:97:G:H1	1.65	0.44
9:A:1062:U:H2'	9:A:1063:C:C6	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:85:SER:HB2	10:B:221:ARG:HH22	1.82	0.44
19:K:82:GLU:N	19:K:82:GLU:OE1	2.51	0.44
24:P:54:LEU:HA	24:P:54:LEU:HD13	1.87	0.44
33:b:885:C:O2'	33:b:886:A:N7	2.38	0.44
33:b:2830:C:H5'	35:d:56:LYS:HE3	1.98	0.44
37:f:8:TYR:HB2	37:f:173:PHE:HZ	1.82	0.44
39:h:94:ILE:HB	39:h:122:LEU:HB2	1.99	0.44
45:p:61:GLN:OE1	45:p:61:GLN:N	2.43	0.44
9:A:491:G:H2'	9:A:491:G:N3	2.33	0.44
9:A:1361:G:O6	9:A:1362:A:N6	2.50	0.44
12:D:84:ASN:HB2	13:E:101:GLY:HA3	1.99	0.44
20:L:35:ARG:HD2	20:L:37:TYR:OH	2.18	0.44
23:O:5:GLU:OE1	23:O:5:GLU:N	2.47	0.44
33:b:640:C:H2'	33:b:641:U:C6	2.52	0.44
33:b:1063:G:N7	33:b:1070:A:H5'	2.33	0.44
33:b:2185:U:C2	33:b:2186:G:N7	2.86	0.44
33:b:2636:C:O2'	35:d:45:TYR:OH	2.35	0.44
39:h:46:PHE:O	39:h:50:ARG:NH1	2.48	0.44
9:A:416:G:H2'	9:A:417:G:H8	1.82	0.44
9:A:430:A:P	12:D:7:LYS:HZ3	2.41	0.44
9:A:506:G:H2'	9:A:507:C:C6	2.52	0.44
11:C:184:ASN:OD1	11:C:185:THR:N	2.48	0.44
12:D:190:LEU:HD21	12:D:194:ILE:HG13	1.99	0.44
16:H:23:ALA:HB1	16:H:59:GLU:OE2	2.17	0.44
30:X:49:G:H2'	30:X:50:C:O4'	2.18	0.44
37:f:117:LEU:H	37:f:178:ARG:H	1.64	0.44
9:A:1056:U:OP1	11:C:161:ILE:HA	2.17	0.44
12:D:171:GLU:HB2	12:D:180:THR:HG22	2.00	0.44
20:L:110:LYS:HE2	20:L:110:LYS:HB2	1.82	0.44
25:Q:67:SER:OG	25:Q:68:LYS:N	2.51	0.44
34:c:180:GLU:HG3	34:c:269:ARG:O	2.18	0.44
55:z:153[B]:SER:HA	55:z:155[B]:TRP:HD1	1.83	0.44
9:A:444:G:C2	9:A:491:G:C2	3.06	0.44
9:A:489:C:H2'	9:A:490:C:H6	1.83	0.44
9:A:1316:G:N2	9:A:1318:A:H3'	2.33	0.44
12:D:18:LEU:HG	12:D:20:LEU:HB2	1.99	0.44
20:L:52:CYS:SG	20:L:66:ILE:HD11	2.58	0.44
21:M:32:ILE:HD11	21:M:62:PHE:HE2	1.81	0.44
33:b:365:U:H2'	33:b:366:C:C6	2.53	0.44
33:b:1870:C:O2'	33:b:1871:A:O5'	2.36	0.44
33:b:2335:A:H5'	45:p:13:ARG:NH2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:n:41:LEU:HD12	43:n:41:LEU:HA	1.89	0.44
9:A:550:G:H2'	9:A:551:U:O2	2.18	0.44
9:A:976:G:N2	9:A:1362:A:O2'	2.48	0.44
9:A:1169:A:H3'	9:A:1170:A:C8	2.53	0.44
33:b:84:A:C2	33:b:98:G:H8	2.35	0.44
33:b:703:U:H2'	33:b:704:G:O4'	2.17	0.44
33:b:1064:C:N4	33:b:1073:A:H5'	2.33	0.44
33:b:2155:U:H5''	33:b:2156:G:OP1	2.17	0.44
9:A:92:U:H2'	9:A:93:U:C2	2.53	0.43
9:A:179:A:H2'	9:A:180:U:O4'	2.17	0.43
9:A:538:G:OP1	20:L:109:ARG:HA	2.18	0.43
18:J:50:THR:OG1	18:J:64:GLN:OE1	2.30	0.43
25:Q:56:ASP:OD1	25:Q:56:ASP:N	2.51	0.43
28:T:14:GLU:O	28:T:18:LYS:HG2	2.18	0.43
33:b:345:A:H1'	33:b:346:A:C2	2.49	0.43
33:b:1532:A:N6	33:b:1533:C:H42	2.16	0.43
48:s:49:ILE:HG21	48:s:54:VAL:N	2.33	0.43
49:t:91:GLY:HA3	55:z:150[A]:TYR:OH	2.17	0.43
50:u:89:GLU:HG2	50:u:90:GLY:H	1.83	0.43
9:A:409:U:OP1	12:D:22:SER:OG	2.36	0.43
10:B:172:ILE:O	10:B:176:ASN:ND2	2.50	0.43
16:H:72:GLU:N	16:H:72:GLU:OE1	2.52	0.43
24:P:34:GLU:OE1	24:P:36:VAL:HG13	2.18	0.43
30:X:49:G:H2'	30:X:50:C:H6	1.83	0.43
31:Y:52:A:O2'	31:Y:53:G:H8	2.00	0.43
33:b:2188:U:H2'	33:b:2189:U:C2	2.54	0.43
33:b:2591:C:H2'	33:b:2592:G:H8	1.82	0.43
35:d:12:THR:HG22	35:d:13:ARG:N	2.28	0.43
37:f:51:ASP:OD1	37:f:51:ASP:N	2.48	0.43
51:v:18:ASP:HB2	51:v:21:LYS:HD2	1.99	0.43
14:F:41:ASP:OD1	14:F:42:TRP:N	2.51	0.43
30:X:44:G:H2'	30:X:45:G:N3	2.33	0.43
33:b:1149:G:H2'	33:b:1150:C:C6	2.53	0.43
33:b:1483:G:N1	33:b:1506:U:N3	2.53	0.43
33:b:2055:C:HO2'	33:b:2056:G:P	2.38	0.43
33:b:2267:A:N6	33:b:2272:U:H3	2.17	0.43
38:g:133:LEU:HD11	38:g:141:ILE:HG13	2.00	0.43
44:o:96:ARG:NH1	44:o:116:VAL:HG12	2.33	0.43
9:A:76:G:H2'	9:A:77:A:H5''	2.00	0.43
9:A:192:A:H2'	9:A:193:C:C6	2.54	0.43
9:A:377:G:O2'	9:A:378:G:H8	2.02	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:744:C:H2'	9:A:745:G:H8	1.83	0.43
9:A:978:A:O2'	9:A:1322:C:H5	2.01	0.43
9:A:1027:C:C2	9:A:1035:A:C6	3.06	0.43
9:A:1343:G:H2'	9:A:1344:C:C6	2.53	0.43
10:B:56:LEU:HD23	10:B:56:LEU:HA	1.82	0.43
15:G:135:LYS:HA	15:G:135:LYS:HD3	1.89	0.43
17:I:52:GLU:HA	17:I:56:MET:HG3	2.01	0.43
33:b:1439:A:N6	33:b:1552:A:H8	2.08	0.43
33:b:1504:A:H2'	33:b:1504:A:N3	2.34	0.43
33:b:2849:U:N3	33:b:2867:G:O4'	2.51	0.43
36:e:176:ASP:OD1	36:e:176:ASP:N	2.51	0.43
9:A:613:C:H2'	9:A:614:C:C6	2.53	0.43
9:A:635:A:H2'	9:A:636:U:C6	2.54	0.43
9:A:1160:G:P	10:B:131:LYS:HZ1	2.39	0.43
14:F:18:VAL:HG21	14:F:58:HIS:CD2	2.53	0.43
18:J:11:LYS:HA	18:J:70:HIS:O	2.18	0.43
24:P:45:GLU:HB2	24:P:46:LYS:HD3	2.01	0.43
25:Q:19:SER:HB3	25:Q:70:LYS:NZ	2.34	0.43
25:Q:67:SER:HB3	25:Q:70:LYS:HB2	2.01	0.43
33:b:151:C:H2'	33:b:152:A:H8	1.84	0.43
33:b:1372:U:HO2'	33:b:2212:A:H8	1.64	0.43
33:b:2480:C:H2'	33:b:2481:G:O4'	2.18	0.43
54:y:41:ARG:HA	54:y:41:ARG:HD3	1.80	0.43
9:A:147:G:H2'	9:A:148:G:C8	2.53	0.43
9:A:262:A:O2'	9:A:263:A:P	2.75	0.43
9:A:687:A:C2	9:A:704:A:C5	3.06	0.43
9:A:737:C:H2'	9:A:738:C:H6	1.84	0.43
9:A:745:G:H2'	9:A:746:A:C8	2.53	0.43
10:B:145:ASN:OD1	10:B:146:SER:N	2.51	0.43
11:C:169:GLU:OE1	11:C:169:GLU:N	2.51	0.43
12:D:63:ILE:HG13	12:D:64:TYR:CD1	2.53	0.43
12:D:187:ARG:HA	12:D:187:ARG:HD2	1.82	0.43
17:I:24:ASN:HA	17:I:58:GLU:O	2.19	0.43
18:J:14:ASP:OD1	18:J:15:HIS:N	2.51	0.43
30:X:7:A:C6	30:X:49:G:C4	3.06	0.43
33:b:1434:A:O2'	33:b:1435:G:OP2	2.26	0.43
48:s:38:VAL:O	48:s:54:VAL:HG12	2.17	0.43
9:A:222:C:H2'	9:A:223:A:C8	2.53	0.43
9:A:262:A:H2'	9:A:263:A:C8	2.53	0.43
10:B:166:ASP:OD2	10:B:190:SER:OG	2.36	0.43
13:E:80:LEU:HB3	13:E:146:MET:SD	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:88:LYS:HE3	16:H:88:LYS:HB3	1.81	0.43
17:I:26:LYS:HA	17:I:26:LYS:HD3	1.80	0.43
33:b:848:C:H2'	33:b:849:A:C8	2.53	0.43
33:b:1040:A:H61	33:b:1115:G:H1	1.66	0.43
33:b:1080:A:H8	33:b:1080:A:P	2.42	0.43
33:b:2187:U:H5''	33:b:2188:U:OP1	2.18	0.43
33:b:2306:C:H2'	33:b:2307:G:H21	1.84	0.43
44:o:103:ARG:HD2	44:o:106:ASP:OD1	2.18	0.43
9:A:131:A:O2'	9:A:262:A:H8	2.01	0.43
9:A:634:C:H2'	9:A:635:A:C8	2.52	0.43
9:A:1256:A:H2'	9:A:1278:G:H1	1.84	0.43
33:b:1361:G:H2'	33:b:1362:C:C6	2.53	0.43
33:b:2250:G:OP1	43:n:84:LYS:NZ	2.52	0.43
36:e:155:GLU:OE1	36:e:155:GLU:N	2.45	0.43
51:v:18:ASP:OD1	51:v:18:ASP:N	2.49	0.43
9:A:411:A:N6	9:A:429:U:O5'	2.52	0.43
9:A:488:C:H2'	9:A:489:C:H6	1.83	0.43
10:B:122:ASP:N	10:B:122:ASP:OD1	2.52	0.43
11:C:11:LEU:HD23	11:C:11:LEU:HA	1.75	0.43
12:D:70:GLN:H	12:D:70:GLN:CD	2.22	0.43
13:E:99:SER:OG	13:E:100:GLU:N	2.50	0.43
30:X:27:C:H2'	30:X:28:G:H8	1.83	0.43
33:b:668:A:H2'	33:b:670:A:H62	1.84	0.43
33:b:1064:C:N3	33:b:1073:A:H5'	2.33	0.43
33:b:1074:G:H8	33:b:1074:G:OP1	2.02	0.43
33:b:1417:C:O2'	33:b:1587:G:O2'	2.26	0.43
33:b:2170:A:H1'	33:b:2171:A:C8	2.54	0.43
36:e:15:SER:N	36:e:197:GLU:OE2	2.47	0.43
39:h:47:PHE:O	39:h:51:ARG:HB2	2.19	0.43
46:q:6:LYS:HE3	46:q:6:LYS:HB3	1.79	0.43
9:A:945:G:C2	9:A:946:A:C8	3.07	0.43
9:A:1391:U:H2'	9:A:1392:G:C8	2.54	0.43
10:B:112:ARG:HH22	10:B:116:LEU:HD13	1.84	0.43
33:b:571:U:H3'	48:s:80:ARG:NH2	2.34	0.43
33:b:2114:A:C6	33:b:2115:G:H1'	2.54	0.43
38:g:154:PRO:HA	38:g:160:LYS:O	2.19	0.43
39:h:144:VAL:HG12	39:h:146:VAL:HG23	2.01	0.43
50:u:37:ASP:OD1	50:u:37:ASP:N	2.52	0.43
5:5:23:THR:OG1	5:5:24:THR:N	2.51	0.42
9:A:323:U:H2'	9:A:324:G:O4'	2.19	0.42
9:A:555:U:H2'	9:A:556:C:C6	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1396:A:H4'	9:A:1397:C:H5'	2.01	0.42
31:Y:66:U:O2'	31:Y:68:U:O4'	2.37	0.42
33:b:1101:U:H2'	33:b:1102:C:H4'	2.00	0.42
33:b:2157:G:H1'	33:b:2158:A:OP2	2.19	0.42
9:A:410:G:H1'	9:A:433:G:N2	2.34	0.42
9:A:1238:A:H2	9:A:1241:G:N3	2.17	0.42
32:a:51:G:O2'	32:a:52:A:OP1	2.30	0.42
33:b:1105:U:C2	33:b:1106:G:N7	2.88	0.42
33:b:1534:U:H1'	33:b:1535:A:H2'	2.01	0.42
33:b:1713:A:C4	33:b:1716:U:H1'	2.53	0.42
35:d:74:GLU:H	35:d:74:GLU:CD	2.24	0.42
36:e:21:ARG:HD3	36:e:106:LYS:HB3	2.01	0.42
49:t:1:MET:HE3	49:t:2:GLU:H	1.85	0.42
9:A:66:A:H4'	9:A:173:U:C5	2.53	0.42
9:A:69:G:H2'	9:A:70:U:C6	2.53	0.42
9:A:361:G:H2'	9:A:362:G:O4'	2.20	0.42
9:A:539:A:H2'	9:A:540:G:H8	1.82	0.42
10:B:166:ASP:O	10:B:169:HIS:ND1	2.52	0.42
33:b:973:A:H5'	33:b:1188:U:H1'	2.02	0.42
33:b:1019:U:O2'	33:b:1021:A:H2	2.02	0.42
33:b:1410:G:H2'	33:b:1411:U:C6	2.53	0.42
33:b:1623:G:H2'	33:b:1624:U:O2	2.19	0.42
33:b:2062:A:C6	55:z:158:ARG:HD2	2.55	0.42
52:w:56:PHE:CE1	52:w:61:LEU:HD21	2.55	0.42
9:A:376:G:O6	9:A:390:U:C5	2.72	0.42
9:A:637:C:H2'	9:A:638:U:C6	2.54	0.42
14:F:3:HIS:ND1	14:F:65:GLU:OE1	2.53	0.42
33:b:886:A:H2'	33:b:887:U:C6	2.54	0.42
33:b:1394:U:H2'	33:b:1395:A:O4'	2.19	0.42
33:b:2025:C:H2'	33:b:2026:U:C6	2.55	0.42
33:b:2649:C:H2'	33:b:2650:U:C6	2.54	0.42
43:n:69:PRO:HA	43:n:94:ALA:HB2	2.02	0.42
44:o:38:LEU:HB3	44:o:39:PRO:HD3	2.01	0.42
9:A:922:G:H2'	9:A:923:A:C8	2.54	0.42
9:A:1071:C:H2'	9:A:1072:G:C8	2.53	0.42
18:J:59:LYS:HE3	18:J:62:ARG:HH21	1.84	0.42
20:L:17:LYS:HA	20:L:17:LYS:HD3	1.86	0.42
20:L:99:GLY:N	20:L:104:SER:O	2.53	0.42
25:Q:46:HIS:HB2	25:Q:70:LYS:HE2	2.02	0.42
33:b:155:A:H2'	33:b:156:A:H8	1.84	0.42
33:b:278:A:C5	33:b:362:A:C5	3.08	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:37:U:O2'	9:A:547:A:N1	2.40	0.42
9:A:80:A:H2'	9:A:81:A:O4'	2.19	0.42
9:A:217:C:H4'	9:A:218:U:C5	2.54	0.42
9:A:1029:U:O2'	9:A:1032:G:N2	2.52	0.42
12:D:49:ASP:OD1	12:D:49:ASP:N	2.52	0.42
12:D:182:LYS:HE2	12:D:182:LYS:HB3	1.89	0.42
19:K:79:LYS:HD2	19:K:80:ASN:N	2.33	0.42
19:K:110:THR:HB	29:U:2:VAL:HG13	2.01	0.42
