



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 03:06 PM UTC

PDB ID : 9GHG / pdb_00009ghg
EMDB ID : EMD-51356
Title : Staphylococcus aureus FusB bound to the small subunit of the S. aureus 70S ribosome (FusB-Sa70S:SSU)
Authors : Gonzalez-Lopez, A.; Selmer, M.
Deposited on : 2024-08-15
Resolution : 2.22 Å (reported)
Based on initial models : 8P2F, ., 4ADN

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:

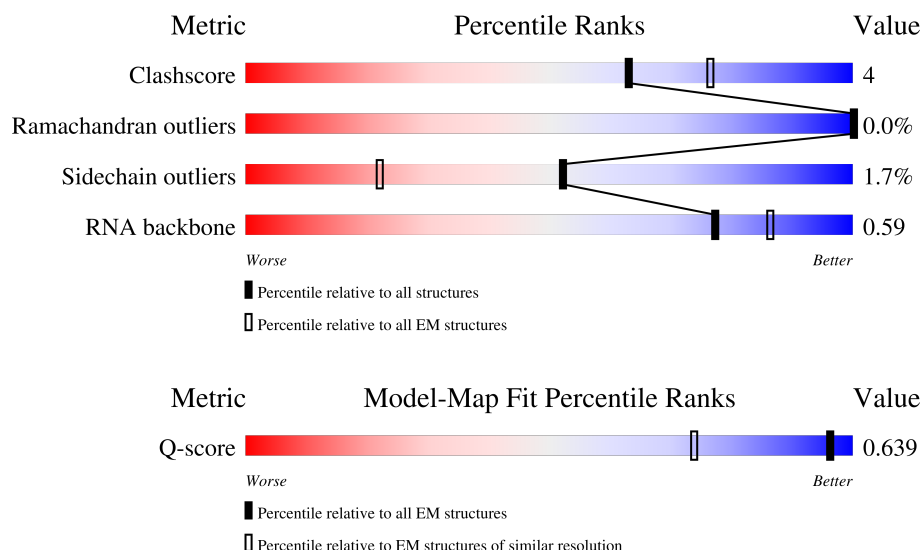
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

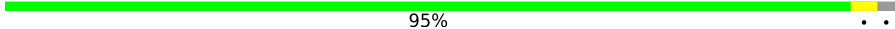
The reported resolution of this entry is 2.22 Å.

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.



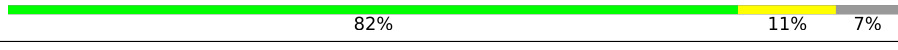
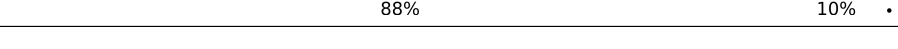
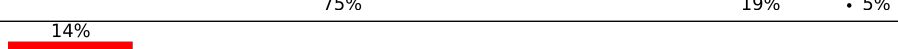
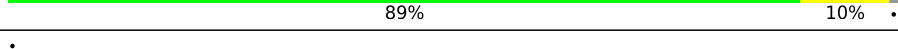
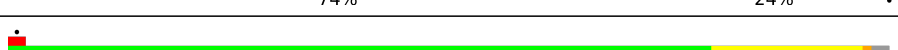
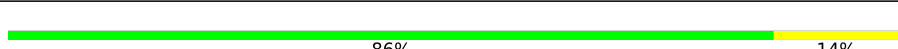
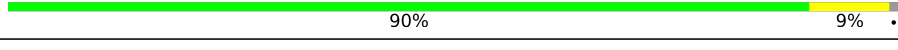
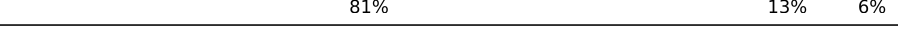
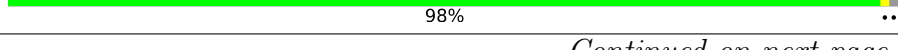
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3277 (1.73 - 2.72)

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	1	62	 95% . .
2	2	69	 87% 7% 6%
3	3	59	 90% 5% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	4	84	
5	5	57	
6	6	49	
7	7	45	
8	8	66	
9	9	37	
10	A	2923	
11	B	115	
12	C	213	
13	D	77	
13	F	77	
14	G	277	
15	H	220	
16	I	207	
17	J	179	
18	K	178	
19	M	145	
20	N	122	
21	O	146	
22	P	144	
23	Q	122	
24	R	119	
25	S	116	
26	T	118	
27	U	102	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	V	117	
29	W	91	
30	X	105	
31	Y	217	
32	Z	94	
33	a	1555	
34	b	24	
35	c	255	
36	d	217	
37	e	200	
38	f	166	
39	g	98	
40	h	156	
41	i	132	
42	j	132	
43	k	102	
44	l	129	
45	m	137	
46	n	121	
47	o	61	
48	p	89	
49	q	91	
50	r	87	
51	s	80	
52	t	92	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	u	83	93%
54	v	58	40% 64% 26% 9%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 150404 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 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	61	Total	C	N	O	S	0	0
			481	298	104	78	1		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	65	Total	C	N	O	S	0	0
			535	329	100	105	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	56	Total	C	N	O	0	0
			436	271	82	83		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	80	Total	C	N	O	S	0	0
			654	417	111	123	3		

- Molecule 5 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	?	-	ARG	deletion	UNP Q2FZF1

- Molecule 6 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	48	Total	C	N	O	S	0	0
			402	245	79	73	5		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2848	Total	C	N	O	P	0	0
			61064	27267	11166	19783	2848		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	G	A	conflict	GB CP000253
A	1584	U	A	conflict	GB CP000253
A	2261	G	A	conflict	GB CP000253

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 12 is a protein called Far1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	203	Total	C	N	O	S	1	0
			1703	1102	278	315	8		

- Molecule 13 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
13	F	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	273	Total	C	N	O	S	0	0
			2085	1297	413	370	5		

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	216	Total	C	N	O	S	0	0
			1637	1024	301	307	5		

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	204	Total	C	N	O	S	0	0
			1564	981	286	295	2		

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	178	Total	C	N	O	S	0	0
			1412	897	244	264	7		

- Molecule 18 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	174	Total	C	N	O	S	0	0
			1361	846	249	263	3		

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	144	Total	C	N	O	S	0	0
			1146	715	210	218	3		

- Molecule 20 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 21 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	145	Total	C	N	O	S	0	0
			1090	674	214	201	1		

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	114	Total	C	N	O		0	0
			922	580	185	157			

- Molecule 26 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 27 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	101	Total	C	N	O	S	0	0
			793	503	141	148	1		

- Molecule 28 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

- Molecule 30 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	102	Total	C	N	O	S	0	0
			787	497	144	144	2		

- Molecule 31 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 32 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Z	82	Total	C	N	O	0	0
			626	386	122	118		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1526	Total	C	N	O	P	0	0
			32707	14608	5975	10598	1526		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	14	Total	C	N	O	P	0	0
			306	137	62	93	14		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	204	Total	C	N	O	S	0	0
			1612	1015	302	293	2		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	156	Total	C	N	O	S	0	0
			1160	730	213	215	2		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	93	Total	C	N	O	S	0	0
			773	489	136	146	2		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	146	Total	C	N	O	S	0	0
			1165	727	222	212	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	128	Total	C	N	O	S	0	0
			1016	629	203	183	1		

- Molecule 43 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	99	Total	C	N	O	S	0	0
			792	499	145	147	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	118	Total	C	N	O	S	0	0
			876	542	166	165	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	113	Total	C	N	O	S	0	0
			902	554	179	168	1		

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	80	Total	C	N	O	S	0	0
			662	419	120	122	1		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	63	Total	C	N	O	S	0	0
			516	330	96	87	3		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	80	Total	C	N	O	S	0	0
			651	419	117	113	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	v	53	Total	C	N	O	0	0
			446	275	93	78		

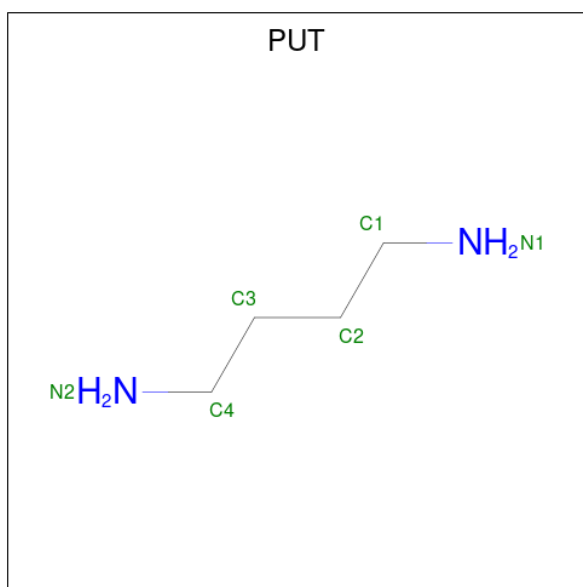
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	5	1	Total	Zn	0
			1	1	
55	9	1	Total	Zn	0
			1	1	
55	C	1	Total	Zn	0
			1	1	
55	o	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	117	Total	Mg	0
			117	117	
56	F	2	Total	Mg	0
			2	2	
56	G	1	Total	Mg	0
			1	1	
56	O	1	Total	Mg	0
			1	1	
56	a	24	Total	Mg	0
			24	24	

- Molecule 57 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
57	A	1	Total	C	N	0
			6	4	2	
57	A	1	Total	C	N	0
			6	4	2	

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	1	8	Total	O	0
			8	8	
58	2	2	Total	O	0
			2	2	
58	3	4	Total	O	0
			4	4	
58	5	18	Total	O	0
			18	18	
58	6	1	Total	O	0
			1	1	
58	7	31	Total	O	0
			31	31	
58	8	32	Total	O	0
			32	32	
58	9	2	Total	O	0
			2	2	
58	A	4272	Total	O	0
			4272	4272	
58	B	24	Total	O	0
			24	24	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	D	5	Total 5	O 5	0
58	F	5	Total 5	O 5	0
58	G	109	Total 109	O 109	0
58	H	63	Total 63	O 63	0
58	I	68	Total 68	O 68	0
58	J	1	Total 1	O 1	0
58	M	29	Total 29	O 29	0
58	N	21	Total 21	O 21	0
58	O	62	Total 62	O 62	0
58	P	24	Total 24	O 24	0
58	Q	26	Total 26	O 26	0
58	S	10	Total 10	O 10	0
58	T	60	Total 60	O 60	0
58	U	34	Total 34	O 34	0
58	V	33	Total 33	O 33	0
58	W	13	Total 13	O 13	0
58	X	1	Total 1	O 1	0
58	Y	1	Total 1	O 1	0
58	Z	13	Total 13	O 13	0
58	a	522	Total 522	O 522	0
58	b	1	Total 1	O 1	0

Continued on next page...

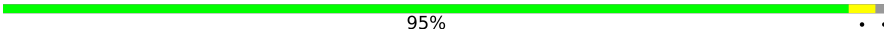
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	c	1	Total 1	O 1	0
58	d	2	Total 2	O 2	0
58	e	1	Total 1	O 1	0
58	f	2	Total 2	O 2	0
58	h	1	Total 1	O 1	0
58	i	2	Total 2	O 2	0
58	k	2	Total 2	O 2	0
58	l	1	Total 1	O 1	0
58	m	1	Total 1	O 1	0
58	o	1	Total 1	O 1	0
58	r	2	Total 2	O 2	0
58	s	1	Total 1	O 1	0
58	u	1	Total 1	O 1	0
58	v	1	Total 1	O 1	0

3 Residue-property plots

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

- Molecule 1: 50S ribosomal protein L28

Chain 1:  95%



- Molecule 2: 50S ribosomal protein L29

Chain 2:  87% 7% 6%



- Molecule 3: 50S ribosomal protein L30

Chain 3:  90% 5% 5%



- Molecule 4: 50S ribosomal protein L31 type B

Chain 4:  65% 29% 5%



- Molecule 5: Large ribosomal subunit protein bL32

Chain 5:  82% 11% 7%



- Molecule 6: Large ribosomal subunit protein bL33A

Chain 6:  88% 10% .



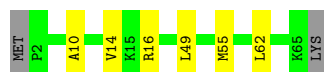
- Molecule 7: 50S ribosomal protein L34

Chain 7:  80% 16% .



- Molecule 8: 50S ribosomal protein L35

Chain 8:  88% 9% .



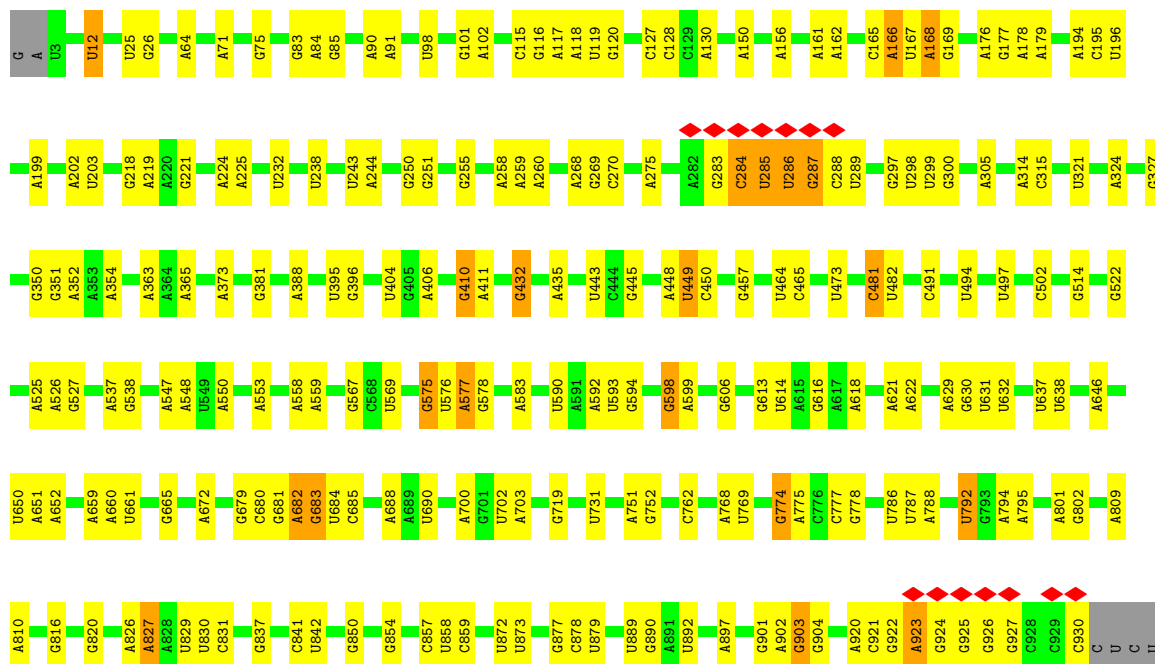
- Molecule 9: 50S ribosomal protein L36

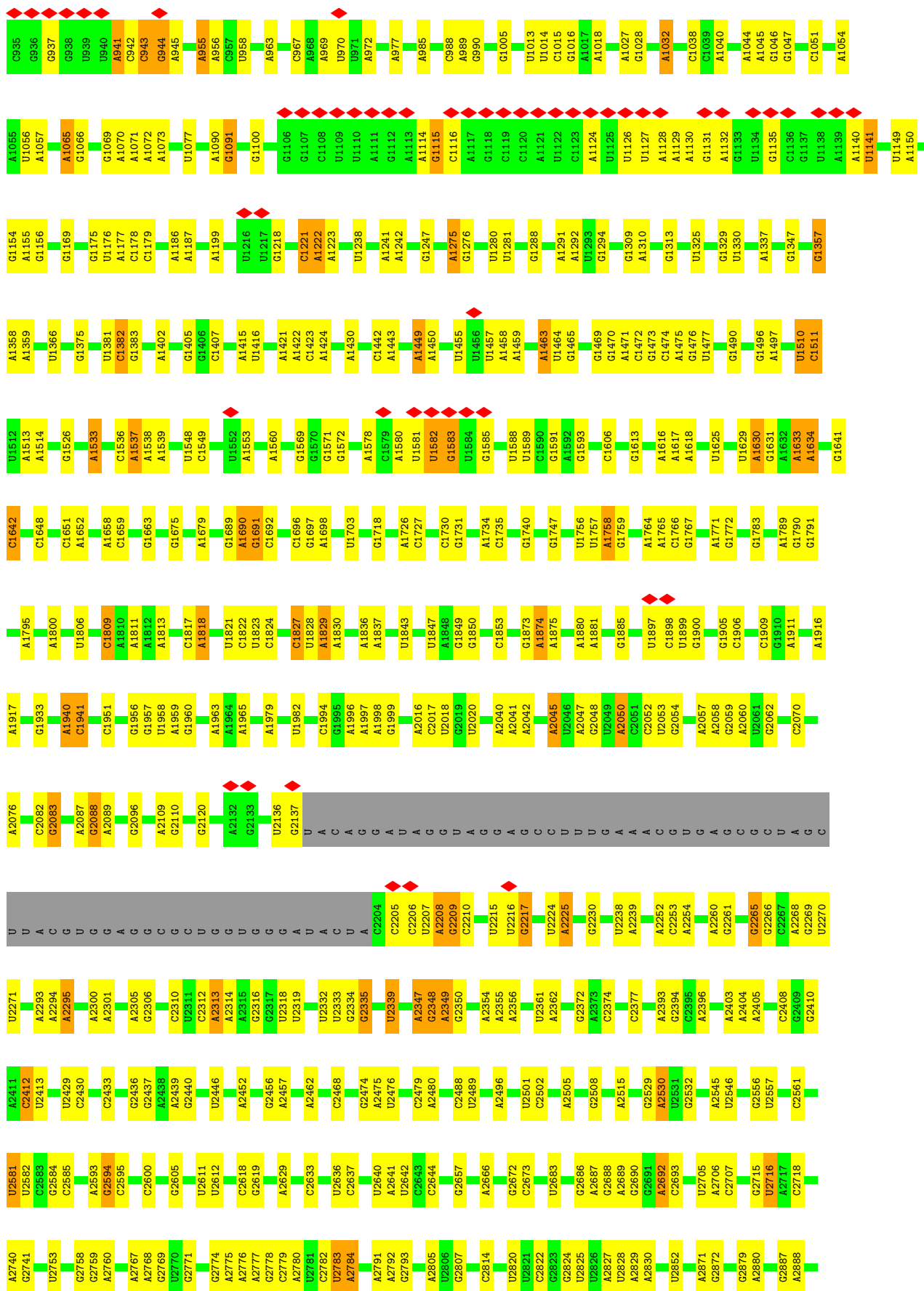
Chain 9:  84% 16%



- Molecule 10: 23S rRNA

Chain A:  73% 22% . .

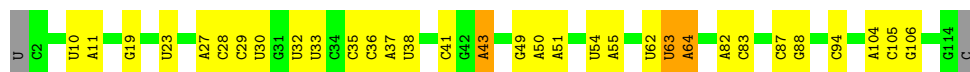






• Molecule 11: 5S rRNA

Chain B: 70% 25% . .



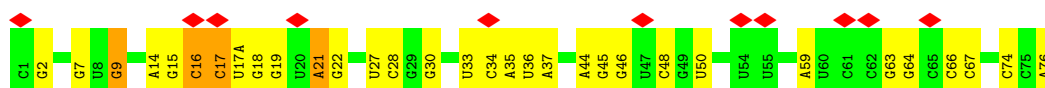
• Molecule 12: Far1

Chain C: 29% 75% 19% 5% . .



• Molecule 13: E-site tRNA

Chain D: 14% 58% 36% 5%



• Molecule 13: E-site tRNA

Chain F: 70% 25% . .



• Molecule 14: 50S ribosomal protein L2

Chain G: 87% 12% .



- Molecule 15: 50S ribosomal protein L3

Chain H:  88% 10%



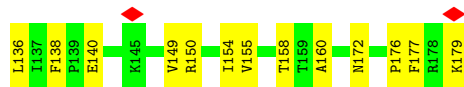
- Molecule 16: 50S ribosomal protein L4

Chain I:  89% 10%



- Molecule 17: 50S ribosomal protein L5

Chain J:  74% 24%



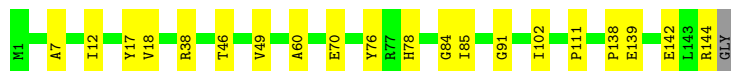
- Molecule 18: 50S ribosomal protein L6

Chain K:  79% 17%



- Molecule 19: 50S ribosomal protein L13

Chain M:  86% 14%



- Molecule 20: 50S ribosomal protein L14

Chain N:  87% 11%



- Molecule 21: 50S ribosomal protein L15

Chain O:  90% 9% .



- Molecule 22: 50S ribosomal protein L16

Chain P:  81% 13% 6%



- Molecule 23: 50S ribosomal protein L17

Chain Q:  84% 15% .

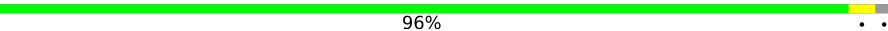


- Molecule 24: 50S ribosomal protein L18

Chain R:  94% 6%



- Molecule 25: 50S ribosomal protein L19

Chain S:  96% . .

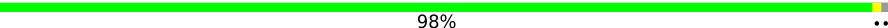


- Molecule 26: 50S ribosomal protein L20

Chain T:  83% 15% .



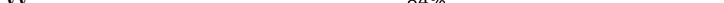
- Molecule 27: 50S ribosomal protein L21

Chain U:  98% . .

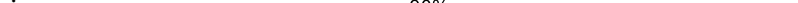


- Molecule 28: 50S ribosomal protein L22

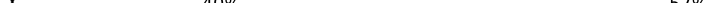
M1	E2	A3	R11	L21	D22	L23	N57	Y62	E73	A74	E78	R92	V106	K111	GLU	GLU	ALA	LYS	GLU	ALA
----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----

- Chain W:  84% 14%

MET	E2	A3	R4	L7	K8	R9	A19	K24	D30	V33	T36	I45	K49	P60	K74	K83	F90	ASN
-----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain X:  5% 90% 7% ..

Protein	Number of Mutations
M1	1
K10	2
I24	2
T48	10
Q49	10
L50	10
N51	10
P52	10
E53	10
I56	1
L70	2
L71	2
K74	2
R92	3
E99	2
K102	1
SER	0
ASN	0
ASN	0

- Chain Y:  40% 57%

Amino Acid	Count
MET	1
ALA	3
SER	17
GLU	11
ARG	16
THR	20
VAL	31
GLY	34
LYS	38
GLN	41
PRO	44
LEU	46
PHE	48
ASN	51
ASP	53
LEU	56
VAL	58
THR	61

[illegible]

ALA	MET	GLU	GLY	GLU	GLN	GLN	THR	GLU	GLU	PRO	GLU	VAL	VAL	GLY	GLU	SER	LYS	GLU	ASP	GLU	GLU	LYS	THR	GLU	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

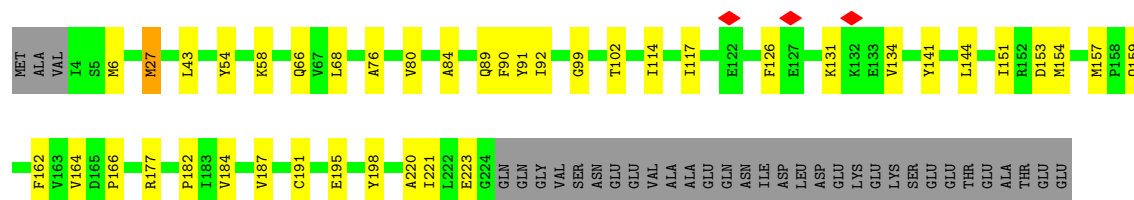
- Chain Z: 78% 10% 13%

MET	LEU	LYS	LEU	ASN	LEU	GLN	PHE	PHE	ALA	SER	K12	A34	T40	N58	L67	I71	D72	K80	K84	V87	A93	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

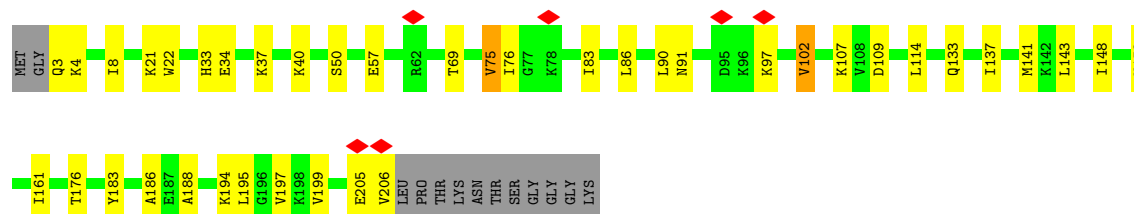
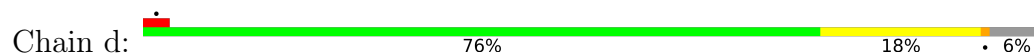
- Chain a: 66% 27%

U	U	U	U	U	A5	U6	G7	G8	A9	G10		U13		A17	U18	C19		G22	G23		C26		G32	A33	A34	C35		G39	G40		C48	C49	U50	A51	A52		U57	G58		C68	G69		A74	G75		G76	G77	A78	G79	A80	A81	G82	C83	U84		U85		G86	C87	U88		U89		C90		G91
---	---	---	---	---	----	----	----	----	----	-----	--	-----	--	-----	-----	-----	--	-----	-----	--	-----	--	-----	-----	-----	-----	--	-----	-----	--	-----	-----	-----	-----	-----	--	-----	-----	--	-----	-----	--	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	--	-----	-----	-----	--	-----	--	-----	--	-----

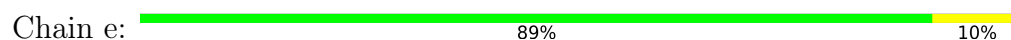
Category	Count
C92	10
U93	10
G94	10
G97	10
U98	10
U99	10
A100	10
A119	10
C120	10
A121	10
A130	10
C131	10
U137	10
A138	10
G147	10
G148	10
A160	10
A161	10
A162	10
C163	10
A171	10
A172	10
U173	10
U183	10
U188	10
G189	10
A190	10
G199	10
U200	10
A206	10
G207	10
A212	10
G213	10
U220	10
U221	10
G222	10
U230	10
U231	10
U237	10
U248	10
G249	10
G255	10



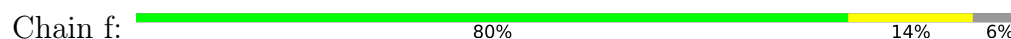
- Molecule 36: 30S ribosomal protein S3



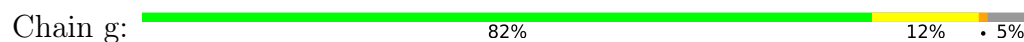
- Molecule 37: 30S ribosomal protein S4



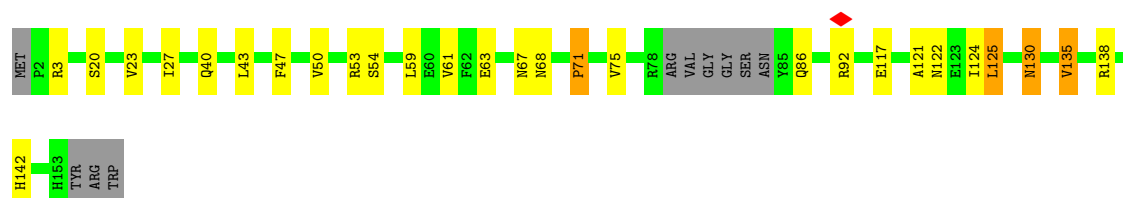
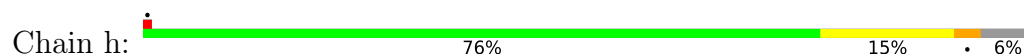
- Molecule 38: 30S ribosomal protein S5



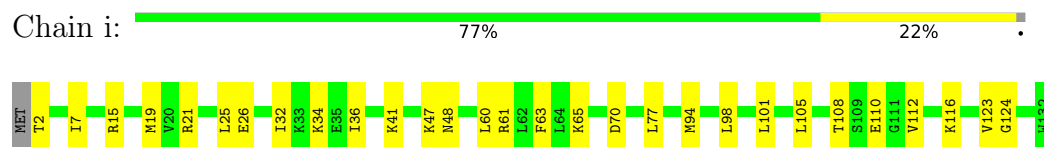
- Molecule 39: 30S ribosomal protein S6



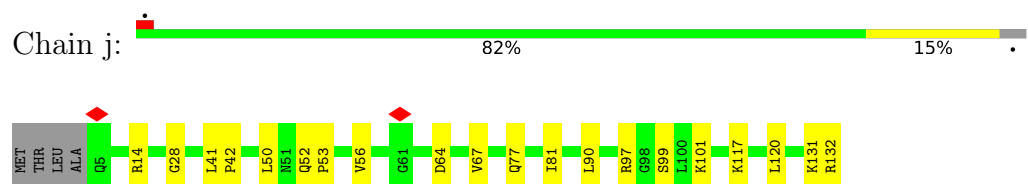
- Molecule 40: 30S ribosomal protein S7



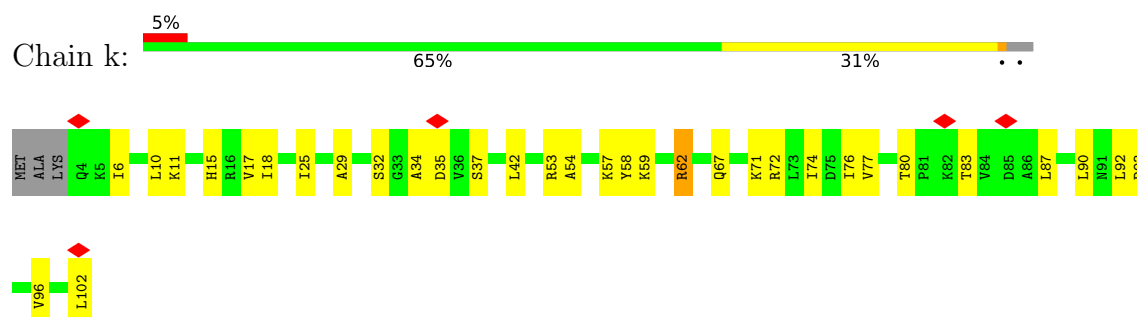
- Molecule 41: 30S ribosomal protein S8



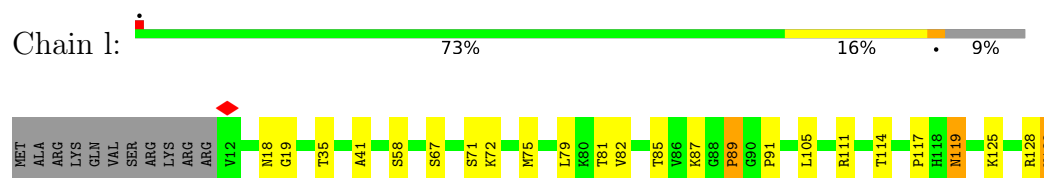
- Molecule 42: 30S ribosomal protein S9



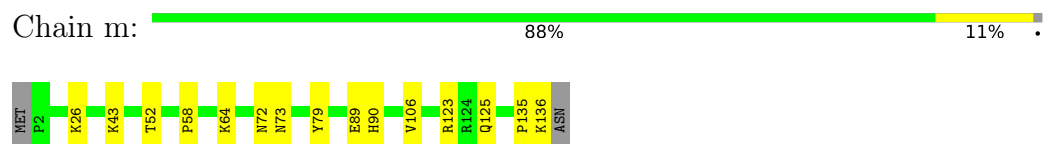
- Molecule 43: Small ribosomal subunit protein uS10



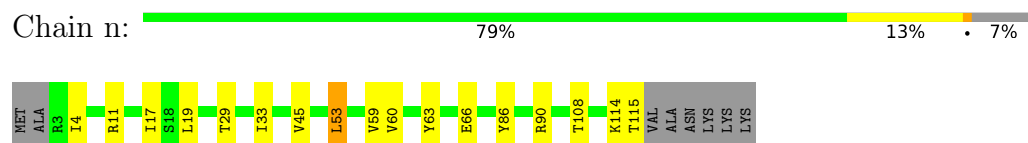
- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S14 type Z

Chain o:  89% 10%



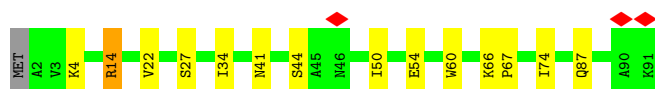
- Molecule 48: 30S ribosomal protein S15

Chain p:  78% 18%



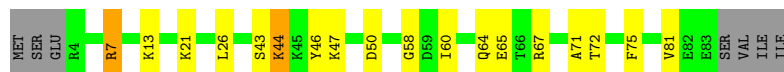
- Molecule 49: 30S ribosomal protein S16

Chain q:  84% 14%



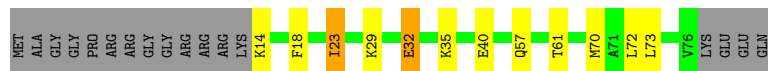
- Molecule 50: 30S ribosomal protein S17

Chain r:  71% 18% 8%



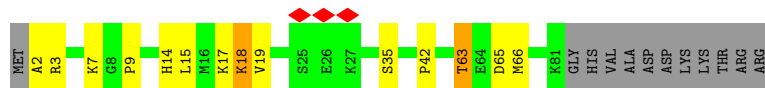
- Molecule 51: 30S ribosomal protein S18

Chain s:  64% 12% 21%

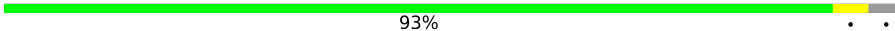


- Molecule 52: 30S ribosomal protein S19

Chain t:  72% 13% 13%

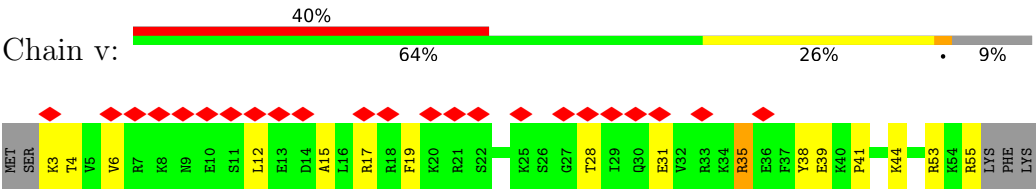


- Molecule 53: 30S ribosomal protein S20

Chain u:  93%



- Molecule 54: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67441	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 ($e^-/\text{\AA}^2$)	28.14	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.255	Depositor
Minimum map value	-0.632	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	436.8, 436.8, 436.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.728, 0.728, 0.728	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, H2U, UR3, ZN, 3TD, MG, MA6, 5MU, 2MA, 5MC, 2MG, 4OC, G7M, PUT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.47	0/487	0.75	0/649
2	2	0.41	0/536	0.91	0/713
3	3	0.45	0/438	0.84	0/590
4	4	0.46	0/671	0.84	0/900
5	5	0.48	0/429	0.79	0/571
6	6	0.43	0/407	0.79	0/545
7	7	0.49	0/371	0.90	0/484
8	8	0.47	0/526	0.84	0/690
9	9	0.49	0/299	0.80	0/393
10	A	0.53	0/68213	0.76	9/106380 (0.0%)
11	B	0.54	0/2692	0.74	0/4193
12	C	0.42	0/1737	0.86	0/2331
13	D	0.54	0/1832	0.78	0/2855
13	F	0.55	0/1813	0.78	0/2825
14	G	0.48	0/2120	0.82	0/2847
15	H	0.47	0/1661	0.83	0/2227
16	I	0.46	0/1587	0.85	0/2143
17	J	0.44	0/1430	0.86	0/1918
18	K	0.47	0/1379	0.84	0/1855
19	M	0.46	0/1168	0.82	0/1573
20	N	0.46	0/927	0.83	0/1243
21	O	0.48	0/1104	0.83	0/1471
22	P	0.46	0/1113	0.82	0/1493
23	Q	0.43	0/956	0.87	0/1277
24	R	0.47	0/931	0.85	0/1244
25	S	0.46	0/934	0.75	0/1249
26	T	0.44	0/955	0.94	0/1265
27	U	0.45	0/803	0.78	0/1073
28	V	0.46	0/861	0.83	0/1159
29	W	0.44	0/733	0.83	0/978
30	X	0.48	0/796	0.81	0/1063
31	Y	0.46	0/746	0.80	0/1000