27:S:15:LEU:HD23	27:S:16:LYS:HD2	2.01	0.42
30:X:9:A:H4'	30:X:45:G:C2'	2.50	0.42
33:b:580:U:H2'	33:b:581:C:C6	2.55	0.42
33:b:890:C:N3	33:b:891:G:O2'	2.50	0.42
33:b:2186:G:H3'	33:b:2187:U:C5	2.54	0.42
39:h:115:VAL:HG12	39:h:132:PHE:CE2	2.55	0.42
9:A:144:G:H2'	9:A:145:G:O4'	2.20	0.42
9:A:493:A:H1'	9:A:494:G:N7	2.35	0.42
9:A:552:U:H2'	9:A:553:A:H8	1.85	0.42
9:A:715:A:H2'	9:A:716:A:C8	2.55	0.42
9:A:838:G:H2'	9:A:839:C:C6	2.55	0.42
9:A:1010:U:H2'	9:A:1011:C:C6	2.54	0.42
9:A:1268:G:H2'	9:A:1269:A:C8	2.55	0.42
10:B:130:LYS:HA	10:B:130:LYS:HD3	1.84	0.42
22:N:30:ILE:HD13	22:N:30:ILE:HA	1.91	0.42
24:P:55:ASP:OD1	24:P:56:ARG:N	2.52	0.42
30:X:19:G:H21	30:X:57:G:H1	1.67	0.42
33:b:172:A:H2'	33:b:173:A:C8	2.54	0.42
33:b:358:U:H2'	33:b:359:G:C8	2.55	0.42
33:b:1177:G:H2'	33:b:1178:C:C6	2.55	0.42
36:e:136:GLN:OE1	36:e:139:LYS:NZ	2.52	0.42
42:m:1:MET:HE2	42:m:1:MET:HA	2.01	0.42
9:A:272:C:H2'	9:A:273:U:C6	2.54	0.42
9:A:580:C:H2'	9:A:581:G:O4'	2.19	0.42
9:A:821:G:H2'	9:A:822:U:C6	2.54	0.42
20:L:42:LYS:HG2	20:L:43:LYS:H	1.85	0.42
22:N:72:PHE:CZ	22:N:77:GLY:HA2	2.55	0.42
33:b:827:U:O2'	33:b:2068:U:C2	2.72	0.42
33:b:1067:A:H61	33:b:1095:A:P	2.42	0.42
33:b:1497:U:H5''	33:b:1498:C:OP2	2.20	0.42
33:b:1548:A:H2'	33:b:1549:A:C8	2.54	0.42
33:b:1713:A:H61	33:b:1745:A:H62	1.67	0.42
33:b:2052:A:H4'	35:d:148:GLN:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:2119:A:C2	33:b:2169:A:H2'	2.55	0.42
34:c:145:GLU:HG2	34:c:151:GLY:C	2.45	0.42
36:e:5:LEU:HB2	36:e:10:SER:H	1.84	0.42
46:q:3:ASN:HA	46:q:6:LYS:HE3	2.02	0.42
51:v:53:ASN:C	51:v:55:PRO:HD3	2.45	0.42
54:y:10:THR:HG22	54:y:12:ASN:H	1.85	0.42
1:0:28:ARG:NH2	33:b:1365:A:H5''	2.35	0.42
2:1:5:GLU:H	2:1:5:GLU:CD	2.24	0.42
9:A:458:U:H3	9:A:474:G:N2	2.18	0.42
9:A:493:A:H1'	9:A:494:G:C5	2.55	0.42
9:A:1035:A:H8	9:A:1036:A:N7	2.17	0.42
9:A:1055:A:C6	9:A:1206:G:C5	3.08	0.42
9:A:1208:C:C2'	9:A:1209:C:H5'	2.49	0.42
9:A:1305:G:HO2'	9:A:1306:A:H8	1.67	0.42
10:B:108:GLN:OE1	10:B:108:GLN:N	2.52	0.42
12:D:113:ALA:O	12:D:117:VAL:HG23	2.19	0.42
14:F:68:GLN:OE1	14:F:68:GLN:N	2.45	0.42
21:M:15:VAL:O	21:M:19:THR:HG23	2.20	0.42
30:X:50:C:H2'	30:X:51:G:H5'	2.01	0.42
33:b:476:G:N1	33:b:479:A:OP2	2.51	0.42
33:b:640:C:H2'	33:b:641:U:H6	1.85	0.42
33:b:2032:G:N2	35:d:151:THR:OG1	2.52	0.42
37:f:8:TYR:HA	37:f:12:VAL:HB	2.02	0.42
52:w:10:LYS:HE2	52:w:10:LYS:HB2	1.86	0.42
9:A:8:A:N6	12:D:201:GLU:O	2.52	0.42
9:A:246:A:C2	9:A:282:A:C5	3.07	0.42
9:A:1033:G:H2'	9:A:1034:G:C8	2.54	0.42
9:A:1072:G:H2'	9:A:1073:U:C6	2.54	0.42
13:E:158:LYS:HB3	13:E:162:GLU:OE2	2.20	0.42
30:X:19:G:C6	33:b:2112:G:H1'	2.55	0.42
33:b:1055:G:C6	33:b:1056:G:N2	2.88	0.42
33:b:2064:C:H2'	33:b:2065:C:H6	1.85	0.42
9:A:186:C:N4	9:A:187:G:C6	2.88	0.41
9:A:744:C:H2'	9:A:745:G:C8	2.54	0.41
12:D:132:ALA:O	12:D:134:TYR:N	2.53	0.41
15:G:78:ARG:HB2	15:G:83:THR:HA	2.01	0.41
15:G:102:TRP:O	15:G:105:GLU:HG3	2.19	0.41
17:I:44:ARG:O	17:I:48:ARG:HG2	2.20	0.41
33:b:886:A:O2'	33:b:887:U:O4'	2.26	0.41
33:b:1094:U:O4	33:b:1099:G:C6	2.73	0.41
33:b:2106:U:C2	33:b:2183:A:C8	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:2142:A:H2'	33:b:2143:C:O4'	2.20	0.41
33:b:2682:A:H61	33:b:2728:U:H1'	1.84	0.41
41:l:40:LYS:HE2	41:l:57:VAL:HG12	2.01	0.41
41:l:92:GLU:HG2	41:l:111:LYS:NZ	2.34	0.41
8:8:16:ILE:HG12	8:8:25:VAL:HG22	2.01	0.41
9:A:259:G:C4	9:A:260:G:C8	3.08	0.41
17:I:87:MET:HE2	17:I:87:MET:HA	2.01	0.41
18:J:17:LEU:HD13	18:J:96:VAL:HG22	2.02	0.41
20:L:87:LYS:C	20:L:89:LEU:H	2.27	0.41
30:X:50:C:C2'	30:X:51:G:H5'	2.49	0.41
31:Y:67:A:H2'	31:Y:68:U:H4'	2.02	0.41
33:b:634:C:H2'	33:b:635:C:C6	2.55	0.41
33:b:1509:A:O2'	33:b:1510:G:C8	2.73	0.41
33:b:2071:A:H2'	33:b:2072:C:C6	2.55	0.41
35:d:157:LYS:HB2	35:d:157:LYS:HE3	1.84	0.41
36:e:5:LEU:HD11	36:e:12:LEU:HD13	2.02	0.41
9:A:1283:U:H2'	9:A:1284:C:O4'	2.20	0.41
9:A:1318:A:H1'	27:S:36:ARG:HH11	1.84	0.41
19:K:79:LYS:CD	19:K:80:ASN:HD22	2.33	0.41
25:Q:57:VAL:HB	25:Q:79:GLU:HB3	2.02	0.41
27:S:19:GLU:O	27:S:22:VAL:HG12	2.20	0.41
33:b:1738:G:O2'	33:b:1739:A:H8	2.03	0.41
33:b:2788:C:H2'	33:b:2789:C:C6	2.56	0.41
39:h:59:ALA:HA	39:h:62:LEU:HD12	2.01	0.41
41:l:51:LYS:HE2	41:l:51:LYS:HB2	1.91	0.41
4:4:9:THR:HG21	33:b:2020:A:H5'	2.02	0.41
5:5:13:SER:HB3	5:5:49:TYR:CZ	2.55	0.41
9:A:78:A:H3'	9:A:79:G:H5''	2.01	0.41
9:A:384:G:H2'	9:A:385:C:H6	1.81	0.41
9:A:478:A:C2'	9:A:479:U:H4'	2.47	0.41
9:A:592:G:H2'	9:A:593:U:C6	2.54	0.41
9:A:1024:G:O2'	9:A:1025:U:O4'	2.19	0.41
9:A:1157:A:H1'	9:A:1181:G:N2	2.36	0.41
10:B:141:GLU:O	10:B:144:GLU:HG3	2.21	0.41
12:D:104:MET:HG2	12:D:172:VAL:HG22	2.02	0.41
14:F:72:ASP:OD1	14:F:72:ASP:N	2.52	0.41
21:M:33:LEU:HD23	21:M:33:LEU:HA	1.89	0.41
22:N:30:ILE:HD11	22:N:44:VAL:N	2.36	0.41
24:P:69:ASP:OD1	24:P:69:ASP:N	2.42	0.41
29:U:4:LYS:HD3	29:U:5:VAL:N	2.34	0.41
30:X:18:G:H4'	30:X:59:G:H1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:54:G:H2'	31:Z:55:U:C6	2.55	0.41
33:b:644:A:H2'	33:b:645:C:O4'	2.20	0.41
33:b:1062:G:H2'	33:b:1063:G:C8	2.56	0.41
33:b:2162:G:H8	33:b:2163:A:C2	2.39	0.41
33:b:2700:A:H2'	33:b:2701:U:C6	2.55	0.41
9:A:39:G:C6	9:A:404:G:C6	3.09	0.41
10:B:83:ALA:C	10:B:85:SER:H	2.29	0.41
10:B:153:MET:HE3	10:B:155:GLY:HA2	2.02	0.41
12:D:8:LEU:HD23	12:D:12:ARG:HD3	2.02	0.41
12:D:104:MET:O	12:D:172:VAL:HG11	2.20	0.41
16:H:58:LEU:HD12	16:H:59:GLU:H	1.86	0.41
33:b:2858:C:O2'	33:b:2859:G:O4'	2.39	0.41
51:v:47:LYS:HE3	51:v:47:LYS:HB2	1.74	0.41
2:1:7:ARG:NH2	33:b:78:U:H5'	2.35	0.41
2:1:10:SER:OG	2:1:11:VAL:N	2.54	0.41
9:A:374:A:O2'	9:A:375:U:O4'	2.37	0.41
9:A:428:G:H5''	12:D:9:LYS:NZ	2.35	0.41
9:A:531:U:H4'	9:A:532:A:H5'	2.02	0.41
9:A:1120:C:H2'	9:A:1121:U:H6	1.85	0.41
26:R:64:LEU:HD23	26:R:64:LEU:HA	1.92	0.41
33:b:2:G:H2'	33:b:3:U:C6	2.56	0.41
33:b:871:U:H2'	33:b:872:U:C6	2.55	0.41
33:b:2813:A:H2'	33:b:2814:A:H8	1.86	0.41
40:k:69:ARG:HD2	40:k:69:ARG:HA	1.80	0.41
55:z:153[A]:SER:HB2	55:z:154[A]:TRP:H	1.58	0.41
9:A:198:G:C6	9:A:219:U:O2	2.73	0.41
9:A:203:G:N2	9:A:204:G:O6	2.53	0.41
9:A:545:C:H5'	12:D:68:GLU:CD	2.46	0.41
10:B:27:LYS:N	10:B:28:PRO:HD2	2.36	0.41
12:D:9:LYS:HA	12:D:9:LYS:HD3	1.93	0.41
26:R:8:LYS:HB2	26:R:8:LYS:HE2	1.82	0.41
27:S:79:TYR:CZ	27:S:81:GLY:HA2	2.56	0.41
33:b:1066:U:O2'	33:b:1095:A:N1	2.44	0.41
33:b:2190:G:H3'	33:b:2191:A:H8	1.86	0.41
33:b:2547:A:H2'	33:b:2548:U:C6	2.56	0.41
36:e:124:PHE:HE2	36:e:141:MET:HE1	1.86	0.41
46:q:33:VAL:HG22	46:q:38:LYS:HB3	2.01	0.41
9:A:32:A:N1	9:A:552:U:H5	2.19	0.41
9:A:235:C:H2'	9:A:236:A:H8	1.86	0.41
9:A:391:G:P	24:P:28:ARG:HH22	2.43	0.41
9:A:613:C:H2'	9:A:614:C:H6	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:908:A:H2'	9:A:909:A:C8	2.55	0.41
17:I:21:LYS:HB3	17:I:61:ASP:HB2	2.02	0.41
19:K:71:ASP:O	19:K:74:LYS:NZ	2.42	0.41
23:O:70:LYS:HE2	23:O:77:TYR:CZ	2.56	0.41
30:X:52:A:H2'	30:X:53:G:H8	1.86	0.41
31:Y:16:C:O2'	31:Y:61:U:O3'	2.38	0.41
31:Z:26:C:C2	31:Z:27:A:C8	3.09	0.41
31:Z:31:C:N4	31:Z:41:G:H22	2.19	0.41
33:b:17:G:H2'	33:b:18:U:C6	2.55	0.41
33:b:2117:A:H61	33:b:2170:A:N6	2.18	0.41
33:b:2162:G:H5''	33:b:2163:A:OP1	2.21	0.41
9:A:299:G:H2'	9:A:300:A:C8	2.55	0.41
9:A:417:G:H2'	9:A:418:C:H6	1.86	0.41
9:A:429:U:OP1	12:D:9:LYS:NZ	2.46	0.41
9:A:472:U:H3'	9:A:473:U:C5	2.56	0.41
9:A:985:C:H2'	9:A:986:U:C6	2.56	0.41
9:A:1412:C:H2'	9:A:1413:A:H8	1.86	0.41
11:C:61:LYS:HD3	11:C:61:LYS:HA	1.88	0.41
12:D:203:TYR:HD1	12:D:203:TYR:HA	1.74	0.41
14:F:67:PRO:HB2	14:F:69:GLU:CD	2.46	0.41
18:J:37:ARG:NH2	18:J:75:ASP:OD2	2.54	0.41
20:L:70:GLY:N	20:L:98:ARG:HH12	2.18	0.41
20:L:73:LEU:HD22	20:L:79:ILE:HD11	2.02	0.41
28:T:70:LYS:HG3	28:T:73:ARG:HH21	1.86	0.41
33:b:118:A:H5'	33:b:119:A:H8	1.86	0.41
33:b:352:A:H2'	33:b:353:C:C6	2.56	0.41
33:b:511:U:O2'	33:b:512:G:OP1	2.26	0.41
33:b:1095:A:OP1	33:b:1096:A:H8	2.04	0.41
33:b:1275:A:H4'	33:b:1276:A:OP1	2.21	0.41
33:b:1353:A:H2'	33:b:1354:A:H8	1.86	0.41
33:b:1432:G:H2'	33:b:1433:A:C8	2.56	0.41
33:b:2130:U:C5	33:b:2131:U:H5	2.39	0.41
33:b:2193:G:H2'	33:b:2194:U:H6	1.86	0.41
33:b:2327:A:H2'	33:b:2328:A:C8	2.56	0.41
37:f:104:ILE:HD12	37:f:104:ILE:HA	1.92	0.41
38:g:117:LEU:HD23	38:g:117:LEU:HA	1.89	0.41
39:h:119:ASN:OD1	39:h:119:ASN:N	2.54	0.41
40:k:12:LYS:HD2	40:k:12:LYS:HA	1.80	0.41
41:l:4:GLU:OE1	41:l:4:GLU:N	2.43	0.41
41:l:109:SER:C	41:l:111:LYS:H	2.29	0.41
42:m:36:LYS:HB3	42:m:36:LYS:HE3	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:t:83:LYS:C	49:t:84:ARG:HD2	2.46	0.41
51:v:33:LYS:HB3	51:v:64:ALA:HB1	2.03	0.41
9:A:736:C:H2'	9:A:737:C:C6	2.56	0.41
11:C:33:ASP:O	11:C:37:LYS:HG2	2.21	0.41
18:J:7:ARG:HB2	18:J:101:SER:OG	2.21	0.41
20:L:43:LYS:HB3	20:L:44:PRO:HD3	2.03	0.41
23:O:19:ASN:OD1	23:O:19:ASN:N	2.52	0.41
27:S:40:PHE:HB2	27:S:43:MET:SD	2.61	0.41
33:b:555:G:O2'	33:b:556:A:H8	2.04	0.41
33:b:1022:G:H22	33:b:1142:A:H2	1.69	0.41
33:b:1304:A:N1	33:b:1624:U:H5	2.18	0.41
33:b:2273:A:H2'	33:b:2274:A:C8	2.56	0.41
33:b:2412:A:H2'	33:b:2413:G:O4'	2.20	0.41
33:b:2667:C:N3	38:g:110:SER:OG	2.48	0.41
35:d:146:ILE:HD13	35:d:146:ILE:HA	1.84	0.41
41:l:71:ARG:HA	41:l:71:ARG:HD3	1.85	0.41
44:o:79:LEU:HD23	44:o:83:LEU:HD12	2.02	0.41
50:u:88:LYS:HB3	50:u:92:ASN:ND2	2.36	0.41
9:A:93:U:H5	9:A:94:G:H21	1.69	0.40