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.47	0/632	0.83	0/838
33	a	0.53	0/36440	0.76	1/56820 (0.0%)
34	b	0.55	0/344	0.78	0/535
35	c	0.44	0/1808	0.90	0/2426
36	d	0.45	0/1634	0.84	0/2195
37	e	0.44	0/1647	0.83	0/2211
38	f	0.46	0/1174	0.86	0/1583
39	g	0.42	0/784	0.84	0/1052
40	h	0.45	0/1181	0.93	1/1587 (0.1%)
41	i	0.45	0/1044	0.85	0/1401
42	j	0.47	0/1032	0.88	0/1386
43	k	0.48	0/804	0.84	0/1083
44	l	0.51	0/891	0.88	1/1203 (0.1%)
45	m	0.49	0/1075	0.83	0/1439
46	n	0.44	0/909	0.92	0/1218
47	o	0.47	0/511	0.83	0/678
48	p	0.43	0/730	0.93	0/975
49	q	0.46	0/723	0.92	0/971
50	r	0.44	0/670	0.83	0/895
51	s	0.46	0/525	1.00	0/704
52	t	0.48	0/668	0.87	0/896
53	u	0.45	0/606	0.98	0/810
54	v	0.44	0/449	0.94	0/589
All	All	0.51	0/156936	0.79	12/234692 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	5	0	1
8	8	0	1
12	C	0	1
14	G	0	3
15	H	0	1
16	I	0	1
20	N	0	1
21	O	0	1
22	P	0	2
26	T	0	1
29	W	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
30	X	0	1
38	f	0	1
39	g	0	1
40	h	0	1
42	j	0	1
43	k	0	2
48	p	0	1
49	q	0	1
50	r	0	2
54	v	0	1
All	All	0	26

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	l	89	PRO	N-CA-CB	-7.23	95.65	103.25
10	A	1065	A	O3'-P-O5'	-6.59	94.11	104.00
10	A	1641	G	O3'-P-O5'	-6.14	94.79	104.00
10	A	826	A	O3'-P-O5'	-5.91	95.13	104.00
33	a	571	A	O3'-P-O5'	-5.79	95.31	104.00
10	A	1996	A	O3'-P-O5'	5.76	112.64	104.00
40	h	71	PRO	N-CA-CB	-5.72	97.24	103.25
10	A	958	U	O3'-P-O5'	-5.63	95.55	104.00
10	A	1275	A	O3'-P-O5'	-5.61	95.59	104.00
10	A	2673	C	O3'-P-O5'	-5.35	95.97	104.00
10	A	2546	U	O3'-P-O5'	-5.30	96.05	104.00
10	A	2641	A	O3'-P-O5'	-5.17	96.24	104.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	5	6	ARG	Sidechain
8	8	16	ARG	Sidechain
12	C	190	ARG	Sidechain
14	G	13	ARG	Sidechain
14	G	189	ARG	Sidechain
14	G	261	ARG	Sidechain
15	H	159	ASP	Peptide
16	I	168	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
20	N	104	ARG	Sidechain
21	O	59	ARG	Sidechain
22	P	134	ARG	Sidechain
22	P	56	ARG	Sidechain
26	T	48	ARG	Sidechain
29	W	9	ARG	Sidechain
30	X	92	ARG	Sidechain
38	f	14	ARG	Sidechain
39	g	88	ARG	Sidechain
40	h	92	ARG	Sidechain
42	j	14	ARG	Sidechain
43	k	62	ARG	Sidechain
43	k	72	ARG	Sidechain
48	p	77	ARG	Sidechain
49	q	14	ARG	Sidechain
50	r	67	ARG	Sidechain
50	r	7	ARG	Sidechain
54	v	35	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	481	0	523	2	0
2	2	535	0	566	4	0
3	3	436	0	473	2	0
4	4	654	0	631	18	0
5	5	422	0	426	6	0
6	6	402	0	413	4	0
7	7	367	0	415	7	0
8	8	521	0	586	3	0
9	9	296	0	339	3	0
10	A	61064	0	30708	290	0
11	B	2408	0	1218	12	0
12	C	1703	0	1739	27	0
13	D	1640	0	837	10	0
13	F	1623	0	825	8	0
14	G	2085	0	2192	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	H	1637	0	1680	15	0
16	I	1564	0	1611	11	0
17	J	1412	0	1470	29	0
18	K	1361	0	1392	16	0
19	M	1146	0	1142	12	0
20	N	920	0	981	10	0
21	O	1090	0	1131	9	0
22	P	1089	0	1155	9	0
23	Q	952	0	999	14	0
24	R	922	0	968	4	0
25	S	922	0	994	2	0
26	T	943	0	1014	14	0
27	U	793	0	831	0	0
28	V	853	0	914	7	0
29	W	725	0	761	7	0
30	X	787	0	853	3	0
31	Y	738	0	787	7	0
32	Z	626	0	645	5	0
33	a	32707	0	16479	257	0
34	b	306	0	153	3	0
35	c	1781	0	1844	24	0
36	d	1612	0	1674	26	0
37	e	1617	0	1646	15	0
38	f	1160	0	1223	15	0
39	g	773	0	772	7	0
40	h	1165	0	1204	20	0
41	i	1032	0	1082	18	0
42	j	1016	0	1039	11	0
43	k	792	0	833	25	0
44	l	876	0	895	14	0
45	m	1058	0	1130	7	0
46	n	902	0	950	14	0
47	o	501	0	523	8	0
48	p	721	0	751	11	0
49	q	712	0	744	10	0
50	r	662	0	702	12	0
51	s	516	0	548	9	0
52	t	651	0	658	10	0
53	u	606	0	650	1	0
54	v	446	0	487	9	0
55	5	1	0	0	0	0
55	9	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	C	1	0	0	0	0
55	o	1	0	0	0	0
56	A	117	0	0	0	0
56	F	2	0	0	0	0
56	G	1	0	0	0	0
56	O	1	0	0	0	0
56	a	24	0	0	0	0
57	A	12	0	24	1	0
58	1	8	0	0	0	0
58	2	2	0	0	0	0
58	3	4	0	0	0	0
58	5	18	0	0	0	0
58	6	1	0	0	0	0
58	7	31	0	0	2	0
58	8	32	0	0	1	0
58	9	2	0	0	0	0
58	A	4272	0	0	19	0
58	B	24	0	0	0	0
58	D	5	0	0	0	0
58	F	5	0	0	0	0
58	G	109	0	0	6	0
58	H	63	0	0	3	0
58	I	68	0	0	3	0
58	J	1	0	0	0	0
58	M	29	0	0	0	0
58	N	21	0	0	0	0
58	O	62	0	0	3	0
58	P	24	0	0	0	0
58	Q	26	0	0	3	0
58	S	10	0	0	0	0
58	T	60	0	0	4	0
58	U	34	0	0	0	0
58	V	33	0	0	0	0
58	W	13	0	0	0	0
58	X	1	0	0	0	0
58	Y	1	0	0	0	0
58	Z	13	0	0	0	0
58	a	522	0	0	1	0
58	b	1	0	0	0	0
58	c	1	0	0	0	0
58	d	2	0	0	0	0
58	e	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	f	2	0	0	0	0
58	h	1	0	0	0	0
58	i	2	0	0	0	0
58	k	2	0	0	0	0
58	l	1	0	0	0	0
58	m	1	0	0	0	0
58	o	1	0	0	0	0
58	r	2	0	0	0	0
58	s	1	0	0	0	0
58	u	1	0	0	0	0
58	v	1	0	0	0	0
All	All	150404	0	97230	1008	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 4.