9:A:435:A:H2'	9:A:436:C:C6	2.56	0.40
9:A:976:G:OP2	9:A:1358:U:O2'	2.37	0.40
9:A:979:C:O2	22:N:58:ARG:NE	2.53	0.40
10:B:132:GLU:HA	10:B:135:MET:HG3	2.03	0.40
11:C:116:ALA:O	11:C:120:THR:HG23	2.21	0.40
18:J:46:LYS:HG2	18:J:68:ARG:HG2	2.02	0.40
20:L:100:ALA:HB3	20:L:103:CYS:SG	2.61	0.40
31:Y:21:U:O4	31:Y:60:A:N6	2.51	0.40
31:Z:54:G:H2'	31:Z:55:U:H6	1.86	0.40
33:b:1532:A:N6	33:b:1540:G:O6	2.53	0.40
34:c:121:ASP:N	34:c:121:ASP:OD1	2.51	0.40
36:e:6:LYS:HB3	36:e:6:LYS:HE3	1.83	0.40
48:s:79:ARG:C	48:s:80:ARG:HG2	2.46	0.40
2:1:5:GLU:OE1	2:1:5:GLU:N	2.44	0.40
9:A:636:U:H2'	9:A:637:C:H6	1.86	0.40
15:G:53:SER:HB2	15:G:55:LYS:HE2	2.03	0.40
31:Z:24:C:H2'	31:Z:25:G:H8	1.86	0.40
33:b:263:G:H2'	33:b:264:C:O4'	2.22	0.40
33:b:709:U:H2'	33:b:710:U:C6	2.56	0.40
33:b:1583:A:O2'	33:b:1585:C:N4	2.54	0.40
33:b:1883:U:H2'	33:b:1884:G:O4'	2.21	0.40
38:g:24:ILE:HD13	38:g:72:LEU:HD11	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:s:31:GLU:OE1	48:s:31:GLU:N	2.39	0.40
49:t:31:GLN:HA	49:t:34:ASP:OD2	2.21	0.40
51:v:81:ASP:OD1	51:v:82:ARG:N	2.51	0.40
9:A:457:G:C4	9:A:458:U:H1'	2.56	0.40
9:A:619:U:H4'	12:D:127:ARG:NH2	2.36	0.40
9:A:841:C:H2'	9:A:843:U:C5	2.57	0.40
9:A:1010:U:H2'	9:A:1011:C:H6	1.86	0.40
10:B:114:LYS:O	10:B:117:GLU:HG3	2.21	0.40
12:D:12:ARG:HB3	12:D:37:PRO:HG3	2.02	0.40
17:I:32:ARG:NH2	17:I:37:TYR:HA	2.36	0.40
19:K:37:GLN:OE1	19:K:37:GLN:N	2.55	0.40
20:L:119:LYS:HD3	20:L:119:LYS:HA	1.83	0.40
33:b:534:U:O2'	47:r:49:ASP:OD2	2.22	0.40
33:b:657:U:H2'	33:b:658:U:C6	2.56	0.40
33:b:980:A:N7	33:b:1136:G:H5''	2.37	0.40
33:b:1022:G:N7	40:k:68:LYS:HE2	2.36	0.40
33:b:1050:A:H2'	33:b:1050:A:N3	2.36	0.40
33:b:1292:G:H2'	33:b:1293:C:C6	2.57	0.40
2:1:47:ARG:NH2	33:b:61:C:OP2	2.55	0.40
9:A:92:U:H2'	9:A:93:U:O2	2.21	0.40
9:A:182:A:C4	9:A:184:G:C8	3.09	0.40
9:A:467:U:H5'	9:A:468:A:N1	2.37	0.40
9:A:486:U:H3'	9:A:487:A:H8	1.86	0.40
9:A:642:A:C5	16:H:106:SER:HA	2.56	0.40
14:F:13:ASP:OD1	14:F:14:GLN:HG2	2.21	0.40
15:G:69:ARG:HA	15:G:70:PRO:HD3	1.98	0.40
23:O:25:GLU:H	23:O:25:GLU:CD	2.28	0.40
25:Q:61:ARG:HD2	25:Q:62:GLU:H	1.87	0.40
27:S:12:LEU:O	27:S:15:LEU:N	2.54	0.40
33:b:219:A:N3	33:b:234:U:O2'	2.52	0.40
33:b:1927:A:O2'	33:b:1928:A:C8	2.69	0.40
33:b:2038:G:H2'	33:b:2039:U:O4'	2.22	0.40
42:m:112:LEU:HD12	42:m:130:GLY:HA3	2.04	0.40
45:p:45:SER:OG	45:p:46:GLU:OE2	2.39	0.40
50:u:69:ARG:HE	50:u:74:ILE:HD13	1.86	0.40
52:w:65:VAL:HG22	52:w:66:ASP:OD1	2.22	0.40
2:1:38:GLN:OE1	2:1:38:GLN:N	2.50	0.40
9:A:235:C:H2'	9:A:236:A:C8	2.57	0.40
9:A:719:C:O2'	9:A:720:C:OP1	2.37	0.40
10:B:100:LEU:HB3	10:B:178:LEU:CD1	2.51	0.40
15:G:16:LYS:HG3	15:G:17:PHE:CD2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:41:GLU:HG2	17:I:42:THR:H	1.86	0.40
17:I:59:LYS:HB2	17:I:59:LYS:HE2	1.83	0.40
21:M:22:TYR:O	21:M:22:TYR:CG	2.74	0.40
33:b:78:U:H2'	33:b:79:C:H6	1.87	0.40
33:b:882:G:N1	33:b:895:U:O2	2.55	0.40
33:b:1425:G:H2'	33:b:1426:G:C8	2.55	0.40
39:h:132:PHE:HE1	39:h:142:VAL:HB	1.86	0.40
47:r:86:ALA:O	47:r:87:SER:OG	2.34	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	
1	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
2	1	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
3	2	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
4	4	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
5	5	50/55 (91%)	47 (94%)	3 (6%)	0	100	100
6	6	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
7	7	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	8	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
10	B	216/241 (90%)	192 (89%)	24 (11%)	0	100	100
11	C	205/233 (88%)	191 (93%)	14 (7%)	0	100	100
12	D	203/206 (98%)	179 (88%)	24 (12%)	0	100	100
13	E	155/167 (93%)	136 (88%)	19 (12%)	0	100	100
14	F	104/135 (77%)	92 (88%)	12 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	G	151/179 (84%)	142 (94%)	9 (6%)	0	100	100
16	H	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
17	I	125/130 (96%)	107 (86%)	18 (14%)	0	100	100
18	J	98/103 (95%)	89 (91%)	9 (9%)	0	100	100
19	K	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
20	L	120/124 (97%)	98 (82%)	22 (18%)	0	100	100
21	M	114/118 (97%)	104 (91%)	10 (9%)	0	100	100
22	N	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
23	O	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
24	P	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
25	Q	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
26	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
27	S	81/92 (88%)	75 (93%)	6 (7%)	0	100	100
28	T	84/87 (97%)	84 (100%)	0	0	100	100
29	U	62/71 (87%)	58 (94%)	4 (6%)	0	100	100
34	c	269/273 (98%)	252 (94%)	17 (6%)	0	100	100
35	d	207/209 (99%)	196 (95%)	11 (5%)	0	100	100
36	e	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
37	f	176/179 (98%)	159 (90%)	17 (10%)	0	100	100
38	g	173/177 (98%)	160 (92%)	13 (8%)	0	100	100
39	h	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
40	k	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
41	l	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
42	m	142/144 (99%)	128 (90%)	14 (10%)	0	100	100
43	n	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
44	o	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
45	p	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
46	q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
47	r	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
48	s	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
49	t	108/110 (98%)	102 (94%)	6 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	u	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
51	v	101/104 (97%)	90 (89%)	11 (11%)	0	100	100
52	w	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
54	y	82/85 (96%)	79 (96%)	3 (4%)	0	100	100
55	z	32/26 (123%)	24 (75%)	8 (25%)	0	100	100
All	All	5582/5869 (95%)	5169 (93%)	413 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	0	67/68 (98%)	67 (100%)	0	100	100
2	1	54/55 (98%)	54 (100%)	0	100	100
3	2	48/49 (98%)	48 (100%)	0	100	100
4	4	47/48 (98%)	47 (100%)	0	100	100
5	5	47/49 (96%)	47 (100%)	0	100	100
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	51 (100%)	0	100	100
8	8	34/34 (100%)	34 (100%)	0	100	100
10	B	180/199 (90%)	180 (100%)	0	100	100
11	C	171/190 (90%)	171 (100%)	0	100	100
12	D	172/173 (99%)	172 (100%)	0	100	100
13	E	119/126 (94%)	119 (100%)	0	100	100
14	F	92/116 (79%)	92 (100%)	0	100	100
15	G	126/147 (86%)	126 (100%)	0	100	100
16	H	104/105 (99%)	104 (100%)	0	100	100
17	I	105/107 (98%)	105 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	J	88/90 (98%)	88 (100%)	0	100	100
19	K	90/99 (91%)	89 (99%)	1 (1%)	65	84
20	L	103/104 (99%)	103 (100%)	0	100	100
21	M	94/96 (98%)	94 (100%)	0	100	100
22	N	83/84 (99%)	83 (100%)	0	100	100
23	O	76/77 (99%)	76 (100%)	0	100	100
24	P	65/65 (100%)	64 (98%)	1 (2%)	57	80
25	Q	74/78 (95%)	74 (100%)	0	100	100
26	R	57/65 (88%)	57 (100%)	0	100	100
27	S	72/79 (91%)	72 (100%)	0	100	100
28	T	65/66 (98%)	65 (100%)	0	100	100
29	U	54/61 (88%)	54 (100%)	0	100	100
34	c	216/218 (99%)	216 (100%)	0	100	100
35	d	164/164 (100%)	164 (100%)	0	100	100
36	e	165/165 (100%)	164 (99%)	1 (1%)	78	91
37	f	149/150 (99%)	146 (98%)	3 (2%)	48	74
38	g	136/138 (99%)	134 (98%)	2 (2%)	57	80
39	h	113/114 (99%)	112 (99%)	1 (1%)	70	87
40	k	116/116 (100%)	116 (100%)	0	100	100
41	l	104/104 (100%)	104 (100%)	0	100	100
42	m	103/103 (100%)	103 (100%)	0	100	100
43	n	109/109 (100%)	109 (100%)	0	100	100
44	o	100/103 (97%)	100 (100%)	0	100	100
45	p	86/87 (99%)	85 (99%)	1 (1%)	63	83
46	q	99/100 (99%)	99 (100%)	0	100	100
47	r	89/90 (99%)	89 (100%)	0	100	100
48	s	84/84 (100%)	83 (99%)	1 (1%)	63	83
49	t	93/93 (100%)	93 (100%)	0	100	100
50	u	84/84 (100%)	84 (100%)	0	100	100
51	v	83/85 (98%)	83 (100%)	0	100	100
52	w	78/78 (100%)	78 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	y	62/63 (98%)	62 (100%)	0	100	100
55	z	27/21 (129%)	22 (82%)	5 (18%)	1	3
All	All	4636/4789 (97%)	4620 (100%)	16 (0%)	84	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	K	108	ASN
24	P	54	LEU
36	e	67	ARG
37	f	91	LEU
37	f	149	VAL
37	f	152	LEU
38	g	10	VAL
38	g	90	VAL
39	h	129	GLU
45	p	83	LEU
48	s	51	VAL
55	z	143	GLU
55	z	146	ARG
55	z	147	GLN
55	z	150[A]	TYR
55	z	150[B]	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	6	GLN
2	1	20	ASN
5	5	26	ASN
10	B	176	ASN
11	C	99	GLN
11	C	101	ASN
12	D	151	GLN
12	D	163	GLN
12	D	195	ASN
13	E	134	ASN
15	G	85	GLN
16	H	3	GLN
16	H	17	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	I	4	GLN
19	K	39	ASN
20	L	74	GLN
22	N	42	ASN
23	O	27	GLN
23	O	50	HIS
24	P	29	ASN
24	P	59	HIS
28	T	12	GLN
28	T	20	ASN
28	T	69	ASN
34	c	25	HIS
34	c	53	HIS
34	c	260	ASN
35	d	140	HIS
36	e	92	HIS
36	e	115	GLN
37	f	5	HIS
39	h	2	GLN
39	h	33	GLN
41	l	3	GLN
41	l	82	ASN
42	m	54	GLN
45	p	19	GLN
46	q	115	ASN
47	r	44	GLN
52	w	75	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	X	75/76 (98%)	32 (42%)	1 (1%)
31	Y	76/77 (98%)	25 (32%)	2 (2%)
31	Z	76/77 (98%)	17 (22%)	1 (1%)
32	a	119/120 (99%)	19 (15%)	0
33	b	2901/2904 (99%)	574 (19%)	0
53	x	13/14 (92%)	3 (23%)	0
9	A	1532/1533 (99%)	338 (22%)	13 (0%)
All	All	4792/4801 (99%)	1008 (21%)	17 (0%)

All (1008) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	2	A
9	A	4	U
9	A	19	A
9	A	32	A
9	A	33	A
9	A	37	U
9	A	39	G
9	A	47	C
9	A	48	C
9	A	50	A
9	A	51	A
9	A	66	A
9	A	71	A
9	A	72	A
9	A	73	C
9	A	74	A
9	A	75	G
9	A	77	A
9	A	78	A
9	A	79	G
9	A	80	A
9	A	81	A
9	A	83	C
9	A	84	U
9	A	85	U
9	A	86	G
9	A	88	U
9	A	89	U
9	A	91	U
9	A	94	G
9	A	95	C
9	A	97	G
9	A	109	A
9	A	121	U
9	A	122	G
9	A	130	A
9	A	138	G
9	A	141	G
9	A	144	G
9	A	159	G
9	A	160	A
9	A	163	C
9	A	181	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	185	U
9	A	189	A
9	A	196	A
9	A	197	A
9	A	200	G
9	A	204	G
9	A	205	A
9	A	208	U
9	A	209	U
9	A	210	C
9	A	214	C
9	A	215	C
9	A	218	U
9	A	219	U
9	A	222	C
9	A	224	U
9	A	226	G
9	A	228	A
9	A	231	U
9	A	239	U
9	A	240	G
9	A	245	U
9	A	247	G
9	A	251	G
9	A	257	G
9	A	262	A
9	A	263	A
9	A	266	G
9	A	267	C
9	A	275	G
9	A	279	A
9	A	280	C
9	A	283	U
9	A	286	C
9	A	289	G
9	A	293	G
9	A	321	A
9	A	328	C
9	A	343	U
9	A	352	C
9	A	354	G
9	A	360	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	364	A
9	A	365	U
9	A	367	U
9	A	369	G
9	A	371	A
9	A	372	C
9	A	374	A
9	A	376	G
9	A	377	G
9	A	378	G
9	A	382	A
9	A	390	U
9	A	391	G
9	A	392	C
9	A	397	A
9	A	398	U
9	A	406	G
9	A	409	U
9	A	411	A
9	A	412	A
9	A	413	G
9	A	414	A
9	A	415	A
9	A	420	U
9	A	421	U
9	A	422	C
9	A	423	G
9	A	424	G
9	A	428	G
9	A	429	U
9	A	435	A
9	A	436	C
9	A	438	U
9	A	439	U
9	A	444	G
9	A	448	A
9	A	449	G
9	A	452	A
9	A	457	G
9	A	458	U
9	A	459	A
9	A	460	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	461	A
9	A	462	G
9	A	467	U
9	A	468	A
9	A	479	U
9	A	481	G
9	A	484	G
9	A	485	U
9	A	486	U
9	A	491	G
9	A	492	C
9	A	493	A
9	A	495	A
9	A	496	A
9	A	497	G
9	A	509	A
9	A	510	A
9	A	511	C
9	A	513	C
9	A	517	G
9	A	518	C
9	A	521	G
9	A	527	G
9	A	530	G
9	A	531	U
9	A	532	A
9	A	533	A
9	A	534	U
9	A	535	A
9	A	541	G
9	A	547	A
9	A	548	G
9	A	549	C
9	A	572	A
9	A	573	A
9	A	576	C
9	A	577	G
9	A	588	G
9	A	589	U
9	A	591	U
9	A	593	U
9	A	615	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	629	A
9	A	632	U
9	A	633	G
9	A	653	U
9	A	665	A
9	A	687	A
9	A	720	C
9	A	721	G
9	A	723	U
9	A	724	G
9	A	731	G
9	A	755	G
9	A	760	G
9	A	761	G
9	A	777	A
9	A	781	A
9	A	787	A
9	A	792	A
9	A	793	U
9	A	794	A
9	A	815	A
9	A	817	C
9	A	821	G
9	A	828	U
9	A	841	C
9	A	842	U
9	A	843	U
9	A	844	G
9	A	849	G
9	A	872	A
9	A	891	U
9	A	900	A
9	A	902	G
9	A	914	A
9	A	918	A
9	A	926	G
9	A	927	G
9	A	933	G
9	A	934	C
9	A	935	A
9	A	945	G
9	A	947	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	960	U
9	A	966	G
9	A	969	A
9	A	971	G
9	A	975	A
9	A	976	G
9	A	977	A
9	A	981	U
9	A	992	U
9	A	993	G
9	A	994	A
9	A	995	C
9	A	998	C
9	A	1003	G
9	A	1004	A
9	A	1013	G
9	A	1019	A
9	A	1020	G
9	A	1022	A
9	A	1024	G
9	A	1028	C
9	A	1029	U
9	A	1030	U
9	A	1034	G
9	A	1035	A
9	A	1036	A
9	A	1039	G
9	A	1041	G
9	A	1046	A
9	A	1049	U
9	A	1053	G
9	A	1065	U
9	A	1066	C
9	A	1094	G
9	A	1095	U
9	A	1101	A
9	A	1121	U
9	A	1134	G
9	A	1137	C
9	A	1138	G
9	A	1139	G
9	A	1140	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1145	A
9	A	1157	A
9	A	1159	U
9	A	1160	G
9	A	1167	A
9	A	1168	U
9	A	1169	A
9	A	1174	G
9	A	1181	G
9	A	1183	U
9	A	1184	G
9	A	1188	A
9	A	1189	U
9	A	1193	G
9	A	1196	A
9	A	1197	A
9	A	1201	A
9	A	1202	U
9	A	1208	C
9	A	1209	C
9	A	1210	C
9	A	1212	U
9	A	1213	A
9	A	1214	C
9	A	1227	A
9	A	1230	C
9	A	1238	A
9	A	1241	G
9	A	1248	A
9	A	1256	A
9	A	1257	A
9	A	1258	G
9	A	1259	C
9	A	1260	G
9	A	1263	C
9	A	1266	G
9	A	1280	A
9	A	1281	C
9	A	1285	A
9	A	1287	A
9	A	1292	G
9	A	1293	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1300	G
9	A	1302	C
9	A	1303	C
9	A	1305	G
9	A	1307	U
9	A	1316	G
9	A	1317	C
9	A	1320	C
9	A	1343	G
9	A	1346	A
9	A	1347	G
9	A	1349	A
9	A	1358	U
9	A	1362	A
9	A	1363	A
9	A	1364	U
9	A	1370	G
9	A	1394	A
9	A	1397	C
9	A	1419	G
9	A	1429	A
9	A	1441	A
9	A	1442	G
9	A	1445	U
9	A	1446	A
9	A	1450	U
9	A	1452	C
9	A	1454	G
9	A	1471	U
9	A	1472	U
9	A	1487	G
9	A	1492	A
9	A	1494	G
9	A	1497	G
9	A	1503	A
9	A	1506	U
9	A	1507	A
9	A	1517	G
9	A	1519	A
9	A	1520	C
9	A	1529	G
9	A	1530	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1533	C
30	X	4	G
30	X	5	G
30	X	6	A
30	X	8	U
30	X	9	A
30	X	16	U
30	X	17	U
30	X	19	G
30	X	21	A
30	X	24	G
30	X	25	C
30	X	29	A
30	X	38	A
30	X	40	G
30	X	42	C
30	X	43	G
30	X	45	G
30	X	46	G
30	X	47	U
30	X	48	C
30	X	49	G
30	X	51	G
30	X	56	C
30	X	57	G
30	X	59	G
30	X	60	U
30	X	61	C
30	X	62	U
30	X	66	U
30	X	67	U
30	X	71	G
30	X	76	A
31	Y	4	U
31	Y	5	G
31	Y	6	A
31	Y	7	U
31	Y	8	U
31	Y	9	G
31	Y	16	C
31	Y	17	C
31	Y	18	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	Y	19	G
31	Y	20	G
31	Y	21	U
31	Y	22	A
31	Y	47	G
31	Y	48	U
31	Y	49	C
31	Y	50	G
31	Y	62	C
31	Y	63	C
31	Y	64	U
31	Y	65	C
31	Y	67	A
31	Y	68	U
31	Y	69	C
31	Y	77	A
31	Z	9	G
31	Z	12	G
31	Z	16	C
31	Z	17	C
31	Z	18	U
31	Z	20	G
31	Z	21	U
31	Z	23	G
31	Z	29	U
31	Z	37	G
31	Z	42	A
31	Z	50	G
31	Z	53	G
31	Z	65	C
31	Z	67	A
31	Z	74	A
31	Z	75	C
32	a	15	A
32	a	24	G
32	a	25	U
32	a	26	C
32	a	30	C
32	a	35	C
32	a	43	C
32	a	52	A
32	a	56	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	57	A
32	a	58	A
32	a	66	A
32	a	67	G
32	a	74	U
32	a	89	U
32	a	90	C
32	a	99	A
32	a	105	G
32	a	109	A
33	b	5	A
33	b	10	A
33	b	34	U
33	b	35	G
33	b	36	G
33	b	39	G
33	b	42	A
33	b	46	G
33	b	51	G
33	b	62	U
33	b	63	A
33	b	64	A
33	b	71	A
33	b	74	A
33	b	75	G
33	b	84	A
33	b	98	G
33	b	100	U
33	b	101	A
33	b	102	U
33	b	103	A
33	b	110	G
33	b	118	A
33	b	119	A
33	b	120	U
33	b	140	C
33	b	142	A
33	b	160	A
33	b	163	C
33	b	174	U
33	b	181	A
33	b	196	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	199	A
33	b	215	G
33	b	216	A
33	b	221	A
33	b	222	A
33	b	223	A
33	b	228	C
33	b	229	C
33	b	230	G
33	b	233	A
33	b	248	G
33	b	250	G
33	b	251	A
33	b	255	A
33	b	264	C
33	b	265	A
33	b	266	G
33	b	267	C
33	b	268	C
33	b	271	G
33	b	272	A
33	b	278	A
33	b	279	A
33	b	282	A
33	b	285	G
33	b	286	U
33	b	295	G
33	b	304	U
33	b	330	A
33	b	346	A
33	b	348	A
33	b	349	U
33	b	353	C
33	b	356	G
33	b	362	A
33	b	363	G
33	b	365	U
33	b	369	U
33	b	371	A
33	b	372	G
33	b	379	G
33	b	380	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	385	C
33	b	386	G
33	b	387	U
33	b	391	A
33	b	396	G
33	b	405	U
33	b	406	G
33	b	412	A
33	b	413	C
33	b	423	A
33	b	424	G
33	b	428	A
33	b	457	A
33	b	473	G
33	b	480	A
33	b	481	G
33	b	482	A
33	b	491	G
33	b	494	G
33	b	505	A
33	b	508	A
33	b	509	C
33	b	512	G
33	b	529	A
33	b	530	G
33	b	531	C
33	b	532	A
33	b	538	A
33	b	546	U
33	b	548	G
33	b	549	G
33	b	563	A
33	b	568	U
33	b	573	U
33	b	575	A
33	b	587	C
33	b	603	A
33	b	604	G
33	b	613	A
33	b	627	A
33	b	632	A
33	b	637	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	643	A
33	b	644	A
33	b	645	C
33	b	646	U
33	b	647	G
33	b	653	U
33	b	654	A
33	b	655	A
33	b	686	U
33	b	701	G
33	b	702	U
33	b	709	U
33	b	716	A
33	b	717	C
33	b	718	A
33	b	727	A
33	b	730	A
33	b	747	U
33	b	752	A
33	b	756	A
33	b	757	G
33	b	764	A
33	b	765	C
33	b	774	G
33	b	775	G
33	b	776	G
33	b	782	A
33	b	784	G
33	b	785	G
33	b	792	A
33	b	805	G
33	b	812	C
33	b	819	A
33	b	827	U
33	b	828	U
33	b	846	U
33	b	847	U
33	b	859	G
33	b	880	G
33	b	881	G
33	b	885	C
33	b	888	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	889	C
33	b	890	C
33	b	891	G
33	b	894	U
33	b	895	U
33	b	896	A
33	b	897	C
33	b	899	A
33	b	900	A
33	b	901	C
33	b	905	A
33	b	910	A
33	b	912	C
33	b	914	G
33	b	927	A
33	b	931	U
33	b	941	A
33	b	946	C
33	b	959	A
33	b	961	C
33	b	974	G
33	b	983	A
33	b	996	A
33	b	1005	C
33	b	1009	A
33	b	1012	U
33	b	1013	C
33	b	1022	G
33	b	1026	G
33	b	1033	U
33	b	1047	G
33	b	1051	G
33	b	1052	C
33	b	1055	G
33	b	1056	G
33	b	1057	A
33	b	1059	G
33	b	1060	U
33	b	1062	G
33	b	1064	C
33	b	1065	U
33	b	1066	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	1068	G
33	b	1069	A
33	b	1070	A
33	b	1072	C
33	b	1073	A
33	b	1074	G
33	b	1075	C
33	b	1076	C
33	b	1077	A
33	b	1078	U
33	b	1079	C
33	b	1081	U
33	b	1082	U
33	b	1083	U
33	b	1084	A
33	b	1085	A
33	b	1086	A
33	b	1087	G
33	b	1088	A
33	b	1092	C
33	b	1093	G
33	b	1094	U
33	b	1095	A
33	b	1096	A
33	b	1097	U
33	b	1098	A
33	b	1101	U
33	b	1102	C
33	b	1103	A
33	b	1104	C
33	b	1105	U
33	b	1107	G
33	b	1109	C
33	b	1112	G
33	b	1132	U
33	b	1133	A
33	b	1134	A
33	b	1135	C
33	b	1136	G
33	b	1142	A
33	b	1174	U
33	b	1175	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	1176	U
33	b	1177	G
33	b	1181	U
33	b	1200	C
33	b	1206	G
33	b	1212	G
33	b	1238	G
33	b	1250	G
33	b	1253	A
33	b	1255	U
33	b	1256	G
33	b	1259	G
33	b	1266	G
33	b	1267	U
33	b	1271	G
33	b	1272	A
33	b	1273	U
33	b	1276	A
33	b	1291	C
33	b	1300	G
33	b	1301	A
33	b	1306	C
33	b	1352	U
33	b	1365	A
33	b	1366	A
33	b	1374	G
33	b	1379	U
33	b	1382	G
33	b	1383	A
33	b	1384	A
33	b	1393	A
33	b	1395	A
33	b	1396	U
33	b	1409	U
33	b	1416	G
33	b	1417	C
33	b	1420	A
33	b	1421	G
33	b	1426	G
33	b	1427	A
33	b	1428	C
33	b	1429	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	1433	A
33	b	1434	A
33	b	1435	G
33	b	1452	G
33	b	1453	A
33	b	1460	U
33	b	1461	C
33	b	1476	U
33	b	1482	G
33	b	1487	U
33	b	1490	A
33	b	1496	A
33	b	1497	U
33	b	1498	C
33	b	1505	A
33	b	1506	U
33	b	1508	A
33	b	1509	A
33	b	1510	G
33	b	1523	U
33	b	1524	G
33	b	1526	C
33	b	1534	U
33	b	1535	A
33	b	1536	C
33	b	1540	G
33	b	1541	C
33	b	1553	A
33	b	1562	U
33	b	1566	A
33	b	1568	G
33	b	1569	A
33	b	1578	U
33	b	1584	U
33	b	1607	C
33	b	1608	A
33	b	1610	A
33	b	1615	C
33	b	1616	A
33	b	1618	A
33	b	1646	C
33	b	1647	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	1648	U
33	b	1664	A
33	b	1674	G
33	b	1677	A
33	b	1716	U
33	b	1717	A
33	b	1718	G
33	b	1730	C
33	b	1733	G
33	b	1736	U
33	b	1744	A
33	b	1745	A
33	b	1763	G
33	b	1764	C
33	b	1773	A
33	b	1775	U
33	b	1776	G
33	b	1799	G
33	b	1800	C
33	b	1801	A
33	b	1807	G
33	b	1808	A
33	b	1811	G
33	b	1816	C
33	b	1829	A
33	b	1840	G
33	b	1847	A
33	b	1848	A
33	b	1857	G
33	b	1871	A
33	b	1877	A
33	b	1884	G
33	b	1901	A
33	b	1906	G
33	b	1913	A
33	b	1914	C
33	b	1919	A
33	b	1922	G
33	b	1927	A
33	b	1928	A
33	b	1929	G
33	b	1930	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	1931	U
33	b	1936	A
33	b	1937	A
33	b	1938	A
33	b	1955	U
33	b	1963	U
33	b	1967	C
33	b	1970	A
33	b	1971	U
33	b	1972	G
33	b	1977	A
33	b	1991	U
33	b	1992	G
33	b	1993	U
33	b	1997	C
33	b	2023	C
33	b	2027	G
33	b	2031	A
33	b	2032	G
33	b	2033	A
33	b	2043	C
33	b	2055	C
33	b	2056	G
33	b	2060	A
33	b	2061	G
33	b	2062	A
33	b	2063	C
33	b	2069	G
33	b	2093	G
33	b	2098	U
33	b	2102	G
33	b	2103	C
33	b	2104	C
33	b	2105	U
33	b	2106	U
33	b	2108	A
33	b	2111	U
33	b	2112	G
33	b	2114	A
33	b	2115	G
33	b	2116	G
33	b	2117	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	2118	U
33	b	2119	A
33	b	2121	G
33	b	2123	G
33	b	2125	G
33	b	2126	A
33	b	2129	C
33	b	2130	U
33	b	2132	U
33	b	2135	A
33	b	2136	G
33	b	2138	G
33	b	2139	U
33	b	2140	G
33	b	2144	G
33	b	2145	C
33	b	2146	C
33	b	2147	A
33	b	2149	U
33	b	2151	U
33	b	2154	A
33	b	2155	U
33	b	2156	G
33	b	2157	G
33	b	2158	A
33	b	2162	G
33	b	2163	A
33	b	2164	C
33	b	2165	C
33	b	2166	U
33	b	2170	A
33	b	2171	A
33	b	2172	U
33	b	2174	C
33	b	2180	U
33	b	2182	U
33	b	2184	A
33	b	2186	G
33	b	2187	U
33	b	2188	U
33	b	2191	A
33	b	2192	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	2193	G
33	b	2198	A
33	b	2204	G
33	b	2212	A
33	b	2213	U
33	b	2214	C
33	b	2225	A
33	b	2229	U
33	b	2238	G
33	b	2239	G
33	b	2250	G
33	b	2252	G
33	b	2256	G
33	b	2283	C
33	b	2287	A
33	b	2288	A
33	b	2300	C
33	b	2305	U
33	b	2308	G
33	b	2311	A
33	b	2320	U
33	b	2322	A
33	b	2325	G
33	b	2326	C
33	b	2333	A
33	b	2335	A
33	b	2336	A
33	b	2345	G
33	b	2346	A
33	b	2347	C
33	b	2348	U
33	b	2357	G
33	b	2361	G
33	b	2377	A
33	b	2383	G
33	b	2385	C
33	b	2396	G
33	b	2402	U
33	b	2406	A
33	b	2407	A
33	b	2419	U
33	b	2422	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	2425	A
33	b	2429	G
33	b	2430	A
33	b	2441	U
33	b	2448	A
33	b	2450	A
33	b	2459	A
33	b	2475	C
33	b	2476	A
33	b	2478	A
33	b	2494	G
33	b	2502	G
33	b	2503	A
33	b	2505	G
33	b	2506	U
33	b	2518	A
33	b	2520	C
33	b	2529	G
33	b	2547	A
33	b	2548	U
33	b	2554	U
33	b	2566	A
33	b	2567	G
33	b	2573	C
33	b	2584	U
33	b	2593	U
33	b	2602	A
33	b	2606	C
33	b	2609	U
33	b	2613	U
33	b	2615	U
33	b	2629	U
33	b	2630	G
33	b	2654	A
33	b	2655	G
33	b	2656	U
33	b	2661	G
33	b	2663	G
33	b	2689	U
33	b	2690	U
33	b	2713	U
33	b	2714	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	2724	U
33	b	2726	A
33	b	2733	A
33	b	2744	G
33	b	2748	A
33	b	2752	C
33	b	2764	A
33	b	2765	A
33	b	2776	A
33	b	2778	A
33	b	2779	U
33	b	2790	U
33	b	2792	A
33	b	2796	U
33	b	2798	U
33	b	2799	A
33	b	2800	A
33	b	2801	G
33	b	2808	G
33	b	2818	U
33	b	2820	A
33	b	2821	A
33	b	2838	G
33	b	2849	U
33	b	2858	C
33	b	2859	G
33	b	2861	U
33	b	2867	G
33	b	2873	A
33	b	2880	C
33	b	2883	A
33	b	2885	G
33	b	2886	A
33	b	2887	A
33	b	2896	C
33	b	2900	A
33	b	2902	C
33	b	2903	U
53	x	14	C
53	x	22	A
53	x	23	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	66	A
9	A	195	A
9	A	262	A
9	A	428	G
9	A	451	A
9	A	719	C
9	A	980	C
9	A	1065	U
9	A	1187	G
9	A	1201	A
9	A	1255	G
9	A	1302	C
9	A	1357	A
30	X	56	C
31	Y	6	A
31	Y	16	C
31	Z	73	G