All (1008) 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)
33:a:939:C:H2'	33:a:940:C:H5''	1.21	1.11
33:a:939:C:C2'	33:a:940:C:H5''	1.87	1.04
10:A:243:U:H3'	58:A:3260:HOH:O	1.69	0.93
44:l:75:MET:HG2	44:l:105:LEU:HD21	1.52	0.92
12:C:13:ILE:HG12	12:C:47:ILE:HD13	1.56	0.86
23:Q:26:ILE:HD11	23:Q:69:VAL:HG21	1.59	0.84
43:k:34:ALA:HB2	43:k:83:THR:HG21	1.58	0.84
10:A:1571:G:H22	10:A:1593:G:H1	1.24	0.83
33:a:525:G:O2'	33:a:538:G:H4'	1.79	0.82
10:A:244:A:H2'	58:A:3260:HOH:O	1.80	0.82
31:Y:7:ILE:HD11	31:Y:65:VAL:HA	1.61	0.82
54:v:39:GLU:HG3	54:v:44:LYS:HG2	1.64	0.80
19:M:7:ALA:HB1	19:M:12:ILE:HD11	1.65	0.78
33:a:1191:G:O2'	33:a:1192:G:N7	2.18	0.76
10:A:942:C:H3'	10:A:943:C:H5''	1.70	0.74
17:J:80:ARG:H	17:J:83:MET:HE2	1.51	0.74
36:d:76:ILE:CG2	36:d:102:VAL:HG11	2.20	0.72
33:a:992:A:H2	33:a:1232:G:H22	1.35	0.72
10:A:1449:A:H8	10:A:1634:A:H62	1.38	0.71
33:a:688:C:O2'	33:a:689:A:H5'	1.91	0.71
10:A:892:U:H5	10:A:977:A:N1	1.88	0.71
33:a:665:U:H3	33:a:757:A:H62	1.38	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:672:G:H22	33:a:749:G:H1	1.40	0.70
33:a:627:U:H5	37:e:127:ASP:HB3	1.55	0.70
33:a:274:G:H3'	50:r:71:ALA:HB2	1.74	0.69
43:k:80:THR:HB	43:k:83:THR:HG23	1.74	0.69
33:a:1155:C:H4'	33:a:1156:A:H5'	1.73	0.69
36:d:76:ILE:HG22	36:d:102:VAL:HG11	1.73	0.69
41:i:34:LYS:HG2	41:i:60:LEU:HD21	1.75	0.69
51:s:18:PHE:HA	51:s:23:ILE:HG23	1.73	0.68
10:A:2776:A:H1'	18:K:63:THR:HG22	1.75	0.68
33:a:525:G:HO2'	33:a:538:G:H4'	1.56	0.68
2:2:1:MET:HE1	2:2:17:GLN:HG2	1.76	0.68
12:C:94:LEU:HG	12:C:104:ILE:HD11	1.74	0.68
33:a:984:A:H4'	33:a:985:G:H5''	1.75	0.67
33:a:199:G:O2'	33:a:200:U:H5'	1.95	0.67
46:n:19:LEU:HD13	46:n:33:ILE:HD11	1.75	0.67
12:C:23:VAL:HG21	12:C:36:ILE:HG21	1.76	0.66
10:A:1806:U:H5	10:A:1811:A:N7	1.94	0.66
4:4:12:VAL:HG12	4:4:44:PRO:HG2	1.78	0.66
10:A:921:C:H2'	10:A:922:G:C8	2.31	0.66
10:A:2216:U:H3'	10:A:2217:G:H5''	1.78	0.66
18:K:115:ILE:HD12	18:K:148:ILE:HG12	1.78	0.66
23:Q:13:ARG:HA	58:Q:226:HOH:O	1.95	0.66
4:4:70:ARG:HG3	52:t:65:ASP:HA	1.79	0.65
22:P:35:GLN:HE22	31:Y:81:PRO:HB2	1.61	0.65
33:a:1011:U:H2'	33:a:1012:G:C8	2.32	0.65
33:a:39:G:H22	33:a:405:A:H5'	1.62	0.65
33:a:777:G:H4'	33:a:1524:A:H4'	1.78	0.65
10:A:1513:A:H2'	10:A:1514:A:C8	2.32	0.65
10:A:2611:U:H2'	10:A:2612:U:H2'	1.79	0.65
18:K:121:ILE:HG21	18:K:144:LEU:HD12	1.78	0.65
39:g:7:MET:HE1	51:s:72:LEU:HD11	1.79	0.65
17:J:8:PHE:HA	17:J:12:VAL:HB	1.79	0.64
41:i:47:LYS:HG3	41:i:65:LYS:HG2	1.80	0.64
12:C:85:PRO:HA	12:C:115:LYS:HA	1.79	0.64
43:k:10:LEU:HB3	43:k:18:ILE:HD11	1.78	0.64
54:v:4:THR:HG21	54:v:19:PHE:HA	1.78	0.64
10:A:165:C:H2'	10:A:166:A:H5'	1.80	0.63
10:A:923:A:N6	10:A:944:G:N7	2.46	0.63
6:6:1:MET:HG2	10:A:2312:C:C5	2.34	0.63
10:A:491:C:H5''	58:T:201:HOH:O	1.98	0.63
33:a:939:C:H2'	33:a:940:C:C5'	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:i:94:MET:HE1	41:i:124:GLY:HA2	1.80	0.63
58:a:1701:HOH:O	51:s:61:THR:HB	1.99	0.63
33:a:1149:G:O5'	33:a:1150:U:H5	1.81	0.63
12:C:85:PRO:HB3	12:C:115:LYS:HG2	1.81	0.63
16:I:54:ARG:HA	58:I:301:HOH:O	1.99	0.63
33:a:759:U:O2'	33:a:760:G:H5'	1.99	0.62
29:W:49:LYS:HB3	29:W:83:LYS:HE3	1.81	0.62
32:Z:40:THR:HA	32:Z:72:ASP:OD1	1.99	0.62
33:a:923:A:H2'	33:a:924:A:H5''	1.82	0.62
36:d:33:HIS:NE2	47:o:25:GLU:HB2	2.14	0.62
33:a:831:G:HO2'	41:i:2:THR:N	1.97	0.62
46:n:33:ILE:HG22	46:n:63:TYR:CE1	2.34	0.62
33:a:464:A:O2'	33:a:465:U:H5'	2.00	0.62
10:A:83:G:H21	10:A:102:A:H2	1.46	0.62
19:M:18:VAL:HG23	19:M:138:PRO:HB2	1.82	0.62
10:A:955:A:H2'	10:A:956:A:C8	2.36	0.61
12:C:79:PHE:HA	12:C:82:TYR:HD1	1.64	0.61
4:4:13:ILE:HG13	4:4:43:TYR:HB2	1.82	0.61
33:a:444:C:O2'	33:a:445:U:H5'	2.01	0.60
33:a:693:G:O2'	33:a:694:U:H5'	2.01	0.60
44:l:72:LYS:HA	44:l:75:MET:HE2	1.81	0.60
7:7:2:VAL:N	10:A:1663:G:HO2'	1.99	0.60
33:a:726:A:H5'	44:l:119:ASN:HB2	1.82	0.60
33:a:459:A:H4'	33:a:460:A:O5'	2.01	0.60
33:a:33:A:H2'	33:a:34:A:C8	2.37	0.60
33:a:1132:U:O2'	33:a:1133:U:H5'	2.02	0.60
13:F:33:U:OP2	42:j:132:ARG:NH2	2.32	0.59
26:T:35:ALA:HB2	58:T:207:HOH:O	2.02	0.59
33:a:390:A:H2'	33:a:391:A:C8	2.37	0.59
33:a:1391:U:O2'	33:a:1392:C:H5'	2.02	0.59
33:a:18:U:H2'	33:a:19:C:C6	2.37	0.59
33:a:68:C:H2'	33:a:69:G:C8	2.37	0.59
20:N:35:ILE:HG21	20:N:103:ALA:HB3	1.84	0.59
10:A:2683:U:H3	10:A:2692:A:H2	1.50	0.59
52:t:63:THR:HG22	52:t:66:MET:HG3	1.84	0.59
10:A:83:G:N2	10:A:101:G:H1'	2.17	0.59
33:a:939:C:C3'	33:a:940:C:H5''	2.32	0.59
15:H:131:ILE:HD11	15:H:149:ARG:HA	1.85	0.59
19:M:70:GLU:HG2	19:M:91:GLY:HA3	1.83	0.59
35:c:76:ALA:HB2	35:c:164:VAL:HG11	1.84	0.59
10:A:631:U:H2'	10:A:632:U:C6	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1221:C:O2'	10:A:1222:A:H8	1.85	0.59
10:A:351:G:H2'	10:A:352:A:C8	2.37	0.59
14:G:219:THR:HG22	58:G:486:HOH:O	2.03	0.58
10:A:1809:C:H1'	10:A:2636:U:H5''	1.85	0.58
10:A:942:C:H3'	10:A:943:C:C5'	2.32	0.58
36:d:76:ILE:HA	36:d:83:ILE:HB	1.85	0.58
48:p:29:ILE:HD11	48:p:66:LEU:HB2	1.85	0.58
10:A:613:G:H2'	10:A:2057:A:N7	2.17	0.58
15:H:132:LYS:HB3	58:H:302:HOH:O	2.01	0.58
10:A:2045:A:H5''	58:A:3252:HOH:O	2.02	0.58
16:I:28:PRO:HD3	16:I:119:GLN:HE22	1.69	0.58
33:a:1167:A:H4'	33:a:1168:C:O5'	2.04	0.58
33:a:1289:A:H4'	33:a:1291:U:H5	1.68	0.58
37:e:46:GLU:OE2	37:e:50:GLN:NE2	2.37	0.58
10:A:830:U:H2'	10:A:831:C:C6	2.38	0.58
33:a:721:G:H2'	33:a:722:G:C8	2.39	0.58
10:A:2715:G:OP1	10:A:2740:A:N6	2.37	0.58
33:a:85:U:H4'	33:a:86:G:H5'	1.86	0.57
7:7:19:PHE:HA	58:7:101:HOH:O	2.03	0.57
16:I:17:ILE:HD12	16:I:196:GLU:HG3	1.84	0.57
45:m:135:PRO:O	45:m:136:LYS:C	2.47	0.57
33:a:1497:G:H2'	33:a:1498:G:C8	2.39	0.57
23:Q:24:LEU:HD23	23:Q:44:VAL:HG21	1.85	0.57
33:a:1029:A:H3'	33:a:1030:G:H5''	1.86	0.57
48:p:36:ILE:HG23	48:p:56:LEU:HD11	1.87	0.57
33:a:1015:A:H2'	33:a:1016:A:C8	2.40	0.57
33:a:1143:C:H2'	33:a:1144:A:C8	2.39	0.57
42:j:67:VAL:HG11	42:j:81:ILE:HG12	1.86	0.57
10:A:622:A:H4'	58:A:3274:HOH:O	2.03	0.57
21:O:40:ALA:HB3	58:O:315:HOH:O	2.04	0.57
17:J:158:THR:HG22	17:J:160:ALA:H	1.70	0.57
22:P:39:THR:OG1	22:P:99:PRO:HD3	2.05	0.57
33:a:1247:C:H3'	33:a:1248:A:H5'	1.87	0.56
44:l:111:ARG:HD3	54:v:3:LYS:HE2	1.87	0.56
10:A:1238:U:H1'	26:T:4:VAL:HG22	1.86	0.56
10:A:1648:C:H1'	58:A:3202:HOH:O	2.05	0.56
58:A:3212:HOH:O	14:G:49:LEU:HB2	2.05	0.56
33:a:756:A:H1'	33:a:757:A:H2	1.70	0.56
33:a:1149:G:O5'	33:a:1150:U:C5	2.58	0.56
33:a:955:A:H2'	33:a:956:G:C8	2.39	0.56
33:a:1484:G:H2'	33:a:1485:G:C8	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:18:ILE:HD13	10:A:2446:U:H5''	1.88	0.56
10:A:688:A:N1	10:A:2396:A:O2'	2.37	0.56
42:j:77:GLN:O	42:j:81:ILE:HG13	2.06	0.56
10:A:778:G:H2'	58:A:3205:HOH:O	2.05	0.56
22:P:104:PHE:HE1	22:P:125:LEU:HD11	1.70	0.56
42:j:90:LEU:HD21	42:j:97:ARG:HA	1.87	0.56
17:J:29:PRO:HB3	17:J:160:ALA:HB2	1.88	0.56
33:a:491:C:O2'	49:q:14:ARG:NH2	2.38	0.56
22:P:78:PRO:HG2	22:P:81:VAL:HG11	1.88	0.55
33:a:262:G:OP1	50:r:72:THR:HG22	2.06	0.55
43:k:67:GLN:NE2	47:o:54:PRO:O	2.37	0.55
14:G:167:LYS:HD2	14:G:172:VAL:HG22	1.87	0.55
13:D:16:C:H3'	13:D:17:C:C6	2.42	0.55
10:A:1885:G:H1'	10:A:1911:A:H61	1.71	0.55
17:J:117:VAL:HG22	17:J:176:PRO:O	2.06	0.55
26:T:76:TYR:CZ	26:T:80:MET:HG3	2.41	0.55
42:j:52:GLN:N	42:j:53:PRO:HD2	2.22	0.55
10:A:2783:U:H1'	10:A:2784:A:H5''	1.89	0.55
33:a:57:U:H2'	33:a:58:G:C8	2.42	0.55
33:a:429:U:H5'	33:a:430:C:H5	1.72	0.55
10:A:1642:C:H5'	29:W:36:THR:OG1	2.07	0.55
38:f:166:ASN:HB2	41:i:116:LYS:HD2	1.88	0.55
4:4:14:PHE:HD2	4:4:48:LEU:HD21	1.70	0.55
10:A:2300:A:H2'	10:A:2301:A:C8	2.41	0.55
33:a:75:A:OP2	33:a:94:G:N2	2.37	0.55
10:A:1072:A:H2'	10:A:1073:A:C8	2.41	0.55
10:A:1100:G:H4'	10:A:1130:A:C8	2.42	0.55
33:a:429:U:H5'	33:a:430:C:C5	2.42	0.55
10:A:1675:G:H1'	10:A:1679:A:N6	2.21	0.55
26:T:66:ASN:O	26:T:70:ARG:HG2	2.06	0.55
33:a:988:C:H1'	33:a:1327:C:N4	2.21	0.55
10:A:794:A:H2'	10:A:795:A:H5'	1.89	0.54
10:A:684:U:H2'	10:A:685:C:C6	2.42	0.54
33:a:1366:G:H2'	33:a:1367:A:C8	2.42	0.54
10:A:194:A:H2'	10:A:195:C:C6	2.42	0.54
33:a:161:A:H2'	33:a:162:A:C8	2.42	0.54
33:a:1174:G:H3'	33:a:1175:U:H5''	1.87	0.54
10:A:250:G:H4'	10:A:432:G:C5	2.41	0.54
33:a:494:U:O2'	33:a:495:A:H5'	2.07	0.54
40:h:27:ILE:HD13	40:h:40:GLN:HG2	1.88	0.54
33:a:10:G:H5'	38:f:108:GLY:HA3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:s:57:GLN:O	51:s:61:THR:HG23	2.07	0.54
17:J:112:ARG:NH2	46:n:66:GLU:OE1	2.41	0.54
32:Z:80:LYS:O	32:Z:84:LYS:HB2	2.08	0.54
33:a:1228:U:H2'	33:a:1229:U:C6	2.43	0.54
33:a:1422:C:H2'	33:a:1423:A:C8	2.43	0.54
23:Q:16:MET:HE2	58:Q:226:HOH:O	2.07	0.54
28:V:73:GLU:HB2	28:V:106:VAL:HB	1.90	0.54
33:a:756:A:H1'	33:a:757:A:C2	2.41	0.54
2:2:26:PHE:CG	29:W:4:ARG:HD2	2.43	0.53
39:g:29:ILE:HA	39:g:32:THR:HG23	1.89	0.53
33:a:1391:U:C2'	33:a:1392:C:H5'	2.38	0.53
36:d:69:THR:HG21	36:d:75:VAL:HG11	1.91	0.53
43:k:25:ILE:HG22	43:k:90:LEU:HD23	1.91	0.53
15:H:38:LYS:HD2	15:H:96:VAL:HB	1.91	0.53
33:a:1306:C:H4'	33:a:1312:U:O4	2.07	0.53
10:A:305:A:N6	10:A:410:G:H22	2.06	0.53
10:A:1885:G:H1'	10:A:1911:A:N6	2.24	0.53
33:a:711:G:H4'	33:a:712:A:H5'	1.91	0.53
33:a:1122:A:N1	36:d:176:THR:HG22	2.24	0.53
20:N:104:ARG:HG2	20:N:121:VAL:HG12	1.91	0.53
41:i:21:ARG:NH1	41:i:70:ASP:O	2.42	0.53
21:O:61:LEU:HB2	58:O:362:HOH:O	2.09	0.53
33:a:1002:G:H2'	33:a:1004:C:H41	1.74	0.53
35:c:166:PRO:HG2	35:c:191:CYS:HB3	1.91	0.53
10:A:621:A:H2'	58:A:3252:HOH:O	2.08	0.53
38:f:56:VAL:HG23	38:f:57:PRO:HD3	1.91	0.53
10:A:2705:U:H2'	10:A:2706:A:C8	2.44	0.52
18:K:16:THR:HG23	18:K:27:LYS:HB2	1.91	0.52
10:A:2354:A:H2'	10:A:2355:A:C8	2.43	0.52
12:C:99:LYS:HD3	12:C:100:LYS:HE3	1.91	0.52
33:a:681:G:H2'	33:a:682:G:C8	2.45	0.52
35:c:58:LYS:HE2	35:c:223:GLU:HB3	1.91	0.52
36:d:22:TRP:CE2	47:o:54:PRO:HG2	2.44	0.52
45:m:123:ARG:HD2	45:m:125:GLN:O	2.09	0.52
35:c:117:ILE:HG21	35:c:141:TYR:HB2	1.91	0.52
10:A:1916:A:H2'	10:A:1917:A:C8	2.45	0.52
37:e:36:HIS:O	37:e:41:ARG:NH1	2.42	0.52
10:A:2672:G:H4'	10:A:2759:G:O2'	2.09	0.52
4:4:50:ILE:HD11	4:4:55:HIS:HA	1.92	0.52
33:a:1312:U:C5	46:n:17:ILE:HG13	2.45	0.52
38:f:38:VAL:HG12	38:f:117:LEU:HD12	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2707:C:H5'	15:H:202:PRO:HA	1.91	0.52
33:a:759:U:C2'	33:a:760:G:H5'	2.40	0.52
40:h:20:SER:HB2	40:h:23:VAL:HG23	1.92	0.52
10:A:1051:C:OP1	19:M:38:ARG:NH1	2.43	0.52
12:C:19:ARG:O	12:C:23:VAL:HG23	2.09	0.52
33:a:1401:U:H2'	33:a:1402:G:C8	2.45	0.52
40:h:68:ASN:O	40:h:138:ARG:NE	2.40	0.52
44:l:71:SER:O	44:l:75:MET:HG3	2.11	0.52
10:A:83:G:N2	10:A:102:A:H2	2.08	0.51
10:A:788:A:O2'	10:A:1703:U:OP1	2.25	0.51
10:A:1072:A:N6	10:A:1169:G:H2'	2.24	0.51
10:A:1836:A:H2'	10:A:1837:A:C8	2.44	0.51
11:B:28:C:H2'	11:B:29:C:H5'	1.92	0.51
12:C:93:LYS:HA	12:C:96:LYS:HD2	1.92	0.51
33:a:412:G:N7	37:e:3:ARG:NH2	2.57	0.51
33:a:1215:U:H4'	36:d:194:LYS:HD3	1.91	0.51
10:A:522:G:H4'	10:A:547:A:N1	2.25	0.51
17:J:135:GLN:HG3	17:J:150:ARG:O	2.10	0.51
33:a:1033:U:C2	33:a:1034:U:H5	2.28	0.51
12:C:193:ILE:HG22	12:C:197:LYS:HE3	1.91	0.51
4:4:1:MET:HG2	11:B:41:C:H5''	1.90	0.51
10:A:363:A:H4'	10:A:365:A:N7	2.26	0.51
10:A:1044:A:H2'	10:A:1045:A:C8	2.46	0.51
10:A:1115:G:H2'	10:A:1116:C:C6	2.46	0.51
10:A:1847:U:H3'	58:A:3206:HOH:O	2.09	0.51
33:a:1445:G:H2'	33:a:1446:C:C6	2.45	0.51
10:A:12:U:H2'	10:A:12:U:O2	2.10	0.51
35:c:187:VAL:HG13	35:c:191:CYS:HB2	1.93	0.51
37:e:178:ARG:NH2	37:e:184:GLU:OE2	2.43	0.51
50:r:44:LYS:HB3	50:r:46:TYR:HE1	1.75	0.51
4:4:31:SER:HB3	4:4:44:PRO:HB2	1.93	0.51
33:a:307:G:H2'	33:a:308:A:C8	2.45	0.51
39:g:7:MET:HG2	51:s:70:MET:HE2	1.93	0.51
10:A:1510:U:O2'	10:A:1593:G:O2'	2.26	0.51
12:C:9:GLN:O	12:C:13:ILE:HG13	2.11	0.51
33:a:13:U:H4'	33:a:534:C:H4'	1.92	0.51
10:A:1469:G:H2'	10:A:1470:G:C8	2.46	0.51
10:A:2879:G:H2'	10:A:2880:A:C8	2.46	0.51
12:C:58:SER:HB3	12:C:75:ILE:HG23	1.92	0.51
23:Q:121:LEU:O	23:Q:122:VAL:HB	2.11	0.51
33:a:538:G:H3'	33:a:538:G:N3	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:k:6:ILE:HB	43:k:76:ILE:HB	1.93	0.51
7:7:25:THR:HG23	7:7:28:GLY:H	1.75	0.51
45:m:89:GLU:O	45:m:90:HIS:HB2	2.09	0.51
4:4:78:PHE:HB2	4:4:80:LEU:HD22	1.94	0.50
10:A:1880:A:H2'	10:A:1881:A:C8	2.46	0.50
33:a:1370:A:OP2	47:o:35:ARG:NH2	2.45	0.50
5:5:2:ALA:HB2	58:A:3538:HOH:O	2.10	0.50
10:A:2355:A:H2'	10:A:2356:A:C8	2.45	0.50
15:H:15:VAL:HG21	15:H:186:VAL:HG11	1.92	0.50
10:A:1533:A:H2'	14:G:98:ASP:HB3	1.93	0.50
10:A:2404:A:H2'	10:A:2405:A:C8	2.47	0.50
25:S:10:VAL:HG23	25:S:11:THR:HG23	1.94	0.50
26:T:3:ARG:N	58:T:201:HOH:O	2.44	0.50
33:a:413:U:H1'	33:a:506:A:H2'	1.94	0.50
33:a:798:A:H2'	33:a:799:G:C8	2.45	0.50
33:a:1011:U:H2'	33:a:1012:G:H8	1.74	0.50
10:A:363:A:H4'	10:A:365:A:C8	2.46	0.50
10:A:1473:G:H2'	10:A:1474:C:C6	2.47	0.50
16:I:200:LYS:O	16:I:204:GLU:HG3	2.12	0.50
30:X:70:LEU:HD11	30:X:92:ARG:NH2	2.26	0.50
33:a:526:C:H2'	33:a:538:G:C8	2.46	0.50
48:p:19:GLU:O	48:p:20:THR:OG1	2.18	0.50
8:8:49:LEU:HD22	58:8:122:HOH:O	2.10	0.50
43:k:18:ILE:HD12	43:k:96:VAL:HG23	1.94	0.50
45:m:26:LYS:O	45:m:43:LYS:NZ	2.45	0.50
48:p:25:PRO:O	48:p:29:ILE:HG12	2.11	0.50
10:A:1821:U:H2'	10:A:1822:C:C6	2.47	0.50
10:A:2372:G:N3	10:A:2408:C:H2'	2.27	0.50
4:4:78:PHE:CE2	52:t:9:PRO:HG3	2.47	0.50
10:A:285:U:H4'	10:A:286:U:C5	2.47	0.50
15:H:169:MET:SD	58:H:301:HOH:O	2.60	0.50
51:s:35:LYS:HG2	51:s:73:LEU:HD21	1.94	0.50
12:C:171:LYS:O	12:C:172:LYS:C	2.55	0.50
35:c:131:LYS:O	35:c:134:VAL:HG22	2.12	0.50
41:i:61:ARG:HD2	41:i:63:PHE:CZ	2.45	0.50
10:A:2318:U:H2'	10:A:2319:U:C6	2.47	0.50
17:J:106:VAL:C	17:J:109:PRO:HD2	2.37	0.50
43:k:80:THR:HB	43:k:83:THR:CG2	2.42	0.50
10:A:2209:G:H2'	10:A:2210:C:O4'	2.12	0.49
13:F:17:C:OP2	13:F:17(A):U:O2'	2.27	0.49
17:J:22:TYR:CE2	17:J:29:PRO:HD3	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:728:C:O2'	51:s:61:THR:HG21	2.12	0.49
35:c:76:ALA:HB1	35:c:164:VAL:HG21	1.93	0.49
54:v:38:TYR:OH	54:v:41:PRO:HD3	2.12	0.49
10:A:2332:U:H5''	17:J:131:GLY:HA3	1.94	0.49
33:a:1188:G:N7	42:j:101:LYS:NZ	2.48	0.49
36:d:34:GLU:HG3	36:d:37:LYS:HE2	1.93	0.49
10:A:787:U:H2'	10:A:788:A:C8	2.47	0.49
33:a:1015:A:H8	33:a:1016:A:N7	2.09	0.49
43:k:11:LYS:HG2	43:k:71:LYS:HG2	1.93	0.49
33:a:99:U:H2'	33:a:100:A:C8	2.46	0.49
49:q:54:GLU:CD	49:q:54:GLU:H	2.21	0.49
4:4:71:VAL:HG23	52:t:42:PRO:HB3	1.94	0.49
13:D:21:A:N1	13:D:46:G:H2'	2.28	0.49
26:T:31:LEU:HB2	26:T:34:VAL:HG12	1.93	0.49
33:a:284:G:H4'	50:r:47:LYS:HZ1	1.76	0.49
33:a:1307:U:H1'	33:a:1308:C:H5	1.77	0.49
38:f:77:VAL:O	38:f:80:THR:HG22	2.11	0.49
17:J:70:ALA:HB2	17:J:79:LEU:HD11	1.95	0.49
48:p:29:ILE:HD11	48:p:66:LEU:CB	2.41	0.49
10:A:719:G:N2	58:A:3215:HOH:O	2.45	0.49
26:T:28:LYS:HG2	26:T:34:VAL:HG22	1.94	0.49
33:a:1283:C:H2'	33:a:1284:A:O4'	2.13	0.49
40:h:138:ARG:HH11	40:h:142:HIS:HD1	1.60	0.49
10:A:1756:U:H2'	10:A:1757:U:O4'	2.12	0.49
14:G:161:SER:HB3	14:G:194:GLN:HG3	1.93	0.49
18:K:164:TYR:HB2	18:K:167:GLU:HB2	1.95	0.49
33:a:532:G:H2'	33:a:533:C:C6	2.47	0.49
33:a:1222:U:H5'	33:a:1223:A:C8	2.48	0.49
35:c:177:ARG:HD2	35:c:195:GLU:HB3	1.95	0.49
42:j:56:VAL:HG12	42:j:99:SER:HB3	1.94	0.49
10:A:1813:A:N6	58:A:3218:HOH:O	2.46	0.49
15:H:128:GLN:HB3	58:H:302:HOH:O	2.13	0.49
33:a:722:G:H2'	33:a:723:A:C8	2.47	0.49
35:c:162:PHE:HA	35:c:184:VAL:O	2.13	0.49
46:n:59:VAL:HG12	46:n:63:TYR:HE1	1.78	0.49
10:A:83:G:H22	10:A:101:G:H1'	1.78	0.49
10:A:702:U:H2'	10:A:703:A:C8	2.48	0.49
10:A:1463:A:H2'	10:A:1465:G:N7	2.27	0.49
13:D:9:G:H1'	13:D:45:G:H2'	1.95	0.49
38:f:115:LEU:HD13	38:f:123:ILE:HG21	1.95	0.49
39:g:26:PHE:HA	39:g:29:ILE:HD12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:k:15:HIS:O	43:k:18:ILE:HG22	2.12	0.49
43:k:32:SER:CB	43:k:83:THR:HG22	2.43	0.49
45:m:79:TYR:HB2	45:m:106:VAL:HG11	1.95	0.49
10:A:1313:G:H4'	23:Q:8:ARG:HH12	1.77	0.48
14:G:165:LEU:HD11	14:G:175:ARG:HB2	1.95	0.48
33:a:688:C:C2'	33:a:689:A:H5'	2.43	0.48
10:A:792:5MU:H4'	28:V:92:ARG:NH2	2.28	0.48
12:C:89:PRO:HB3	12:C:141:LEU:HD22	1.94	0.48
12:C:140:GLN:HB2	12:C:142:LYS:HE3	1.95	0.48
20:N:24:VAL:HG13	20:N:33:ALA:HB2	1.95	0.48
20:N:90:ASP:O	20:N:91:LYS:HB2	2.13	0.48
30:X:10:LYS:HB2	30:X:71:LEU:HD21	1.95	0.48
44:l:19:GLY:HA3	44:l:79:LEU:HD11	1.95	0.48
10:A:569:U:H4'	10:A:598:G:H4'	1.96	0.48
43:k:25:ILE:HD11	43:k:74:ILE:HD13	1.95	0.48
10:A:2584:G:H2'	10:A:2585:C:C6	2.48	0.48
18:K:17:VAL:HG13	18:K:26:VAL:HG22	1.94	0.48
33:a:685:U:H3	33:a:721:G:H22	1.60	0.48
10:A:1091:G:N2	10:A:1154:G:O2'	2.46	0.48
10:A:2716:U:H5''	10:A:2740:A:C2	2.48	0.48
22:P:32:PHE:HD1	22:P:133:LYS:HG2	1.78	0.48
36:d:50:SER:O	36:d:69:THR:HA	2.13	0.48
41:i:26:GLU:HG3	41:i:61:ARG:HG3	1.95	0.48
10:A:2088:G:H5'	58:A:3204:HOH:O	2.12	0.48
33:a:957:C:OP1	46:n:108:THR:HG22	2.14	0.48
48:p:12:ILE:HG13	48:p:13:LYS:N	2.27	0.48
48:p:87:ILE:O	48:p:88:ARG:HB2	2.14	0.48
10:A:1423:C:H2'	10:A:1424:A:C8	2.48	0.48
10:A:1588:U:H2'	10:A:1589:U:C6	2.49	0.48
10:A:2339:U:H5'	17:J:85:ILE:HD11	1.95	0.48
33:a:9:A:N6	37:e:196:GLU:O	2.47	0.48
10:A:1827:C:OP1	14:G:260:ARG:NH2	2.45	0.48
14:G:103:TYR:HB3	58:G:469:HOH:O	2.13	0.48
14:G:145:GLU:HG2	14:G:151:GLY:C	2.38	0.48
17:J:12:VAL:HG22	17:J:172:ASN:HB3	1.95	0.48
33:a:1064:G:N7	33:a:1210:C:H5''	2.29	0.48
10:A:2335:G:N3	10:A:2335:G:H2'	2.28	0.48
58:A:4013:HOH:O	26:T:34:VAL:HB	2.13	0.48
13:F:58:A:O2'	13:F:60:U:OP2	2.20	0.48
14:G:133:GLN:HG2	14:G:186:SER:HB2	1.96	0.48
33:a:828:U:H4'	33:a:829:G:OP2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:1388:C:OP2	40:h:3:ARG:NH2	2.47	0.48
42:j:131:LYS:O	42:j:132:ARG:HB2	2.14	0.48
10:A:2479:C:H2'	10:A:2480:A:C8	2.49	0.47
23:Q:52:LYS:NZ	23:Q:96:ARG:O	2.47	0.47
31:Y:7:ILE:HD13	31:Y:41:VAL:HB	1.95	0.47
52:t:2:ALA:HB3	52:t:7:LYS:HB2	1.95	0.47
53:u:39:VAL:HG11	53:u:81:ALA:HB1	1.96	0.47
10:A:25:U:H5'	28:V:78:GLU:O	2.14	0.47
10:A:827:A:N7	14:G:220:VAL:HG21	2.30	0.47
10:A:2778:G:N3	10:A:2778:G:H2'	2.29	0.47
18:K:23:HIS:HA	18:K:36:THR:HA	1.96	0.47
33:a:550:U:H5'	37:e:34:GLY:HA3	1.95	0.47
33:a:1143:C:H2'	33:a:1144:A:H8	1.77	0.47
33:a:1238:C:H4'	46:n:115:THR:HA	1.96	0.47
33:a:1297:A:H2'	33:a:1298:A:C8	2.49	0.47
36:d:8:ILE:HD11	36:d:183:TYR:H	1.79	0.47
44:l:128:ARG:O	44:l:129:VAL:HB	2.12	0.47
12:C:100:LYS:HE2	12:C:100:LYS:HA	1.97	0.47
13:D:14:A:N1	13:D:21:A:O2'	2.45	0.47
17:J:129:THR:HG23	17:J:155:VAL:HG22	1.96	0.47
33:a:754:G:O2'	33:a:755:U:H5'	2.15	0.47
10:A:2052:C:H2'	10:A:2053:U:C6	2.49	0.47
17:J:44:VAL:HG13	17:J:83:MET:HE1	1.95	0.47
33:a:1172:C:H2'	33:a:1173:G:H8	1.79	0.47
46:n:11:ARG:HA	46:n:45:VAL:HB	1.96	0.47
3:3:11:SER:HB2	10:A:1032:A:H5''	1.95	0.47
10:A:287:G:H2'	10:A:287:G:N3	2.30	0.47
15:H:30:ALA:HB3	15:H:107:VAL:HG12	1.95	0.47
28:V:3:ALA:HB1	28:V:57:ASN:OD1	2.15	0.47
33:a:32:G:H3'	33:a:33:A:H5''	1.95	0.47
33:a:171:A:H2'	33:a:172:A:C8	2.50	0.47
10:A:2594:G:H2'	10:A:2595:C:C6	2.50	0.47
33:a:517:A:H2'	33:a:518:A:C8	2.48	0.47
38:f:56:VAL:CG2	38:f:57:PRO:HD3	2.45	0.47
46:n:114:LYS:O	46:n:115:THR:C	2.58	0.47
54:v:53:ARG:HG3	54:v:53:ARG:HH11	1.78	0.47
10:A:221:G:N2	10:A:238:U:H4'	2.30	0.47
10:A:1940:A:H4'	10:A:1941:C:OP2	2.12	0.47
11:B:62:U:O2'	11:B:63:U:H5'	2.14	0.47
33:a:748:U:O2'	33:a:749:G:H5'	2.15	0.47
33:a:1141:A:O2'	33:a:1142:U:H5'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:1151:U:O2'	33:a:1152:G:O5'	2.33	0.47
33:a:1286:G:H2'	33:a:1287:C:O4'	2.15	0.47
35:c:54:TYR:CD2	35:c:220:ALA:HB2	2.50	0.47
35:c:157:MET:HE2	35:c:157:MET:HA	1.96	0.47
36:d:22:TRP:CZ2	47:o:54:PRO:HG2	2.50	0.47
36:d:205:GLU:O	36:d:206:VAL:C	2.58	0.47
39:g:3:THR:O	39:g:93:ARG:O	2.32	0.47
46:n:4:ILE:HG22	46:n:60:VAL:HG11	1.96	0.47
54:v:31:GLU:HG3	54:v:35:ARG:HE	1.80	0.47
11:B:38:U:H1'	11:B:43:A:H61	1.79	0.47
33:a:496:C:O2'	33:a:497:C:H5'	2.15	0.47
33:a:1045:G:H2'	33:a:1046:G:C8	2.49	0.47
33:a:1379:C:H2'	33:a:1380:G:C8	2.50	0.47
33:a:1390:U:C5	40:h:3:ARG:HB2	2.50	0.47
43:k:54:ALA:O	47:o:41:ARG:NH1	2.48	0.47
5:5:17:ARG:HG3	58:A:3283:HOH:O	2.14	0.47
10:A:1047:G:O2'	10:A:1054:A:N1	2.44	0.47
10:A:2687:A:H2'	10:A:2688:G:O4'	2.15	0.47
24:R:78:GLU:HG3	24:R:111:ALA:HB1	1.95	0.47
41:i:47:LYS:HG3	41:i:65:LYS:CG	2.42	0.47
10:A:1828:U:OP2	14:G:150:LYS:NZ	2.45	0.47
11:B:35:C:H2'	11:B:36:C:O4'	2.15	0.47
32:Z:58:ASN:HB3	32:Z:71:ILE:HG12	1.97	0.47
33:a:464:A:C2'	33:a:465:U:H5'	2.45	0.47
33:a:1323:U:O4	52:t:3:ARG:HG2	2.15	0.47
8:8:14:VAL:HG21	8:8:62:LEU:HD13	1.97	0.46
10:A:1221:C:O2'	10:A:1222:A:O5'	2.33	0.46
36:d:21:LYS:HB2	36:d:57:GLU:HG2	1.96	0.46
41:i:110:GLU:HG3	41:i:123:VAL:HG21	1.97	0.46
10:A:537:A:H2'	10:A:538:G:O4'	2.15	0.46
10:A:2916:U:H2'	10:A:2917:U:C6	2.50	0.46
17:J:43:ALA:HA	17:J:46:ASN:O	2.16	0.46
26:T:32:TYR:HA	58:T:253:HOH:O	2.14	0.46
33:a:728:C:H2'	33:a:729:A:C8	2.50	0.46
33:a:929:U:H2'	33:a:930:U:C6	2.49	0.46
33:a:1135:G:H5''	43:k:37:SER:HB2	1.97	0.46
33:a:1348:G:H2'	33:a:1349:A:C8	2.50	0.46
10:A:774:G:C6	14:G:207:LYS:HB2	2.50	0.46
10:A:2820:U:H2'	10:A:2822:C:C5	2.50	0.46
17:J:38:MET:HE2	17:J:57:LEU:HD22	1.97	0.46
10:A:1659:C:N4	58:A:3225:HOH:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:33:U:H3'	13:D:35:A:OP2	2.16	0.46
33:a:345:G:H2'	33:a:346:A:C8	2.51	0.46
33:a:385:G:OP1	49:q:4:LYS:HD3	2.16	0.46
33:a:563:C:H2'	33:a:564:C:C6	2.51	0.46
33:a:1394:C:O2'	33:a:1395:G:H5'	2.16	0.46
40:h:63:GLU:O	40:h:67:ASN:ND2	2.48	0.46
45:m:52:THR:HG22	45:m:64:LYS:HD3	1.98	0.46
10:A:120:G:H4'	10:A:150:A:H5'	1.97	0.46
16:I:34:PHE:CE1	21:O:8:PRO:HB3	2.51	0.46
5:5:5:LYS:NZ	10:A:2083:G:O3'	2.48	0.46
9:9:22:LYS:HD3	9:9:35:ARG:HD3	1.97	0.46
10:A:1149:U:H2'	10:A:1150:A:H8	1.80	0.46
33:a:1085:G:O2'	33:a:1112:A:N1	2.44	0.46
33:a:1221:U:H1'	33:a:1223:A:C2	2.50	0.46
36:d:188:ALA:HB3	36:d:195:LEU:HB2	1.97	0.46
49:q:66:LYS:HA	49:q:67:PRO:HD3	1.85	0.46
10:A:12:U:O2	10:A:12:U:C2'	2.62	0.46
10:A:1823:U:H2'	10:A:1824:C:C6	2.50	0.46
10:A:2109:A:H2'	10:A:2110:G:O4'	2.15	0.46
11:B:37:A:H2'	11:B:38:U:C6	2.51	0.46
23:Q:105:LYS:HA	23:Q:117:VAL:HG12	1.98	0.46
33:a:409:C:OP2	37:e:66:ARG:NH1	2.44	0.46
33:a:670:A:H2'	33:a:671:A:C8	2.51	0.46
10:A:2436:G:H2'	10:A:2437:G:O4'	2.16	0.46
33:a:1002:G:H2'	33:a:1002:G:N3	2.31	0.46
33:a:1014:C:H5'	33:a:1050:A:O4'	2.16	0.46
10:A:127:C:H2'	10:A:128:C:C6	2.50	0.46
10:A:2403:A:N3	24:R:113:ARG:NH2	2.64	0.46
33:a:1071:U:H5''	43:k:53:ARG:HG2	1.97	0.46
40:h:47:PHE:HA	40:h:50:VAL:HG12	1.97	0.46
10:A:841:C:H2'	10:A:842:U:C6	2.51	0.46
10:A:1013:U:H2'	10:A:1014:U:C6	2.51	0.46
10:A:2912:A:H4'	10:A:2913:G:N3	2.31	0.46
10:A:305:A:H61	10:A:410:G:H22	1.63	0.45
14:G:221:ARG:HG3	58:G:486:HOH:O	2.16	0.45
16:I:79:ARG:HB3	58:I:301:HOH:O	2.15	0.45
33:a:703:A:H2'	33:a:704:A:O4'	2.16	0.45
33:a:1450:U:H2'	33:a:1451:G:C8	2.50	0.45
38:f:15:VAL:HG12	38:f:37:VAL:HG22	1.98	0.45
49:q:22:VAL:HG21	49:q:60:TRP:CD1	2.51	0.45
10:A:1474:C:H2'	10:A:1475:A:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:107:ALA:O	26:T:111:THR:HG23	2.16	0.45
33:a:469:U:H2'	33:a:470:A:C8	2.51	0.45
39:g:7:MET:HE2	51:s:70:MET:HB3	1.98	0.45
46:n:29:THR:O	46:n:33:ILE:HG23	2.16	0.45
48:p:8:LYS:O	48:p:12:ILE:HG23	2.17	0.45
10:A:395:U:H2'	10:A:396:G:C8	2.51	0.45
10:A:788:A:OP1	15:H:144:GLY:HA2	2.17	0.45
10:A:963:A:H5''	11:B:94:C:O2'	2.16	0.45
10:A:1537:A:H2'	10:A:1538:A:C8	2.52	0.45
16:I:83:TRP:CD1	58:I:309:HOH:O	2.70	0.45
33:a:1177:A:H3'	33:a:1178:C:H5''	1.97	0.45
10:A:926:G:H2'	10:A:926:G:N3	2.30	0.45
10:A:2208:A:H3'	10:A:2209:G:H5''	1.98	0.45
36:d:107:LYS:HB3	36:d:143:LEU:HD13	1.98	0.45
41:i:36:ILE:HG23	41:i:105:LEU:HD22	1.97	0.45
48:p:75:ILE:HD12	48:p:75:ILE:H	1.81	0.45
4:4:55:HIS:HB3	4:4:58:TYR:CD1	2.52	0.45
10:A:1817:C:H5'	58:A:6759:HOH:O	2.16	0.45
10:A:1850:G:H3'	58:A:4173:HOH:O	2.16	0.45
21:O:58:PHE:HD1	58:O:362:HOH:O	1.99	0.45
37:e:15:LEU:HD13	37:e:56:LYS:HA	1.97	0.45
37:e:88:ILE:HG22	37:e:185:LEU:HD11	1.97	0.45
10:A:1065:A:H3'	10:A:1065:A:N3	2.31	0.45
10:A:1689:G:H4'	10:A:1690:A:C8	2.52	0.45
10:A:2774:G:O6	10:A:2782:C:H5''	2.17	0.45
17:J:136:LEU:HD13	17:J:149:VAL:HG12	1.98	0.45
18:K:9:ILE:HD11	18:K:69:ARG:HG2	1.98	0.45
33:a:160:A:H2'	33:a:161:A:O4'	2.17	0.45
33:a:917:A:H2'	33:a:918:A:C8	2.51	0.45
10:A:858:U:H2'	10:A:859:C:C6	2.51	0.45
18:K:97:GLN:HG3	18:K:104:ILE:HB	1.98	0.45
33:a:50:U:O4	33:a:373:U:H5	2.00	0.45
33:a:986:A:O2'	33:a:988:C:OP2	2.31	0.45
10:A:901:G:H2'	10:A:902:A:C8	2.52	0.45
10:A:903:G:N3	10:A:2295:A:H2'	2.31	0.45
10:A:1829:A:H2'	10:A:1830:A:C8	2.52	0.45
10:A:2041:A:H2'	10:A:2042:A:C8	2.52	0.45
11:B:64:A:N6	11:B:104:A:H2'	2.32	0.45
14:G:107:PRO:HD2	14:G:110:LEU:HD22	1.98	0.45
33:a:810:A:H2'	33:a:811:G:O4'	2.17	0.45
50:r:7:ARG:HB2	50:r:64:GLN:HE21	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:878:C:H2'	10:A:879:U:C6	2.51	0.45
10:A:2439:A:H2'	10:A:2440:G:O4'	2.16	0.45
33:a:78:A:N3	33:a:78:A:H2'	2.32	0.45
33:a:1246:A:H2'	33:a:1247:C:C6	2.51	0.45
50:r:26:LEU:HD11	50:r:43:SER:HB3	1.99	0.45
1:1:10:ARG:HD3	10:A:443:U:OP2	2.17	0.45
2:2:1:MET:HE3	2:2:6:ILE:HG12	1.98	0.45
10:A:1140:A:H3'	10:A:1141:U:H5''	1.99	0.45
18:K:45:GLN:HG3	18:K:50:ILE:HG12	1.98	0.45
34:b:19:G:H2'	34:b:20:C:C6	2.52	0.45
36:d:137:ILE:HA	36:d:148:ILE:HD13	1.99	0.45
42:j:41:LEU:HA	42:j:42:PRO:HD3	1.85	0.45
10:A:525:A:H1'	10:A:526:A:H5''	1.99	0.44
10:A:892:U:C5	10:A:977:A:N1	2.77	0.44
10:A:967:C:O2'	32:Z:34:ALA:HB2	2.16	0.44
15:H:194:VAL:HG11	25:S:10:VAL:HG11	2.00	0.44
33:a:22:G:H2'	33:a:23:G:C8	2.52	0.44
33:a:923:A:C2'	33:a:924:A:H5''	2.46	0.44
36:d:109:ASP:HB2	36:d:143:LEU:HD12	1.99	0.44
10:A:84:A:N1	10:A:98:U:O2'	2.44	0.44
10:A:1071:A:C2	10:A:2515:A:H5'	2.52	0.44
10:A:1697:G:C6	23:Q:5:LYS:HB2	2.51	0.44
10:A:1766:C:H2'	10:A:1767:G:O4'	2.18	0.44
13:D:36:U:H2'	13:D:37:A:O4'	2.17	0.44
14:G:72:ASP:OD2	14:G:189:ARG:NH2	2.50	0.44
33:a:34:A:H2'	33:a:35:C:C6	2.53	0.44
33:a:130:A:OP1	50:r:7:ARG:NH2	2.41	0.44
33:a:745:U:H2'	33:a:746:U:C6	2.51	0.44
33:a:995:A:H2'	33:a:996:A:C8	2.52	0.44
33:a:1150:U:H2'	33:a:1151:U:C6	2.52	0.44
33:a:1154:G:N2	33:a:1156:A:H62	2.15	0.44
44:l:35:THR:HG22	44:l:41:ALA:HA	1.99	0.44
10:A:1698:A:O2'	15:H:127:PHE:O	2.35	0.44
23:Q:75:ASP:O	23:Q:76:GLU:HB2	2.17	0.44
33:a:147:G:H2'	33:a:148:G:C8	2.53	0.44
41:i:15:ARG:HG2	41:i:19:MET:HE3	1.99	0.44
44:l:117:PRO:HG2	54:v:35:ARG:NH1	2.32	0.44
10:A:195:C:H2'	10:A:196:U:H5'	1.99	0.44
10:A:1222:A:H2'	10:A:1223:A:C8	2.52	0.44
35:c:151:ILE:HB	35:c:154:MET:HE2	1.99	0.44
36:d:186:ALA:HB3	36:d:197:VAL:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:k:57:LYS:HE3	43:k:58:TYR:CZ	2.52	0.44
10:A:2633:C:H4'	58:A:3218:HOH:O	2.16	0.44
21:O:91:VAL:HA	21:O:95:LEU:HD23	1.98	0.44
33:a:26:C:H5'	33:a:532:G:H1'	1.99	0.44
40:h:50:VAL:HG23	40:h:125:LEU:HD22	2.00	0.44
43:k:67:GLN:OE1	47:o:36:LYS:HE2	2.18	0.44
52:t:14:HIS:HA	52:t:17:LYS:HE3	1.98	0.44
10:A:26:G:H1'	10:A:559:A:N6	2.33	0.44
10:A:682:A:H4'	10:A:683:G:H5'	2.00	0.44
10:A:877:G:H2'	10:A:878:C:C6	2.52	0.44
10:A:941:A:H2'	10:A:942:C:H5'	1.99	0.44
10:A:2686:G:O2'	18:K:175:LYS:NZ	2.50	0.44
11:B:82:A:O2'	11:B:83:C:H5'	2.18	0.44
12:C:138:LYS:HB2	12:C:140:GLN:HG2	1.99	0.44
13:F:44:A:H2'	13:F:45:G:C8	2.53	0.44
33:a:119:A:O2'	33:a:121:A:OP1	2.31	0.44
33:a:504:G:N2	33:a:505:A:H3'	2.33	0.44
35:c:27:MET:HE2	35:c:27:MET:HB3	1.92	0.44
10:A:629:A:N1	10:A:854:G:O2'	2.47	0.44
14:G:29:PRO:HG2	14:G:34:LEU:HD11	1.99	0.44
43:k:17:VAL:HG13	43:k:93:PRO:HG2	1.99	0.44
43:k:35:ASP:HB3	43:k:77:VAL:HB	2.00	0.44
10:A:665:G:N3	10:A:665:G:H2'	2.33	0.44
10:A:1381:U:O2	10:A:1422:A:H5'	2.18	0.44
10:A:1382:C:H2'	10:A:1383:G:H8	1.82	0.44
17:J:103:LEU:HA	17:J:107:SER:HB3	1.99	0.44
29:W:19:ALA:HB1	29:W:24:LYS:HB2	2.00	0.44
49:q:14:ARG:HG3	49:q:14:ARG:HH11	1.83	0.44
54:v:6:VAL:HG22	54:v:15:ALA:CB	2.47	0.44
10:A:161:A:H2'	10:A:162:A:C8	2.52	0.44
10:A:1357:G:C2	10:A:1366:U:H5''	2.52	0.44
10:A:1510:U:H4'	10:A:1593:G:H21	1.83	0.44
10:A:2053:U:H2'	10:A:2054:G:O4'	2.18	0.44
10:A:2917:U:H2'	10:A:2918:A:C8	2.53	0.44
33:a:755:U:H2'	33:a:756:A:O4'	2.17	0.44
33:a:1090:G:H5'	38:f:134:ILE:HD13	1.99	0.44
33:a:1534:G:OP1	44:l:128:ARG:NH2	2.51	0.44
35:c:153:ASP:OD1	35:c:153:ASP:N	2.51	0.44
10:A:259:A:H2'	10:A:260:A:C8	2.53	0.43
10:A:1241:A:H2'	10:A:1242:A:C8	2.53	0.43
10:A:1873:G:H2'	10:A:1874:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:118:ASP:HA	21:O:139:LYS:HE2	2.00	0.43
22:P:111:GLU:O	22:P:115:ARG:HG3	2.18	0.43
33:a:416:G:OP1	37:e:106:THR:HG21	2.17	0.43
33:a:1031:C:H2'	33:a:1032:C:C6	2.53	0.43
33:a:1327:C:N4	47:o:19:ARG:HH21	2.15	0.43
35:c:89:GLN:HG3	35:c:221:ILE:HD13	2.00	0.43
10:A:1582:U:O2'	10:A:1583:G:O5'	2.36	0.43
10:A:1951:C:H4'	13:F:13:C:H4'	2.00	0.43
10:A:2814:C:H1'	15:H:72:PRO:HG3	2.01	0.43
18:K:2:SER:O	18:K:6:LYS:HG2	2.18	0.43
18:K:76:VAL:O	18:K:80:SER:OG	2.35	0.43
33:a:884:C:H4'	41:i:19:MET:HE1	2.00	0.43
33:a:1008:C:H2'	33:a:1009:U:C6	2.53	0.43
33:a:1333:G:H2'	33:a:1334:A:C8	2.53	0.43
40:h:23:VAL:HG13	40:h:43:LEU:HD21	1.99	0.43
10:A:1817:C:H2'	10:A:1818:A:C5	2.53	0.43
28:V:1:MET:SD	28:V:62:TYR:HB3	2.58	0.43
31:Y:7:ILE:C	31:Y:7:ILE:HD12	2.43	0.43
33:a:797:U:O2'	33:a:799:G:N7	2.49	0.43
48:p:64:ARG:HH12	48:p:88:ARG:HH22	1.66	0.43
50:r:47:LYS:HG3	50:r:72:THR:HG23	2.01	0.43
33:a:744:U:H2'	33:a:745:U:C6	2.53	0.43
33:a:757:A:H2'	33:a:758:C:O4'	2.19	0.43
33:a:1159:C:H2'	33:a:1160:U:C6	2.53	0.43
33:a:1324:C:H41	52:t:3:ARG:HB3	1.84	0.43
36:d:34:GLU:O	36:d:37:LYS:HG2	2.18	0.43
44:l:58:SER:O	44:l:91:PRO:HG2	2.18	0.43
10:A:922:G:H22	10:A:944:G:P	2.41	0.43
10:A:2265:G:N3	10:A:2265:G:H2'	2.34	0.43
12:C:168:LEU:HD13	12:C:187:TYR:CE1	2.54	0.43
14:G:91:ILE:HB	58:G:469:HOH:O	2.19	0.43
18:K:23:HIS:NE2	18:K:34:SER:HB2	2.33	0.43
19:M:76:TYR:HB3	19:M:85:ILE:HD11	2.01	0.43
33:a:381:A:O2'	33:a:459:A:N7	2.51	0.43
33:a:1077:C:O2'	33:a:1078:A:H5'	2.18	0.43
7:7:15:LYS:HD3	10:A:816:G:OP1	2.18	0.43
7:7:32:LEU:HD21	58:7:101:HOH:O	2.18	0.43
10:A:481:C:H2'	10:A:482:U:H5'	2.00	0.43
10:A:577:A:H2'	26:T:28:LYS:HE3	1.99	0.43
10:A:2268:A:H2'	10:A:2269:G:C8	2.54	0.43
17:J:80:ARG:HB3	17:J:83:MET:HG3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:137:U:O2'	33:a:138:A:H5'	2.18	0.43
33:a:237:U:H5''	49:q:34:ILE:HD13	1.99	0.43
33:a:418:G:H2'	33:a:437:U:C4	2.53	0.43
33:a:641:U:O2	33:a:641:U:H2'	2.18	0.43
33:a:736:A:H2'	33:a:737:A:C8	2.54	0.43
33:a:1216:G:H2'	33:a:1217:C:O4'	2.18	0.43
10:A:792:5MU:O2	10:A:2041:A:H1'	2.19	0.43
31:Y:16:SER:O	31:Y:20:GLN:HG2	2.18	0.43
33:a:1479:A:H2'	33:a:1480:A:O4'	2.19	0.43
44:l:18:ASN:HD22	44:l:81:THR:HB	1.83	0.43
50:r:21:LYS:HA	50:r:50:ASP:O	2.19	0.43
2:2:6:ILE:HG23	2:2:53:LEU:HD23	2.00	0.43
6:6:19:THR:OG1	10:A:2313:A:N6	2.45	0.43
10:A:85:G:H21	10:A:102:A:H8	1.60	0.43
10:A:221:G:H22	10:A:238:U:H4'	1.83	0.43
10:A:435:A:C8	10:A:2440:G:H4'	2.53	0.43
10:A:1329:G:H2'	10:A:1330:U:C6	2.54	0.43
10:A:1375:G:N3	10:A:1430:A:H2	2.16	0.43
10:A:2224:U:O2'	10:A:2225:A:H2'	2.19	0.43
10:A:2618:C:H2'	10:A:2619:G:C8	2.54	0.43
11:B:49:G:H2'	11:B:50:A:C8	2.52	0.43
16:I:8:LYS:HB2	16:I:10:ASP:OD1	2.18	0.43
20:N:15:GLY:HA2	20:N:47:THR:HG23	2.00	0.43
33:a:1246:A:H4'	33:a:1314:G:H4'	1.99	0.43
38:f:56:VAL:N	38:f:57:PRO:CD	2.82	0.43
40:h:75:VAL:HB	40:h:86:GLN:HB3	2.01	0.43
40:h:130:ASN:HA	40:h:135:VAL:HG21	2.00	0.43
4:4:78:PHE:HB2	4:4:80:LEU:CD2	2.49	0.43
5:5:22:ILE:O	28:V:23:LEU:HD21	2.19	0.43
10:A:1726:A:H2'	10:A:1727:C:C6	2.54	0.43
10:A:2253:C:H2'	10:A:2254:A:O4'	2.18	0.43
11:B:27:A:H2'	11:B:28:C:O4'	2.19	0.43
17:J:57:LEU:HD23	17:J:65:PRO:HB3	2.01	0.43
20:N:86:ILE:HG22	20:N:94:ARG:HG3	1.99	0.43
21:O:124:LYS:HG2	21:O:144:GLU:HB3	2.01	0.43
29:W:30:ASP:O	29:W:33:VAL:HG22	2.19	0.43
33:a:230:U:H2'	33:a:231:U:C6	2.54	0.43
33:a:527:C:H2'	33:a:528:A:C8	2.54	0.43
43:k:29:ALA:HB2	43:k:87:LEU:HD21	2.01	0.43
10:A:768:A:H2'	10:A:769:U:O4'	2.19	0.43
10:A:2270:U:H2'	10:A:2271:U:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2412:C:H2'	10:A:2413:U:C6	2.52	0.43
12:C:13:ILE:HD11	12:C:47:ILE:HG21	2.01	0.43
12:C:109:PHE:HB2	12:C:114:LEU:HD21	2.00	0.43
23:Q:44:VAL:O	23:Q:48:ILE:HG12	2.19	0.43
32:Z:67:LEU:HD13	32:Z:87:VAL:HG12	2.01	0.43
35:c:68:LEU:HD11	35:c:92:ILE:HG12	2.00	0.43
10:A:350:G:N2	10:A:352:A:H3'	2.34	0.42
10:A:1734:A:H2'	10:A:1735:C:O4'	2.19	0.42
10:A:2206:C:H2'	10:A:2207:U:O4'	2.19	0.42
29:W:7:LEU:HD12	29:W:45:ILE:HD12	2.00	0.42
29:W:60:PRO:HG3	29:W:74:LYS:HB3	2.01	0.42
33:a:413:U:H3'	33:a:414:G:H5'	2.01	0.42
33:a:504:G:H21	33:a:505:A:H3'	1.84	0.42
33:a:1318:U:O2'	33:a:1319:G:H5'	2.18	0.42
39:g:11:ARG:NE	39:g:13:ASN:OD1	2.52	0.42
42:j:28:GLY:N	42:j:64:ASP:OD1	2.52	0.42
51:s:32:GLU:CD	51:s:32:GLU:H	2.27	0.42
4:4:11:GLN:HB3	4:4:24:LEU:HD11	2.01	0.42
10:A:575:G:N3	10:A:575:G:H2'	2.33	0.42
10:A:1959:A:H2'	10:A:1960:G:O4'	2.19	0.42
13:D:44:A:H2'	13:D:45:G:C8	2.54	0.42
33:a:277:U:H2'	33:a:278:A:C8	2.54	0.42
33:a:550:U:O2'	33:a:551:G:H5'	2.19	0.42
40:h:121:ALA:HA	40:h:124:ILE:HG12	2.01	0.42
41:i:32:ILE:HD12	41:i:112:VAL:HG21	2.02	0.42
41:i:41:LYS:HE2	41:i:48:ASN:HA	2.02	0.42
10:A:1280:U:H2'	10:A:1281:U:C6	2.53	0.42
10:A:1288:G:N7	21:O:18:ARG:NH2	2.59	0.42
10:A:1442:C:H2'	10:A:1443:A:C8	2.54	0.42
10:A:1629:U:O2'	10:A:1630:A:H5''	2.19	0.42
10:A:1905:G:H2'	10:A:1906:C:O4'	2.19	0.42
17:J:46:ASN:HB3	17:J:49:VAL:HG23	2.01	0.42
33:a:310:G:N3	33:a:564:C:H4'	2.33	0.42
33:a:469:U:H2'	33:a:470:A:H8	1.83	0.42
33:a:1390:U:O4	40:h:3:ARG:HB2	2.19	0.42
35:c:184:VAL:HG22	35:c:198:TYR:HB2	2.01	0.42
43:k:32:SER:HB3	43:k:83:THR:HG22	2.01	0.42
48:p:18:HIS:CD2	48:p:21:ASP:HB2	2.54	0.42
49:q:41:ASN:ND2	49:q:44:SER:HB3	2.34	0.42
10:A:2348:G:H3'	10:A:2348:G:N3	2.34	0.42
10:A:2758:G:H2'	10:A:2759:G:C8	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:81:PRO:HB3	16:I:89:VAL:HG23	2.02	0.42
19:M:12:ILE:HD13	19:M:12:ILE:HA	1.91	0.42
22:P:118:LEU:HD12	22:P:131:PHE:CD1	2.54	0.42
33:a:1278:G:H2'	33:a:1279:A:C8	2.54	0.42
33:a:1498:G:O2'	33:a:1499:G:H5'	2.19	0.42
35:c:84:ALA:CB	35:c:91:TYR:HB3	2.50	0.42
35:c:99:GLY:HA2	35:c:102:THR:OG1	2.19	0.42
9:9:9:PRO:HB3	9:9:14:CYS:HB2	2.01	0.42
10:A:268:A:N1	10:A:473:U:O2'	2.48	0.42
10:A:365:A:OP2	16:I:169:ASN:HB2	2.19	0.42
11:B:29:C:O2'	11:B:30:U:H5'	2.20	0.42
12:C:138:LYS:O	12:C:139:LYS:HB2	2.20	0.42
14:G:53:HIS:CE1	14:G:219:THR:HG23	2.54	0.42
14:G:247:MET:HB2	58:G:480:HOH:O	2.19	0.42
15:H:21:GLU:HA	20:N:73:ASP:HA	2.02	0.42
33:a:51:A:O2'	33:a:368:G:N2	2.52	0.42
33:a:1179:A:H2'	33:a:1180:A:C8	2.55	0.42
33:a:1285:A:H2'	33:a:1286:G:O4'	2.19	0.42
3:3:45:GLY:HA3	10:A:897:A:H5'	2.02	0.42
4:4:7:PRO:HG3	17:J:58:GLU:HG2	2.02	0.42
10:A:115:C:H2'	10:A:116:G:O4'	2.20	0.42
10:A:1038:C:OP1	26:T:53:ARG:NH2	2.52	0.42
10:A:2767:A:H2'	10:A:2768:A:C8	2.55	0.42
26:T:78:ARG:HD3	26:T:78:ARG:HA	1.77	0.42
33:a:6:U:O2'	33:a:7:G:OP2	2.34	0.42
33:a:221:U:H4'	33:a:222:G:O5'	2.20	0.42
38:f:75:PRO:HG2	38:f:147:LEU:HB3	2.02	0.42
5:5:4:PRO:HA	10:A:2642:U:C2	2.55	0.42
6:6:17:TYR:CE2	6:6:34:LYS:HB3	2.54	0.42
10:A:877:G:N3	21:O:52:GLY:HA3	2.35	0.42
10:A:889:U:H2'	10:A:890:G:O4'	2.19	0.42
10:A:1015:C:H2'	10:A:1016:G:O4'	2.20	0.42
10:A:1824:C:H4'	14:G:257:LYS:O	2.20	0.42
10:A:2777:A:H1'	10:A:2779:C:N4	2.35	0.42
12:C:59:LEU:O	12:C:63:MET:HG2	2.20	0.42
12:C:79:PHE:HA	12:C:82:TYR:CD1	2.51	0.42
15:H:139:GLY:HA3	15:H:147:PHE:HD1	1.85	0.42
33:a:470:A:H2'	33:a:471:A:C8	2.55	0.42
33:a:708:G:H2'	33:a:709:C:C6	2.54	0.42
37:e:139:ILE:N	37:e:139:ILE:HD12	2.35	0.42
9:9:25:VAL:HB	9:9:34:GLN:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1359:A:N7	57:A:3101:PUT:N2	2.68	0.42
31:Y:31:VAL:O	31:Y:38:ASN:HA	2.20	0.42
33:a:88:U:H2'	33:a:89:U:C6	2.55	0.42
33:a:509:C:H1'	33:a:557:C:H1'	2.01	0.42
33:a:722:G:N3	33:a:785:A:H1'	2.35	0.42
33:a:1149:G:C2	33:a:1151:U:C5	3.08	0.42
41:i:108:THR:CG2	41:i:123:VAL:HB	2.49	0.42
46:n:86:TYR:CZ	46:n:90:ARG:HD2	2.55	0.42
10:A:2016:A:H2'	10:A:2017:C:O4'	2.19	0.42
13:D:66:C:H2'	13:D:67:C:C6	2.55	0.42
33:a:100:A:O5'	33:a:100:A:H8	2.03	0.42
33:a:287:A:H5''	33:a:289:G:O4'	2.20	0.42
33:a:343:C:H2'	33:a:344:A:C8	2.55	0.42
33:a:417:U:H2'	33:a:418:G:O4'	2.20	0.42
33:a:495:A:H2'	33:a:496:C:O4'	2.19	0.42
33:a:525:G:H4'	33:a:527:C:C2	2.55	0.42
33:a:612:G:H2'	33:a:613:U:O4'	2.20	0.42
36:d:137:ILE:O	36:d:141:MET:HG2	2.20	0.42
40:h:54:SER:HB2	40:h:125:LEU:HD11	2.01	0.42
1:l:52:ARG:NH1	10:A:445:G:N7	2.56	0.42
10:A:448:A:H2'	10:A:449:U:O4'	2.20	0.42
10:A:672:A:N1	10:A:681:G:O2'	2.52	0.42
10:A:1325:U:O2'	10:A:1691:G:N2	2.53	0.42
10:A:1382:C:H2'	10:A:1383:G:C8	2.54	0.42
19:M:38:ARG:HD2	19:M:111:PRO:CD	2.50	0.42
23:Q:8:ARG:HD2	58:Q:226:HOH:O	2.19	0.42
33:a:17:A:N1	33:a:928:A:H2	2.17	0.42
33:a:206:A:H2'	33:a:207:G:C8	2.54	0.42
33:a:1297:A:H8	33:a:1297:A:H5''	1.84	0.42
34:b:12:A:N3	34:b:12:A:H2'	2.35	0.42
35:c:6:MET:HE3	35:c:43:LEU:HB2	2.01	0.42
41:i:7:ILE:HD11	41:i:32:ILE:HG12	2.02	0.42
10:A:1149:U:H2'	10:A:1150:A:C8	2.54	0.41
10:A:1696:C:H2'	10:A:1697:G:O4'	2.20	0.41
10:A:1979:A:C2	20:N:22:ILE:HG23	2.55	0.41
13:F:23:C:H2'	13:F:24:U:C6	2.55	0.41
17:J:138:PHE:HZ	17:J:154:ILE:HD11	1.85	0.41
19:M:46:THR:HB	19:M:49:VAL:HG22	2.02	0.41
33:a:477:U:H2'	33:a:478:G:O4'	2.19	0.41
36:d:91:ASN:HD21	36:d:97:LYS:HA	1.85	0.41
40:h:50:VAL:HG23	40:h:125:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:l:87:LYS:HG3	44:l:114:THR:HA	2.01	0.41
49:q:50:ILE:HG21	49:q:74:ILE:HG23	2.01	0.41
50:r:65:GLU:HG3	50:r:75:PHE:CE2	2.55	0.41
10:A:168:A:H3'	10:A:169:G:H8	1.84	0.41
10:A:1175:G:O2'	10:A:2053:U:H5'	2.20	0.41
10:A:2403:A:H2'	10:A:2404:A:O4'	2.20	0.41
33:a:505:A:H2'	33:a:505:A:N3	2.36	0.41
33:a:1235:A:H2'	33:a:1236:C:C5	2.55	0.41
40:h:53:ARG:NH1	40:h:122:ASN:OD1	2.54	0.41
49:q:22:VAL:HG21	49:q:60:TRP:CG	2.54	0.41
10:A:283:G:H3'	10:A:284:C:C5'	2.50	0.41
15:H:205:LYS:O	15:H:206:LYS:HB2	2.21	0.41
19:M:17:TYR:HA	19:M:139:GLU:O	2.21	0.41
20:N:47:THR:HA	20:N:48:PRO:HD3	1.95	0.41
33:a:435:C:OP1	37:e:13:ARG:NH2	2.53	0.41
33:a:918:A:H2'	33:a:919:C:O4'	2.20	0.41
33:a:1168:C:C5	33:a:1170:G:H1'	2.55	0.41
10:A:178:A:H2'	10:A:179:A:C8	2.56	0.41
10:A:1247:G:O2'	10:A:1275:A:N1	2.46	0.41
10:A:2349:A:H2'	10:A:2350:G:O4'	2.20	0.41
12:C:65:ILE:HG13	12:C:66:ARG:HG3	2.03	0.41
24:R:43:GLN:HG2	24:R:55:GLN:HG2	2.02	0.41
33:a:1023:A:C2	33:a:1229:U:H1'	2.55	0.41
35:c:159:GLN:O	35:c:182:PRO:HD2	2.20	0.41
10:A:777:C:H2'	10:A:778:G:O4'	2.21	0.41
33:a:692:U:H2'	33:a:693:G:O4'	2.21	0.41
33:a:1277:C:O2	33:a:1337:A:H4'	2.20	0.41
43:k:32:SER:HB2	43:k:83:THR:HG22	2.01	0.41
4:4:55:HIS:HB3	4:4:58:TYR:HD1	1.85	0.41
10:A:1045:A:H2'	10:A:1046:G:O4'	2.19	0.41
10:A:1829:A:N1	10:A:1849:G:H1'	2.36	0.41
10:A:1853:C:H5'	14:G:241:ILE:HD11	2.03	0.41
10:A:2779:C:H2'	10:A:2780:A:O4'	2.21	0.41
17:J:59:LEU:HB3	17:J:140:GLU:CG	2.50	0.41
23:Q:101:THR:HG22	23:Q:121:LEU:HD23	2.02	0.41
33:a:352:A:H4'	33:a:353:C:OP2	2.20	0.41
33:a:407:G:H2'	33:a:408:C:C6	2.55	0.41
33:a:456:A:H2'	33:a:457:A:O4'	2.20	0.41
36:d:3:GLN:HB3	36:d:4:LYS:HE3	2.02	0.41
36:d:50:SER:HB3	36:d:114:LEU:HD22	2.01	0.41
45:m:72:ASN:O	45:m:73:ASN:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:r:60:ILE:HG22	50:r:81:VAL:HB	2.02	0.41
8:8:10:ALA:O	8:8:14:VAL:HG22	2.20	0.41
10:A:275:A:H61	10:A:297:G:H1'	1.86	0.41
10:A:1617:A:H2'	10:A:1618:A:C8	2.56	0.41
10:A:1916:A:N1	10:A:2261:G:H1'	2.35	0.41
10:A:2293:A:H4'	10:A:2294:A:O5'	2.21	0.41
33:a:271:A:H2'	33:a:272:C:C6	2.56	0.41
33:a:511:A:O2'	33:a:512:C:H5'	2.20	0.41
33:a:869:A:H2'	33:a:870:G:O4'	2.20	0.41
36:d:133:GLN:OE1	36:d:152:VAL:HG12	2.21	0.41
36:d:183:TYR:HA	36:d:199:VAL:O	2.21	0.41
46:n:53:LEU:HD13	46:n:53:LEU:HA	1.93	0.41
54:v:39:GLU:HG3	54:v:44:LYS:CG	2.43	0.41
4:4:2:LYS:HD2	4:4:5:ILE:HD13	2.02	0.41
10:A:637:U:H2'	10:A:638:U:C6	2.56	0.41
10:A:651:A:H2'	10:A:652:A:C8	2.56	0.41
10:A:2347:A:H2'	10:A:2347:A:N3	2.36	0.41
10:A:2581:U:H2'	10:A:2582:U:C6	2.56	0.41
12:C:62:LEU:HG	12:C:75:ILE:HD13	2.02	0.41
19:M:142:GLU:O	19:M:144:ARG:NH1	2.53	0.41
33:a:985:G:H5'	33:a:1368:U:O2'	2.21	0.41
33:a:1036:C:O2	33:a:1036:C:H2'	2.21	0.41
33:a:1081:U:H2'	33:a:1082:C:C6	2.56	0.41
35:c:126:PHE:CZ	35:c:134:VAL:HB	2.55	0.41
38:f:61:LYS:HB2	38:f:61:LYS:HE3	1.90	0.41
50:r:13:LYS:HE3	50:r:58:GLY:HA2	2.03	0.41
52:t:15:LEU:O	52:t:19:VAL:HG23	2.20	0.41
4:4:16:ASP:O	4:4:20:ASN:N	2.53	0.41
10:A:464:U:H2'	10:A:465:C:C6	2.56	0.41
10:A:1572:G:C6	10:A:1591:G:C6	3.08	0.41
10:A:1764:A:H2'	10:A:1765:A:C8	2.55	0.41
10:A:2050:A:H5'	10:A:2644:C:H4'	2.03	0.41
10:A:2260:A:H2'	10:A:2261:G:C8	2.56	0.41
13:F:61:C:H2'	13:F:62:C:C6	2.56	0.41
18:K:28:GLY:HA3	18:K:79:VAL:HB	2.03	0.41
20:N:104:ARG:HG3	20:N:122:LEU:C	2.46	0.41
24:R:49:LYS:HB2	24:R:51:VAL:HG22	2.03	0.41
31:Y:7:ILE:HD13	31:Y:41:VAL:CG1	2.51	0.41
33:a:86:G:H1'	33:a:87:C:N1	2.36	0.41
33:a:188:U:H2'	33:a:189:G:H8	1.86	0.41
33:a:588:C:H2'	33:a:589:G:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:786:U:H2'	33:a:787:C:O4'	2.21	0.41
33:a:1391:U:H2'	33:a:1392:C:C5'	2.51	0.41
34:b:21:A:H2'	34:b:22:A:C8	2.55	0.41
37:e:13:ARG:HD2	37:e:29:ARG:O	2.21	0.41
40:h:27:ILE:HG13	40:h:43:LEU:HD23	2.01	0.41
43:k:42:LEU:HB2	43:k:71:LYS:HB2	2.03	0.41
7:7:40:ARG:NH2	10:A:514:G:N7	2.54	0.41
10:A:679:G:H2'	10:A:680:C:C6	2.56	0.41
10:A:1450:A:N1	10:A:1633:A:H8	2.19	0.41
10:A:2088:G:H5''	10:A:2530:2MA:C2	2.51	0.41
10:A:2488:C:H2'	10:A:2489:U:C6	2.56	0.41
10:A:2688:G:H2'	10:A:2689:A:C8	2.56	0.41
10:A:2829:A:H2'	10:A:2830:A:C8	2.56	0.41
16:I:148:GLN:HB3	16:I:152:VAL:HG21	2.03	0.41
17:J:16:LEU:HD13	17:J:29:PRO:HD2	2.02	0.41
17:J:177:PHE:O	17:J:179:LYS:HD3	2.21	0.41
18:K:12:PRO:HD2	18:K:15:VAL:HB	2.02	0.41
19:M:60:ALA:HB1	19:M:102:ILE:HG13	2.03	0.41
33:a:6:U:H4'	33:a:7:G:O5'	2.21	0.41
33:a:1082:C:H2'	33:a:1083:G:C8	2.56	0.41
40:h:50:VAL:HB	40:h:124:ILE:HD11	2.03	0.41
42:j:117:LYS:HB2	42:j:120:LEU:HD12	2.03	0.41
4:4:5:ILE:HD12	17:J:64:LYS:HE2	2.02	0.40
10:A:659:A:H2'	10:A:660:A:C8	2.56	0.40
10:A:786:U:H2'	10:A:787:U:O4'	2.21	0.40
10:A:1476:G:H2'	10:A:1477:U:C6	2.55	0.40
10:A:1538:A:H2'	10:A:1539:A:C8	2.56	0.40
10:A:1582:U:O2'	10:A:1583:G:O4'	2.36	0.40
10:A:1730:C:H2'	10:A:1731:G:O4'	2.21	0.40
10:A:1897:U:H2'	10:A:1898:C:C6	2.56	0.40
10:A:2871:A:H2'	10:A:2872:G:O4'	2.20	0.40
12:C:78:LYS:HG2	12:C:82:TYR:HE1	1.86	0.40
13:D:50:U:H3	13:D:64:G:H1	1.69	0.40
22:P:65:TRP:HB2	22:P:105:GLU:HB2	2.03	0.40
33:a:212:A:H4'	33:a:213:G:OP1	2.20	0.40
33:a:489:G:O2'	33:a:491:C:N4	2.50	0.40
33:a:954:G:H2'	33:a:954:G:N3	2.36	0.40
33:a:1015:A:H2'	33:a:1016:A:N7	2.36	0.40
33:a:1082:C:H2'	33:a:1083:G:H8	1.86	0.40
33:a:1260:A:H2'	33:a:1261:A:O4'	2.21	0.40
33:a:1489:A:H2'	33:a:1490:A:C8	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:114:ILE:HG12	35:c:144:LEU:HB3	2.02	0.40
10:A:1510:U:HO2'	10:A:1511:C:P	2.45	0.40
10:A:1548:U:H2'	10:A:1549:C:C6	2.56	0.40
10:A:2692:A:H2'	10:A:2693:C:O4'	2.21	0.40
13:F:19:G:H1	17:J:80:ARG:HH22	1.69	0.40
14:G:218:PRO:HB2	58:G:485:HOH:O	2.21	0.40
30:X:74:LYS:HG3	30:X:99:GLU:HG3	2.04	0.40
33:a:86:G:H1'	33:a:87:C:C6	2.56	0.40
33:a:1091:A:H5''	38:f:21:VAL:HG11	2.02	0.40
33:a:1191:G:O2'	33:a:1192:G:C8	2.67	0.40
33:a:1325:U:H2'	33:a:1326:G:O4'	2.21	0.40
35:c:66:GLN:HB3	35:c:90:PHE:CE2	2.56	0.40
38:f:47:GLY:HA3	38:f:71:LEU:HD23	2.03	0.40
41:i:108:THR:HG23	41:i:124:GLY:O	2.21	0.40
43:k:92:LEU:HB3	43:k:96:VAL:HG11	2.03	0.40
7:7:25:THR:CG2	7:7:28:GLY:H	2.34	0.40
10:A:751:A:H2'	10:A:752:G:O4'	2.22	0.40
10:A:1127:U:O3'	10:A:1128:A:H3'	2.21	0.40
10:A:1764:A:H2'	10:A:1765:A:O4'	2.21	0.40
12:C:3:THR:HB	12:C:48:PHE:HD1	1.85	0.40
33:a:476:C:H2'	33:a:477:U:C6	2.56	0.40
33:a:794:G:H2'	33:a:795:A:O4'	2.21	0.40
33:a:1423:A:H2	33:a:1498:G:H22	1.69	0.40
37:e:17:ILE:HG13	37:e:56:LYS:HE3	2.04	0.40
38:f:40:GLY:HA3	38:f:117:LEU:HB3	2.02	0.40
43:k:59:LYS:O	43:k:62:ARG:NE	2.51	0.40
46:n:86:TYR:CE2	46:n:90:ARG:HD2	2.56	0.40
5:5:2:ALA:HB3	10:A:2083:G:N2	2.37	0.40
10:A:801:A:H2'	10:A:802:G:O4'	2.21	0.40
10:A:2048:G:N3	10:A:2048:G:H2'	2.36	0.40
10:A:2393:A:H2'	10:A:2394:G:O4'	2.22	0.40
13:D:14:A:H2'	13:D:15:G:C8	2.57	0.40
19:M:78:HIS:HA	19:M:84:GLY:O	2.22	0.40
22:P:58:MET:HE2	22:P:62:GLY:HA3	2.04	0.40
26:T:85:LYS:HD2	26:T:117:LEU:HD23	2.03	0.40
28:V:21:LEU:HD22	28:V:74:ALA:HB1	2.04	0.40
33:a:75:A:H2'	33:a:75:A:N3	2.36	0.40
33:a:1515:G:H4'	33:a:1516:G:C4	2.56	0.40
52:t:14:HIS:O	52:t:18:LYS:NZ	2.54	0.40
10:A:1758:A:H61	10:A:1771:A:H2	1.69	0.40
23:Q:121:LEU:O	23:Q:122:VAL:CB	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:788:A:H5''	44:l:125:LYS:HD3	2.03	0.40
33:a:1390:U:C4	40:h:3:ARG:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1	59/62 (95%)	59 (100%)	0	0	100	100
2	2	63/69 (91%)	63 (100%)	0	0	100	100
3	3	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
4	4	78/84 (93%)	78 (100%)	0	0	100	100
5	5	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
6	6	46/49 (94%)	46 (100%)	0	0	100	100
7	7	41/45 (91%)	41 (100%)	0	0	100	100
8	8	62/66 (94%)	62 (100%)	0	0	100	100
9	9	35/37 (95%)	35 (100%)	0	0	100	100
12	C	200/213 (94%)	199 (100%)	1 (0%)	0	100	100
14	G	271/277 (98%)	266 (98%)	5 (2%)	0	100	100
15	H	214/220 (97%)	205 (96%)	9 (4%)	0	100	100
16	I	202/207 (98%)	202 (100%)	0	0	100	100
17	J	176/179 (98%)	174 (99%)	2 (1%)	0	100	100
18	K	172/178 (97%)	171 (99%)	1 (1%)	0	100	100
19	M	142/145 (98%)	140 (99%)	2 (1%)	0	100	100
20	N	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
21	O	143/146 (98%)	138 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	P	134/144 (93%)	134 (100%)	0	0	100	100
23	Q	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
24	R	117/119 (98%)	117 (100%)	0	0	100	100
25	S	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
26	T	114/118 (97%)	114 (100%)	0	0	100	100
27	U	99/102 (97%)	99 (100%)	0	0	100	100
28	V	109/117 (93%)	109 (100%)	0	0	100	100
29	W	87/91 (96%)	87 (100%)	0	0	100	100
30	X	100/105 (95%)	100 (100%)	0	0	100	100
31	Y	92/217 (42%)	92 (100%)	0	0	100	100
32	Z	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
35	c	219/255 (86%)	217 (99%)	2 (1%)	0	100	100
36	d	202/217 (93%)	197 (98%)	5 (2%)	0	100	100
37	e	197/200 (98%)	193 (98%)	4 (2%)	0	100	100
38	f	154/166 (93%)	152 (99%)	2 (1%)	0	100	100
39	g	91/98 (93%)	91 (100%)	0	0	100	100
40	h	142/156 (91%)	141 (99%)	0	1 (1%)	18	18
41	i	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
42	j	126/132 (96%)	124 (98%)	2 (2%)	0	100	100
43	k	97/102 (95%)	94 (97%)	3 (3%)	0	100	100
44	l	116/129 (90%)	113 (97%)	3 (3%)	0	100	100
45	m	133/137 (97%)	130 (98%)	3 (2%)	0	100	100
46	n	111/121 (92%)	109 (98%)	2 (2%)	0	100	100
47	o	58/61 (95%)	58 (100%)	0	0	100	100
48	p	84/89 (94%)	83 (99%)	1 (1%)	0	100	100
49	q	88/91 (97%)	87 (99%)	1 (1%)	0	100	100
50	r	78/87 (90%)	78 (100%)	0	0	100	100
51	s	61/80 (76%)	61 (100%)	0	0	100	100
52	t	78/92 (85%)	77 (99%)	1 (1%)	0	100	100
53	u	78/83 (94%)	78 (100%)	0	0	100	100
54	v	51/58 (88%)	51 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5584/6046 (92%)	5510 (99%)	73 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	h	71	PRO