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	PRO	Z	101	31	6,7,8	0.71	0	7,8,10	1.32	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PRO	Z	101	31	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	Z	101	PRO	O-C-CA	-2.41	118.57	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	Z	101	PRO	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

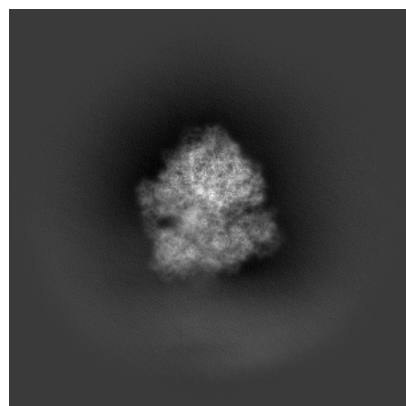
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66121. These allow visual inspection of the internal detail of the map and identification of artifacts.

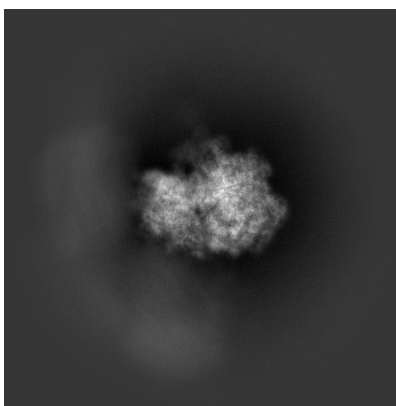
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