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	1	51/52 (98%)	51 (100%)	0	100	100
2	2	59/62 (95%)	59 (100%)	0	100	100
3	3	51/53 (96%)	50 (98%)	1 (2%)	48	63
4	4	71/75 (95%)	67 (94%)	4 (6%)	19	22
5	5	48/50 (96%)	48 (100%)	0	100	100
6	6	46/47 (98%)	46 (100%)	0	100	100
7	7	39/40 (98%)	39 (100%)	0	100	100
8	8	55/57 (96%)	54 (98%)	1 (2%)	51	66
9	9	35/35 (100%)	35 (100%)	0	100	100
12	C	196/204 (96%)	192 (98%)	4 (2%)	48	63
14	G	220/224 (98%)	220 (100%)	0	100	100
15	H	174/177 (98%)	174 (100%)	0	100	100
16	I	168/169 (99%)	166 (99%)	2 (1%)	63	76
17	J	157/158 (99%)	150 (96%)	7 (4%)	24	31
18	K	152/155 (98%)	146 (96%)	6 (4%)	28	37
19	M	123/123 (100%)	123 (100%)	0	100	100
20	N	100/100 (100%)	99 (99%)	1 (1%)	68	80
21	O	111/112 (99%)	111 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	P	113/119 (95%)	113 (100%)	0	100	100
23	Q	101/102 (99%)	101 (100%)	0	100	100
24	R	95/95 (100%)	95 (100%)	0	100	100
25	S	100/102 (98%)	99 (99%)	1 (1%)	68	80
26	T	96/98 (98%)	96 (100%)	0	100	100
27	U	86/86 (100%)	85 (99%)	1 (1%)	63	76
28	V	90/94 (96%)	89 (99%)	1 (1%)	65	78
29	W	80/82 (98%)	80 (100%)	0	100	100
30	X	87/90 (97%)	85 (98%)	2 (2%)	44	58
31	Y	83/190 (44%)	83 (100%)	0	100	100
32	Z	64/75 (85%)	64 (100%)	0	100	100
35	c	192/221 (87%)	190 (99%)	2 (1%)	68	80
36	d	166/175 (95%)	160 (96%)	6 (4%)	31	40
37	e	174/175 (99%)	173 (99%)	1 (1%)	78	88
38	f	122/131 (93%)	120 (98%)	2 (2%)	55	70
39	g	81/86 (94%)	76 (94%)	5 (6%)	16	18
40	h	124/132 (94%)	118 (95%)	6 (5%)	23	28
41	i	112/113 (99%)	108 (96%)	4 (4%)	31	40
42	j	106/109 (97%)	105 (99%)	1 (1%)	70	82
43	k	89/91 (98%)	88 (99%)	1 (1%)	65	78
44	l	94/104 (90%)	88 (94%)	6 (6%)	16	18
45	m	117/119 (98%)	116 (99%)	1 (1%)	70	82
46	n	98/104 (94%)	97 (99%)	1 (1%)	68	80
47	o	52/53 (98%)	52 (100%)	0	100	100
48	p	79/81 (98%)	78 (99%)	1 (1%)	61	75
49	q	76/77 (99%)	74 (97%)	2 (3%)	40	53
50	r	75/82 (92%)	74 (99%)	1 (1%)	61	75
51	s	56/68 (82%)	51 (91%)	5 (9%)	9	9
52	t	70/80 (88%)	67 (96%)	3 (4%)	26	33
53	u	67/69 (97%)	66 (98%)	1 (2%)	57	71
54	v	49/54 (91%)	45 (92%)	4 (8%)	10	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4850/5150 (94%)	4766 (98%)	84 (2%)	52 68

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	9	THR
4	4	45	VAL
4	4	49	ASP
4	4	71	VAL
4	4	76	LYS
8	8	55	MET
12	C	33	VAL
12	C	54	ASP
12	C	99	LYS
12	C	104	ILE
16	I	49	HIS
16	I	58	SER
17	J	42	ASP
17	J	80	ARG
17	J	89	VAL
17	J	101	ASP
17	J	117	VAL
17	J	132	VAL
17	J	135	GLN
18	K	16	THR
18	K	43	PHE
18	K	73	ASN
18	K	80	SER
18	K	107	VAL
18	K	136	ILE
20	N	47	THR
25	S	2	THR
27	U	86	LYS
28	V	11	ARG
30	X	24	ILE
30	X	56	ILE
35	c	27	MET
35	c	80	VAL
36	d	40	LYS
36	d	75	VAL
36	d	86	LEU
36	d	90	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	d	102	VAL
36	d	161	ILE
37	e	64	THR
38	f	39	VAL
38	f	156	LEU
39	g	36	GLU
39	g	43	TRP
39	g	65	VAL
39	g	84	ASP
39	g	88	ARG
40	h	59	LEU
40	h	61	VAL
40	h	117	GLU
40	h	125	LEU
40	h	130	ASN
40	h	135	VAL
41	i	25	LEU
41	i	77	LEU
41	i	98	LEU
41	i	101	LEU
42	j	50	LEU
43	k	102	LEU
44	l	67	SER
44	l	82	VAL
44	l	85	THR
44	l	89	PRO
44	l	119	ASN
44	l	129	VAL
45	m	58	PRO
46	n	53	LEU
48	p	12	ILE
49	q	27	SER
49	q	87	GLN
50	r	44	LYS
51	s	14	LYS
51	s	23	ILE
51	s	29	LYS
51	s	32	GLU
51	s	40	GLU
52	t	18	LYS
52	t	35	SER
52	t	63	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	u	28	MET
54	v	12	LEU
54	v	17	ARG
54	v	28	THR
54	v	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	17	GLN
3	3	48	ASN
12	C	11	ASN
12	C	204	GLN
14	G	163	GLN
15	H	14	GLN
15	H	136	GLN
15	H	167	GLN
15	H	181	GLN
16	I	119	GLN
16	I	179	GLN
16	I	188	ASN
17	J	52	ASN
17	J	161	ASN
18	K	99	GLN
19	M	81	HIS
22	P	13	HIS
22	P	35	GLN
23	Q	61	ASN
23	Q	73	ASN
23	Q	79	GLN
24	R	55	GLN
29	W	69	GLN
30	X	39	ASN
31	Y	38	ASN
31	Y	84	ASN
31	Y	85	GLN
35	c	55	ASN
35	c	94	GLN
36	d	91	ASN
37	e	40	GLN
37	e	137	GLN
38	f	145	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	f	146	ASN
39	g	69	ASN
40	h	18	HIS
40	h	67	ASN
40	h	130	ASN
41	i	18	ASN
42	j	70	HIS
43	k	78	ASN
44	l	15	ASN
44	l	18	ASN
44	l	64	GLN
46	n	76	ASN
46	n	104	ASN
49	q	41	ASN
49	q	73	ASN
49	q	87	GLN
50	r	64	GLN
51	s	25	HIS
52	t	43	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2845/2923 (97%)	345 (12%)	47 (1%)
11	B	112/115 (97%)	13 (11%)	5 (4%)
13	D	76/77 (98%)	19 (25%)	2 (2%)
13	F	75/77 (97%)	12 (16%)	2 (2%)
33	a	1523/1555 (97%)	194 (12%)	0
34	b	13/24 (54%)	6 (46%)	0
All	All	4644/4771 (97%)	589 (12%)	56 (1%)