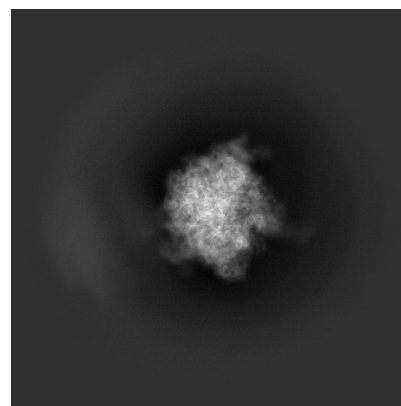
6.1.1 Primary map



X

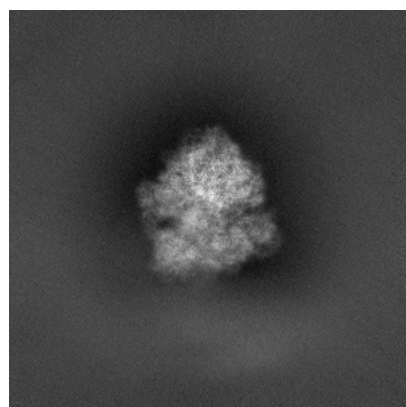


Y

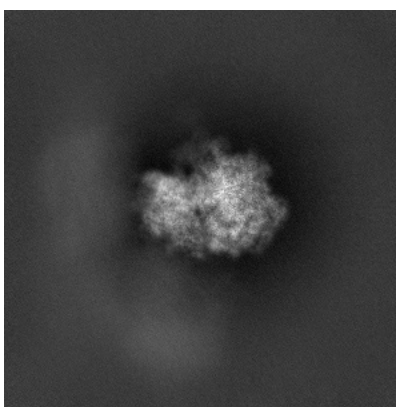


Z

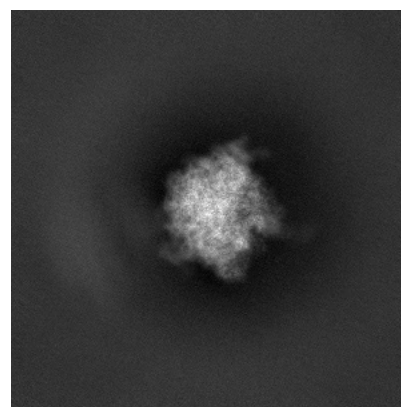
6.1.2 Raw map



X



Y

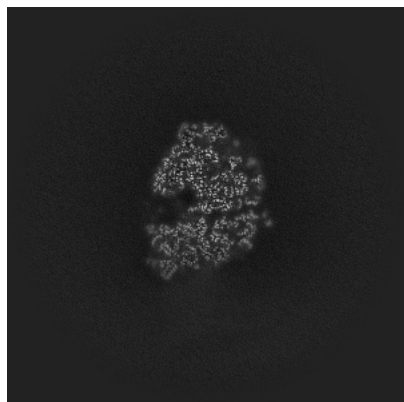


Z

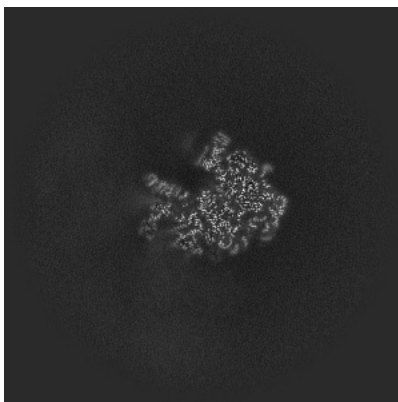
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

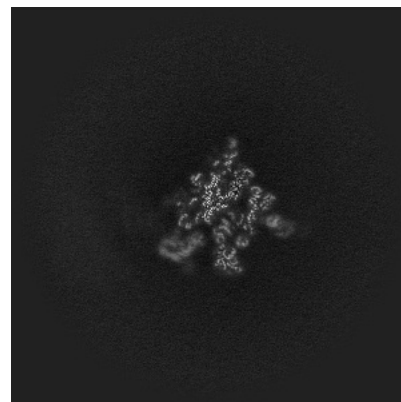
6.2.1 Primary map



X Index: 310

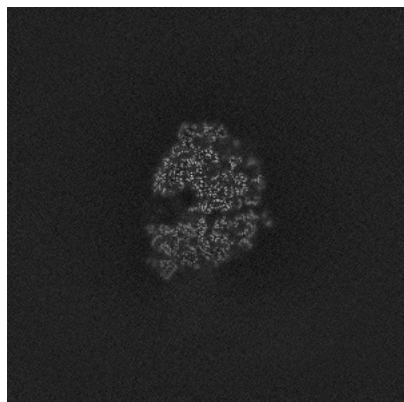


Y Index: 310

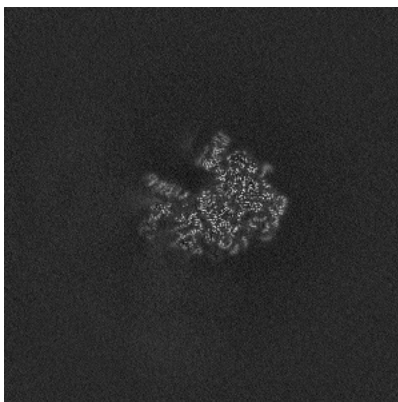


Z Index: 310

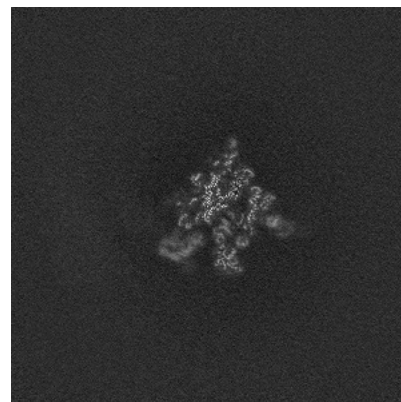
6.2.2 Raw map



X Index: 310



Y Index: 310

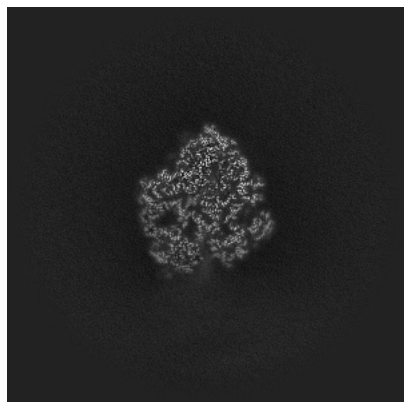


Z Index: 310

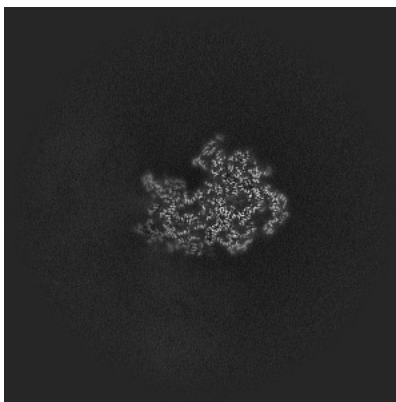
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

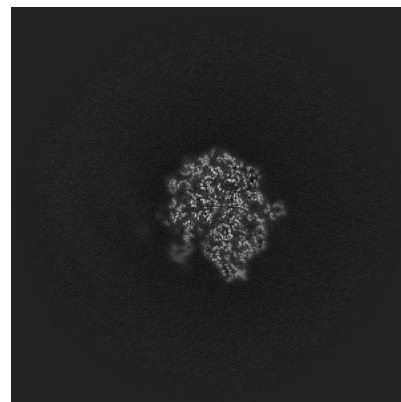
6.3.1 Primary map



X Index: 324

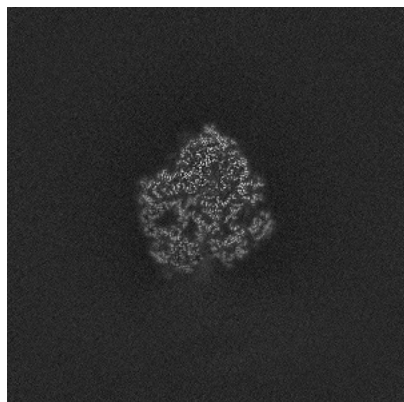


Y Index: 318

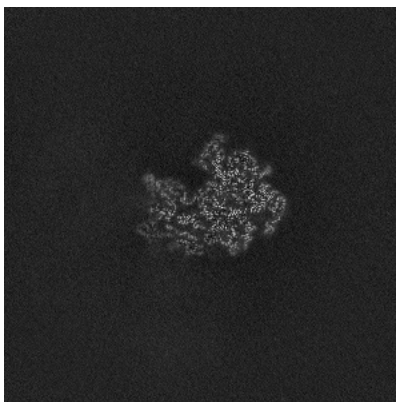


Z Index: 340

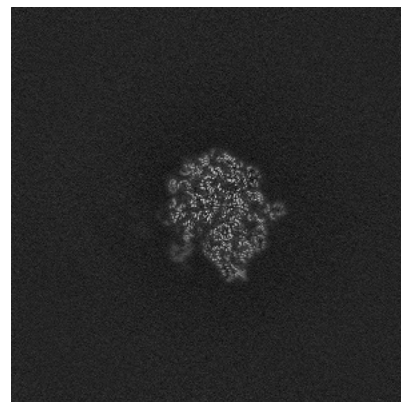
6.3.2 Raw map



X Index: 324



Y Index: 315

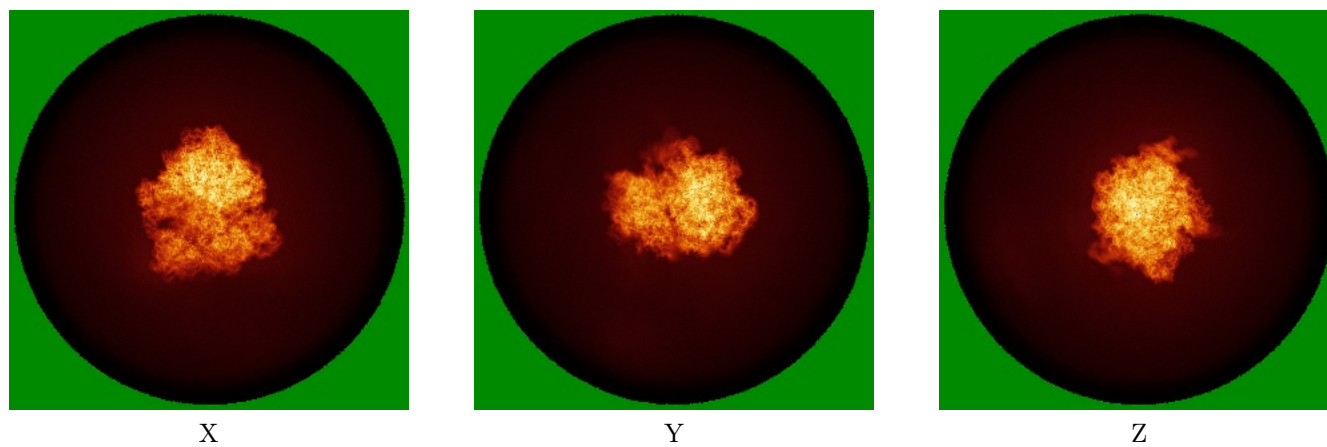


Z Index: 340

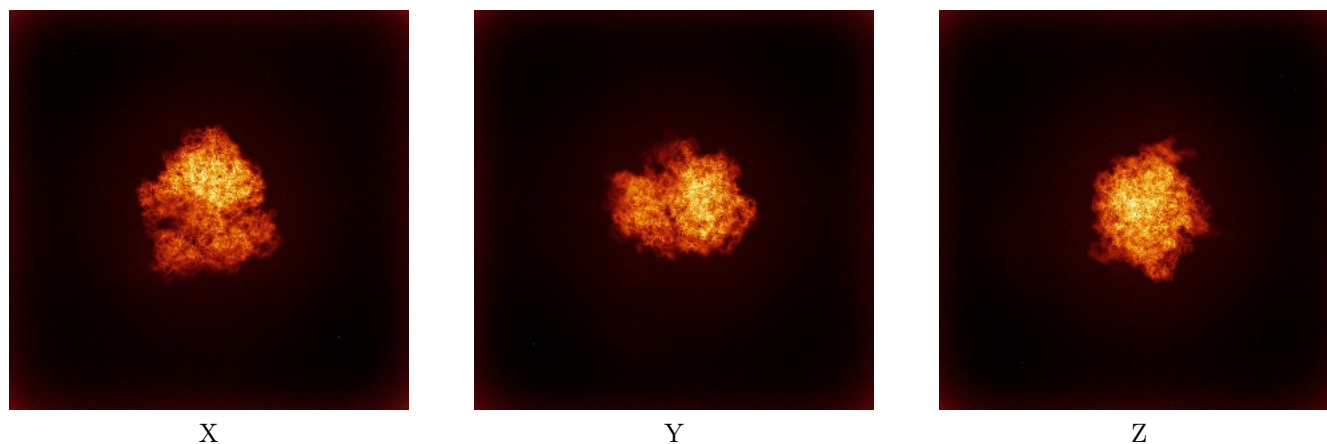
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

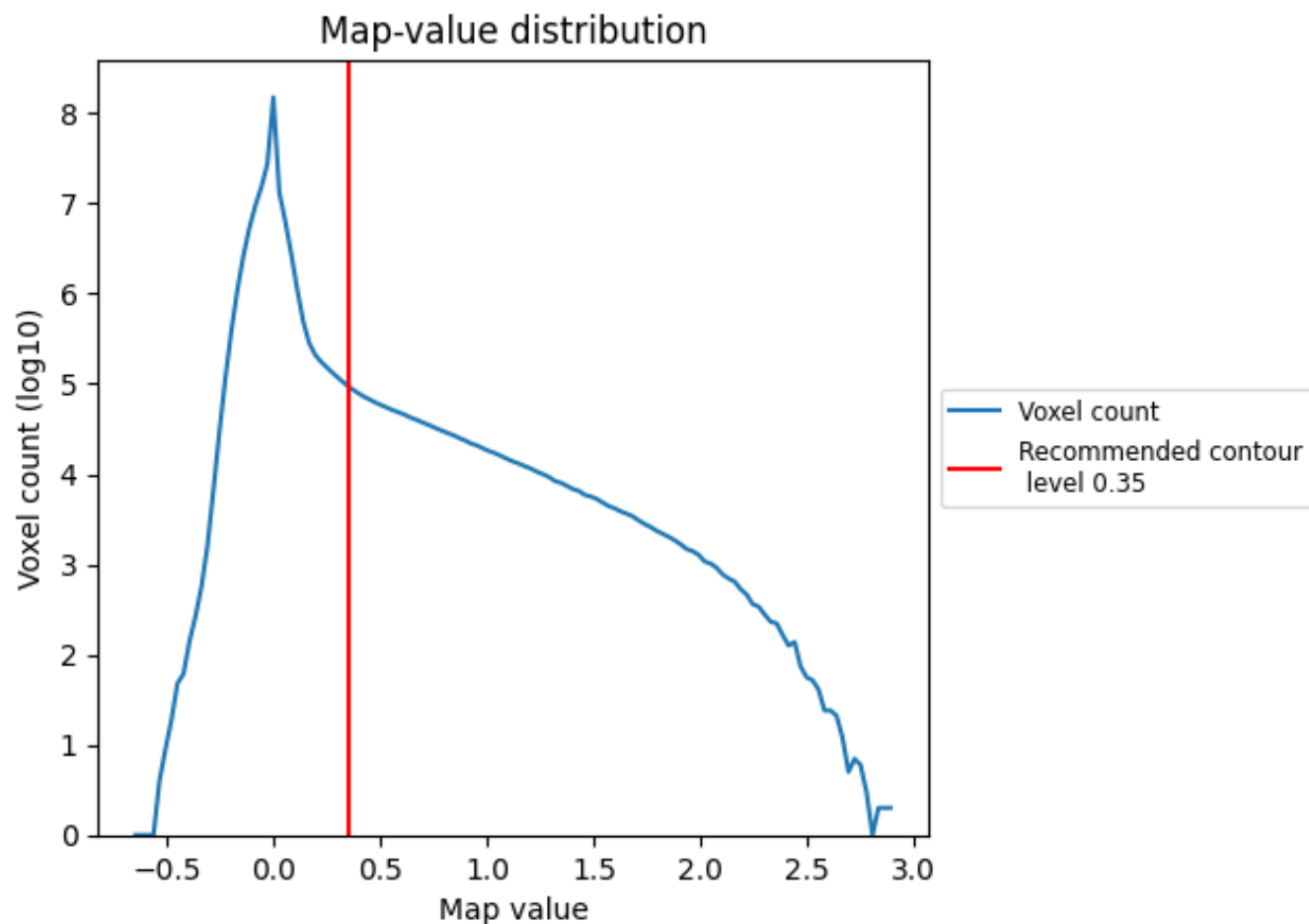
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

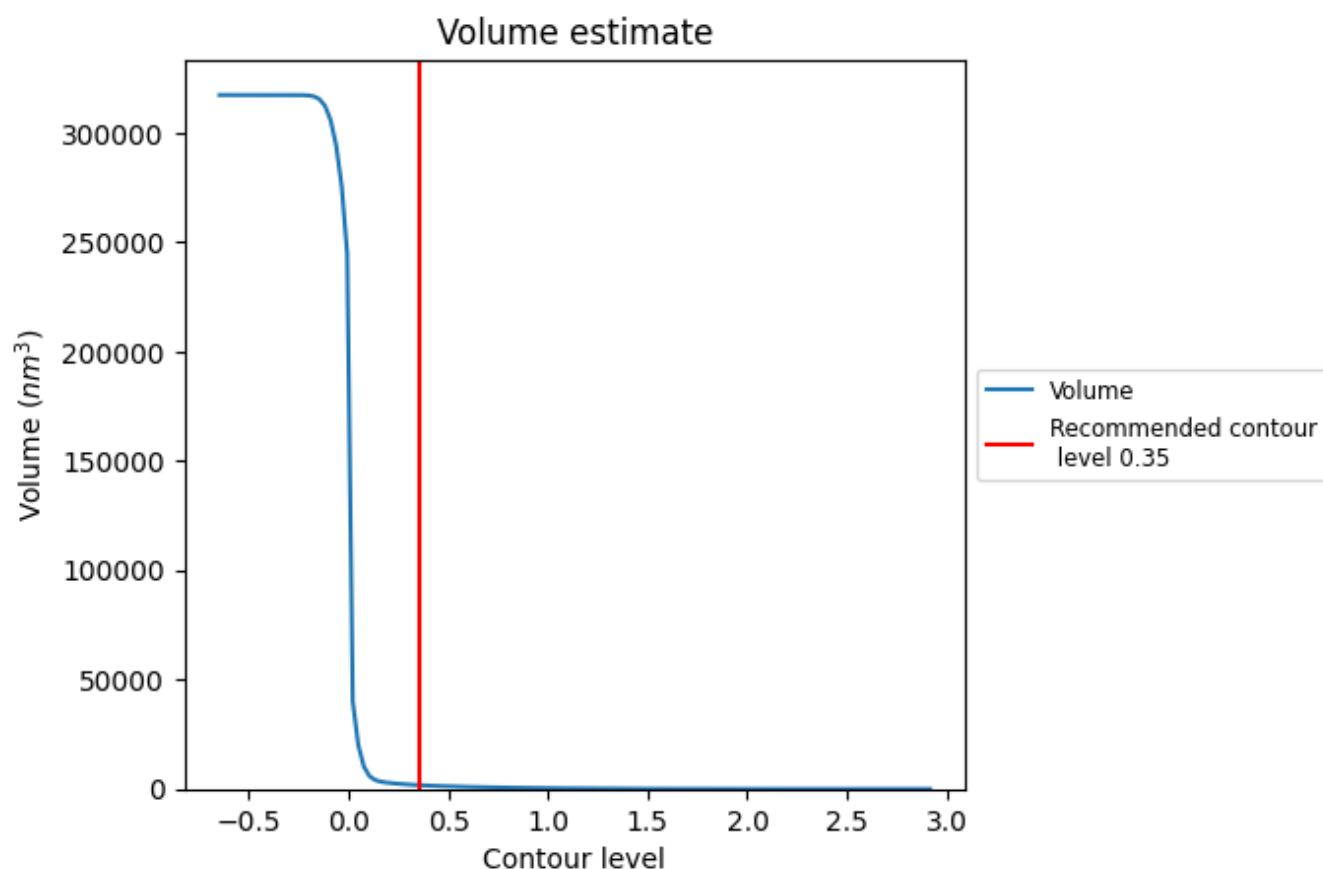
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

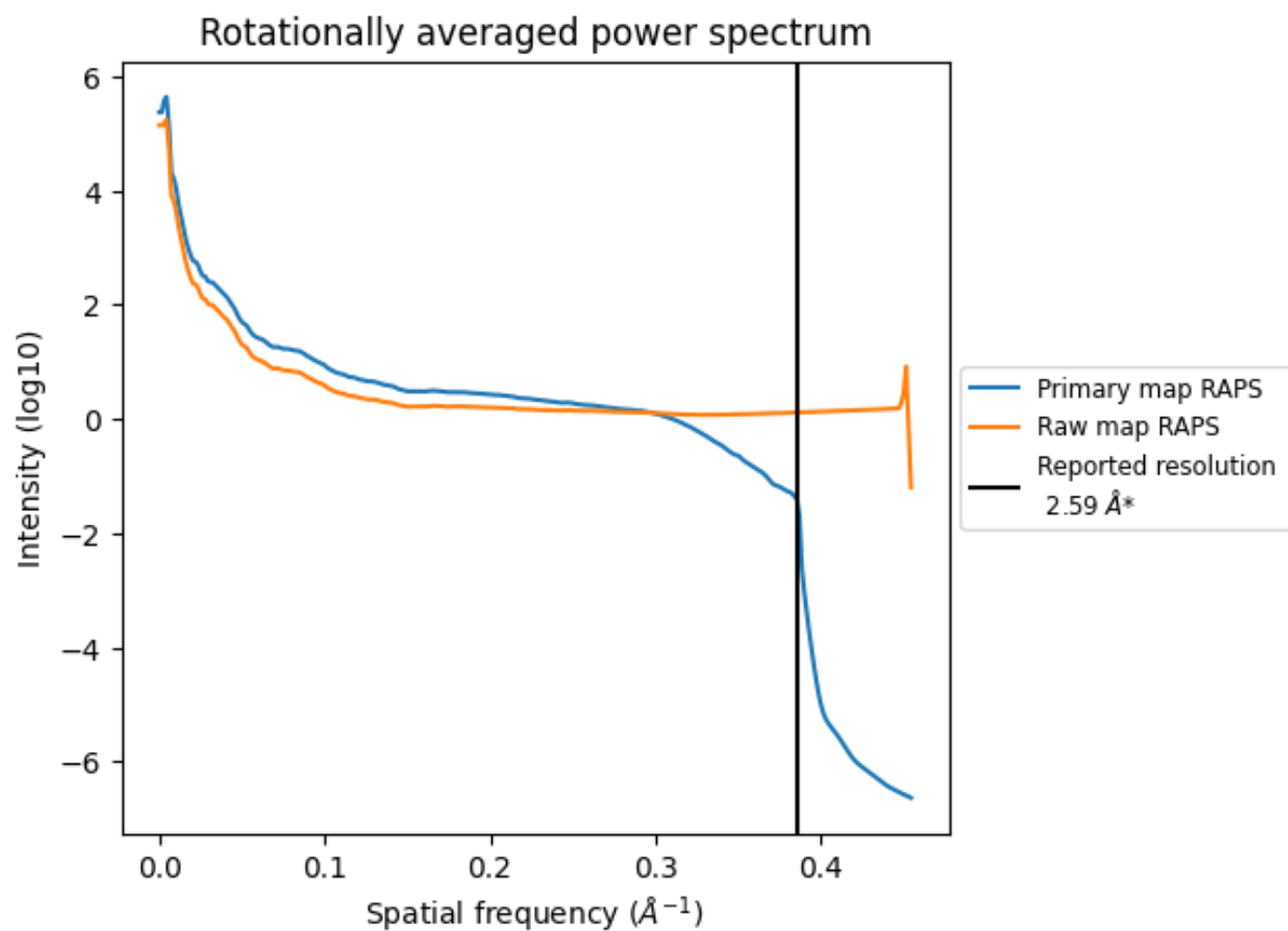
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1749 nm^3 ; this corresponds to an approximate mass of 1580 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 ⓘ

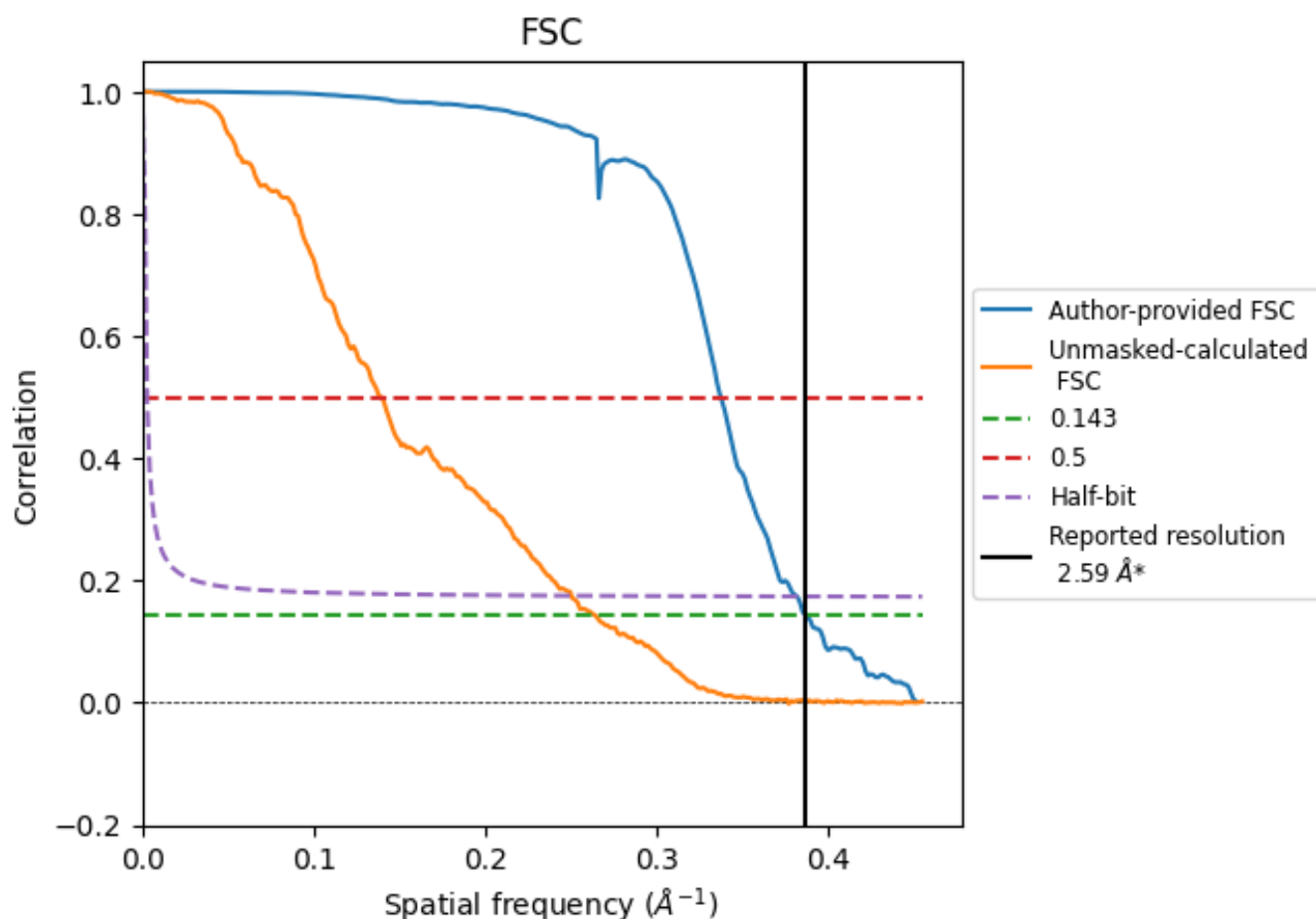


*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.386 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

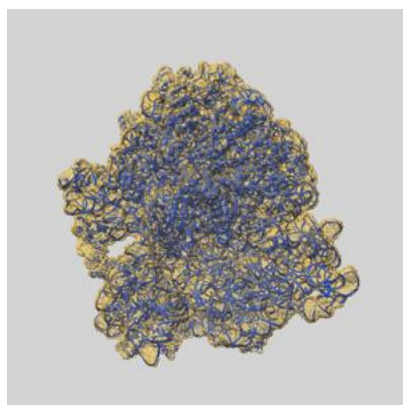
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	2.97	2.62
Unmasked-calculated*	3.79	7.17	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 2.59 by more than 10 %

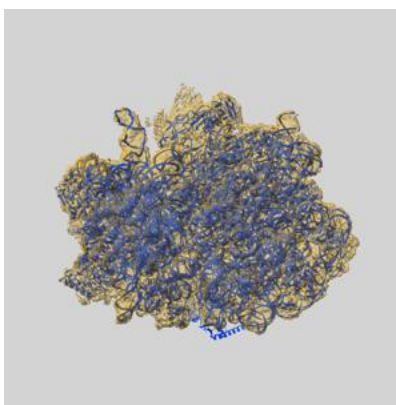
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66121 and PDB model 9WNQ. Per-residue inclusion information can be found in section 3 on page 15.

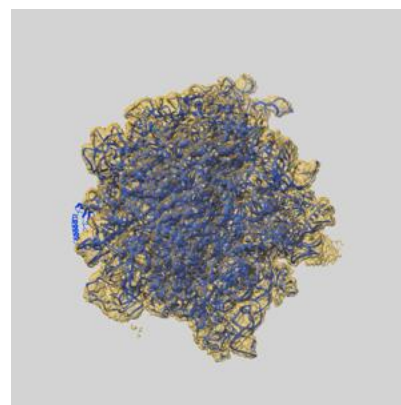
9.1 Map-model overlay [i](#)



X



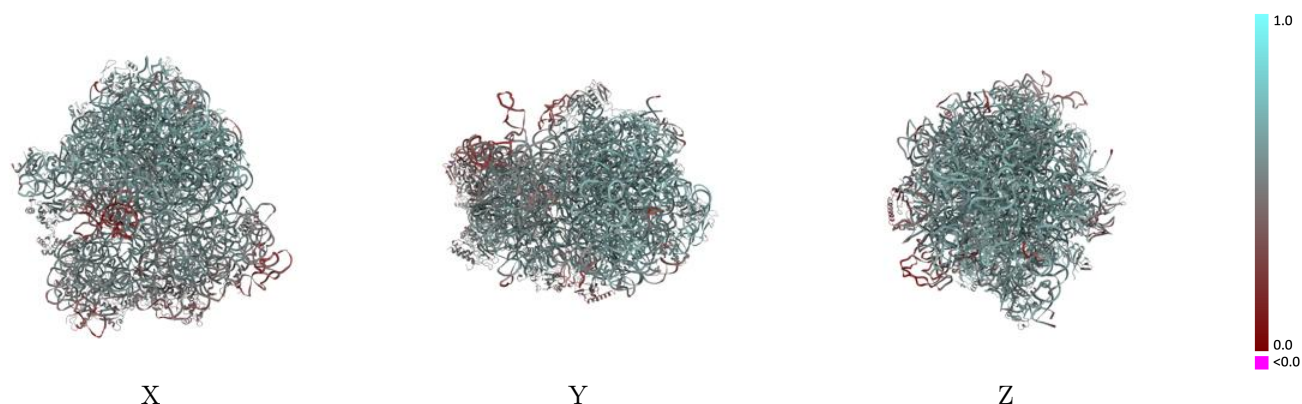
Y



Z

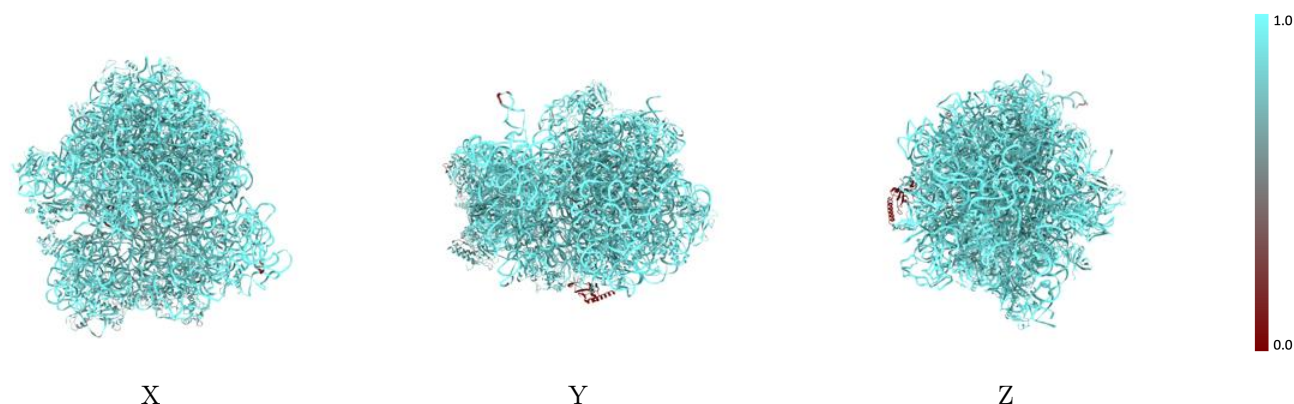
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



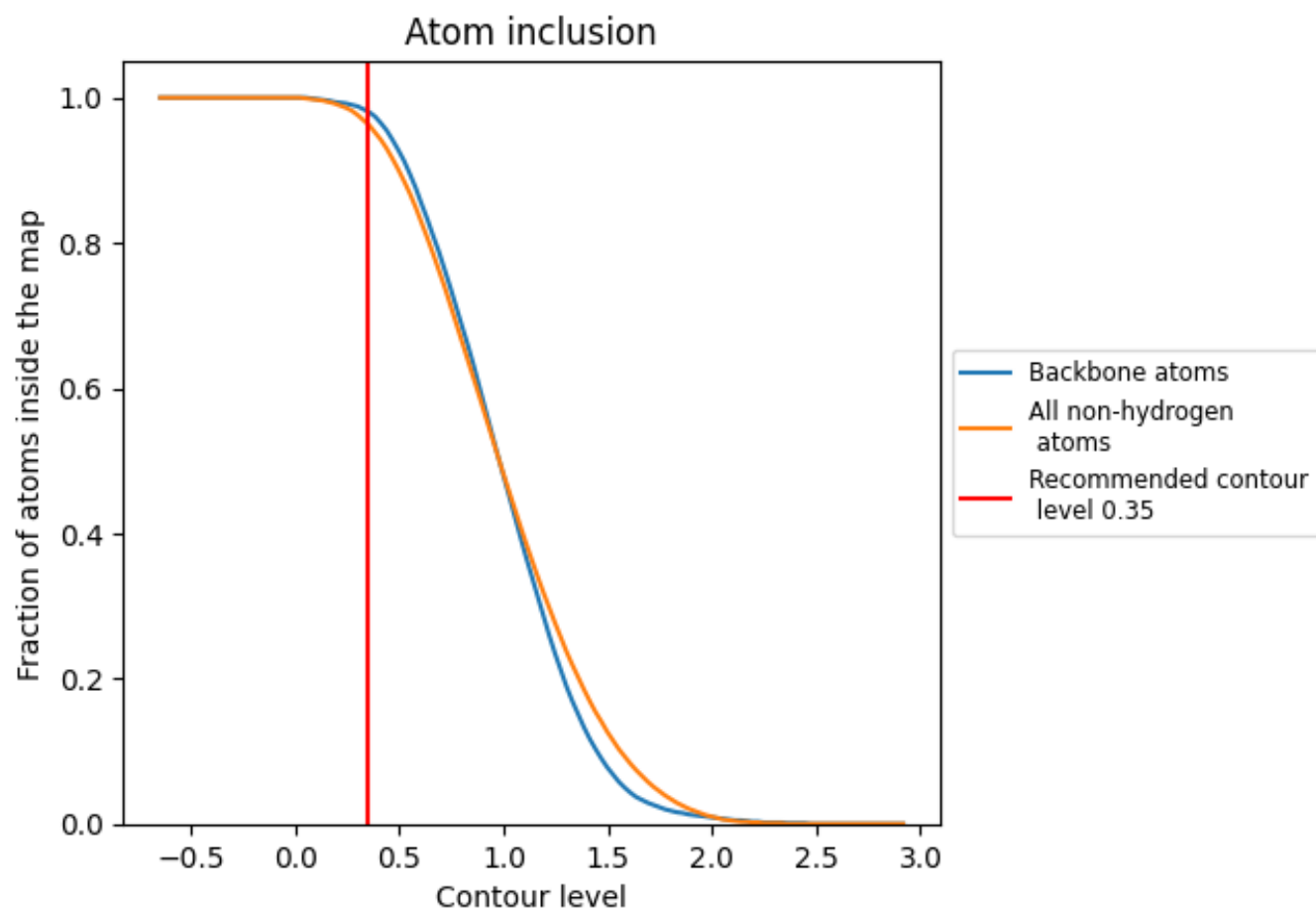
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.5530
0	 0.9670	 0.5930
1	 0.9460	 0.5350
2	 0.9500	 0.5770
4	 0.9490	 0.5800
5	 0.9090	 0.5580
6	 0.9830	 0.6220
7	 0.9800	 0.6190
8	 0.9860	 0.5990
A	 0.9900	 0.5300
B	 0.6920	 0.4700
C	 0.8780	 0.5130
D	 0.7940	 0.4030
E	 0.9140	 0.5370
F	 0.8930	 0.4860
G	 0.8650	 0.4800
H	 0.9410	 0.5410
I	 0.9200	 0.4990
J	 0.7900	 0.4470
K	 0.9280	 0.5370
L	 0.8500	 0.4690
M	 0.9160	 0.5000
N	 0.9440	 0.5160
O	 0.9450	 0.5350
P	 0.9260	 0.4740
Q	 0.9270	 0.4990
R	 0.9330	 0.5410
S	 0.9290	 0.4950
T	 0.9300	 0.4730
U	 0.7490	 0.4670
X	 0.9090	 0.3940
Y	 0.9640	 0.5070
Z	 0.8840	 0.5280
a	 0.9950	 0.5730
b	 0.9940	 0.5830



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	 0.9740	 0.6070
d	 0.9690	 0.6010
e	 0.9470	 0.5770
f	 0.9360	 0.5060
g	 0.9370	 0.5100
h	 0.2770	 0.3890
k	 0.9770	 0.5990
l	 0.9540	 0.5820
m	 0.9700	 0.5880
n	 0.9560	 0.5890
o	 0.9850	 0.6090
p	 0.9510	 0.5480
q	 0.9550	 0.5890
r	 0.9860	 0.6130
s	 0.9570	 0.5740
t	 0.9520	 0.5910
u	 0.9190	 0.5410
v	 0.9530	 0.5540
w	 0.9540	 0.5540
x	 0.9100	 0.5100
y	 0.9640	 0.6040
z	 0.7060	 0.4700