All (589) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	12	U
10	A	64	A
10	A	71	A
10	A	75	G
10	A	90	A
10	A	91	A
10	A	117	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	118	A
10	A	119	U
10	A	130	A
10	A	156	A
10	A	166	A
10	A	167	U
10	A	168	A
10	A	177	G
10	A	199	A
10	A	202	A
10	A	203	U
10	A	218	G
10	A	219	A
10	A	224	A
10	A	225	A
10	A	251	G
10	A	255	G
10	A	269	G
10	A	270	C
10	A	284	C
10	A	285	U
10	A	286	U
10	A	287	G
10	A	288	C
10	A	289	U
10	A	298	U
10	A	299	U
10	A	300	G
10	A	314	A
10	A	315	C
10	A	321	U
10	A	324	A
10	A	327	G
10	A	354	A
10	A	373	A
10	A	381	G
10	A	404	U
10	A	406	A
10	A	410	G
10	A	411	A
10	A	432	G
10	A	449	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	450	C
10	A	457	G
10	A	481	C
10	A	494	U
10	A	497	U
10	A	502	C
10	A	527	G
10	A	550	A
10	A	553	A
10	A	558	A
10	A	567	G
10	A	575	G
10	A	576	U
10	A	577	A
10	A	578	G
10	A	583	A
10	A	590	U
10	A	592	A
10	A	593	U
10	A	594	G
10	A	598	G
10	A	599	A
10	A	606	G
10	A	616	G
10	A	618	A
10	A	630	G
10	A	646	A
10	A	650	U
10	A	682	A
10	A	683	G
10	A	690	U
10	A	700	A
10	A	731	U
10	A	762	C
10	A	774	G
10	A	775	A
10	A	792	5MU
10	A	809	A
10	A	810	A
10	A	820	G
10	A	827	A
10	A	829	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	837	G
10	A	850	G
10	A	857	C
10	A	872	U
10	A	873	U
10	A	903	G
10	A	904	G
10	A	920	A
10	A	923	A
10	A	924	G
10	A	925	G
10	A	927	G
10	A	930	C
10	A	937	G
10	A	941	A
10	A	943	C
10	A	944	G
10	A	945	A
10	A	955	A
10	A	970	U
10	A	972	A
10	A	985	A
10	A	988	C
10	A	989	A
10	A	990	G
10	A	1005	G
10	A	1018	A
10	A	1027	A
10	A	1032	A
10	A	1040	A
10	A	1056	U
10	A	1057	A
10	A	1066	G
10	A	1070	A
10	A	1077	U
10	A	1090	A
10	A	1091	G
10	A	1114	A
10	A	1115	G
10	A	1124	A
10	A	1126	U
10	A	1129	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1131	G
10	A	1132	A
10	A	1141	U
10	A	1155	A
10	A	1156	G
10	A	1176	U
10	A	1177	A
10	A	1178	C
10	A	1179	C
10	A	1186	A
10	A	1187	A
10	A	1199	A
10	A	1218	G
10	A	1222	A
10	A	1276	G
10	A	1291	A
10	A	1292	A
10	A	1294	G
10	A	1309	G
10	A	1310	A
10	A	1337	A
10	A	1358	A
10	A	1382	C
10	A	1402	A
10	A	1405	G
10	A	1415	A
10	A	1416	U
10	A	1421	A
10	A	1449	A
10	A	1455	U
10	A	1457	U
10	A	1458	A
10	A	1459	A
10	A	1463	A
10	A	1464	U
10	A	1471	A
10	A	1472	C
10	A	1490	G
10	A	1496	G
10	A	1497	A
10	A	1510	U
10	A	1511	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1526	G
10	A	1533	A
10	A	1536	C
10	A	1537	A
10	A	1553	A
10	A	1560	A
10	A	1569	G
10	A	1578	A
10	A	1580	A
10	A	1581	U
10	A	1582	U
10	A	1583	G
10	A	1585	G
10	A	1606	C
10	A	1613	G
10	A	1616	A
10	A	1625	U
10	A	1630	A
10	A	1631	G
10	A	1633	A
10	A	1634	A
10	A	1642	C
10	A	1651	C
10	A	1652	A
10	A	1658	A
10	A	1690	A
10	A	1691	G
10	A	1692	C
10	A	1718	G
10	A	1740	G
10	A	1747	G
10	A	1758	A
10	A	1759	G
10	A	1772	G
10	A	1783	G
10	A	1789	A
10	A	1790	G
10	A	1791	G
10	A	1795	A
10	A	1800	A
10	A	1809	C
10	A	1818	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1827	C
10	A	1829	A
10	A	1843	U
10	A	1874	A
10	A	1875	A
10	A	1899	U
10	A	1900	G
10	A	1909	C
10	A	1933	G
10	A	1940	A
10	A	1941	C
10	A	1956	G
10	A	1957	G
10	A	1958	U
10	A	1963	A
10	A	1965	A
10	A	1982	U
10	A	1994	C
10	A	1997	A
10	A	1998	A
10	A	1999	G
10	A	2018	U
10	A	2020	U
10	A	2040	A
10	A	2045	A
10	A	2047	A
10	A	2050	A
10	A	2058	A
10	A	2059	G
10	A	2060	A
10	A	2070	C
10	A	2076	A
10	A	2082	C
10	A	2083	G
10	A	2087	A
10	A	2088	G
10	A	2089	A
10	A	2096	G
10	A	2120	G
10	A	2136	U
10	A	2137	G
10	A	2205	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	2208	A
10	A	2209	G
10	A	2215	U
10	A	2217	G
10	A	2225	A
10	A	2230	G
10	A	2238	U
10	A	2239	A
10	A	2252	A
10	A	2265	G
10	A	2266	G
10	A	2295	A
10	A	2305	A
10	A	2306	G
10	A	2310	C
10	A	2314	A
10	A	2316	G
10	A	2333	U
10	A	2334	G
10	A	2335	G
10	A	2339	U
10	A	2347	A
10	A	2348	G
10	A	2349	A
10	A	2361	U
10	A	2362	A
10	A	2374	C
10	A	2377	C
10	A	2410	G
10	A	2412	C
10	A	2429	U
10	A	2430	C
10	A	2433	C
10	A	2452	A
10	A	2456	G
10	A	2457	A
10	A	2462	A
10	A	2468	C
10	A	2474	G
10	A	2475	A
10	A	2476	H2U
10	A	2496	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	2502	C
10	A	2505	A
10	A	2529	G
10	A	2532	G
10	A	2545	A
10	A	2556	G
10	A	2557	U
10	A	2561	C
10	A	2581	U
10	A	2593	A
10	A	2594	G
10	A	2600	C
10	A	2605	G
10	A	2629	A
10	A	2637	C
10	A	2640	U
10	A	2657	G
10	A	2666	A
10	A	2690	G
10	A	2692	A
10	A	2716	U
10	A	2718	C
10	A	2741	G
10	A	2753	U
10	A	2760	A
10	A	2769	G
10	A	2771	G
10	A	2775	A
10	A	2784	A
10	A	2791	A
10	A	2792	A
10	A	2793	G
10	A	2805	A
10	A	2807	G
10	A	2824	G
10	A	2825	U
10	A	2827	A
10	A	2828	U
10	A	2852	U
10	A	2887	G
10	A	2888	A
10	A	2892	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	2903	A
10	A	2913	G
11	B	10	U
11	B	11	A
11	B	23	U
11	B	32	U
11	B	33	U
11	B	43	A
11	B	51	A
11	B	54	U
11	B	55	A
11	B	64	A
11	B	87	C
11	B	88	G
11	B	106	G
13	D	2	G
13	D	7	G
13	D	9	G
13	D	16	C
13	D	17	C
13	D	17(A)	U
13	D	18	G
13	D	19	G
13	D	21	A
13	D	22	G
13	D	27	U
13	D	28	C
13	D	30	G
13	D	34	C
13	D	48	C
13	D	59	A
13	D	63	G
13	D	74	C
13	D	76	A
13	F	7	G
13	F	8	U
13	F	9	G
13	F	17(A)	U
13	F	18	G
13	F	19	G
13	F	21	A
13	F	47	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	F	48	C
13	F	52	G
13	F	58	A
13	F	76	A
33	a	6	U
33	a	7	G
33	a	8	G
33	a	9	A
33	a	10	G
33	a	33	A
33	a	40	G
33	a	48	C
33	a	49	C
33	a	52	A
33	a	74	G
33	a	75	A
33	a	81	A
33	a	82	G
33	a	83	C
33	a	84	U
33	a	85	U
33	a	89	U
33	a	91	U
33	a	94	G
33	a	97	G
33	a	120	C
33	a	131	C
33	a	163	C
33	a	173	U
33	a	183	U
33	a	190	A
33	a	212	A
33	a	213	G
33	a	220	U
33	a	221	U
33	a	222	G
33	a	248	U
33	a	249	G
33	a	255	G
33	a	258	A
33	a	259	G
33	a	274	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	a	275	C
33	a	278	A
33	a	297	G
33	a	313	G
33	a	314	A
33	a	329	A
33	a	336	C
33	a	337	A
33	a	340	G
33	a	355	G
33	a	360	C
33	a	362	G
33	a	375	U
33	a	380	C
33	a	405	A
33	a	414	G
33	a	419	A
33	a	420	U
33	a	421	G
33	a	429	U
33	a	432	G
33	a	437	U
33	a	447	U
33	a	456	A
33	a	461	C
33	a	492	G
33	a	493	G
33	a	505	A
33	a	513	G
33	a	519	C
33	a	526	C
33	a	529	G
33	a	534	C
33	a	535	G7M
33	a	540	A
33	a	541	A
33	a	544	C
33	a	555	A
33	a	567	A
33	a	580	A
33	a	581	A
33	a	584	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	a	626	C
33	a	649	A
33	a	650	A
33	a	661	U
33	a	662	G
33	a	673	A
33	a	695	A
33	a	696	G
33	a	710	A
33	a	711	G
33	a	731	U
33	a	732	G
33	a	757	A
33	a	763	G
33	a	785	A
33	a	801	U
33	a	802	A
33	a	823	A
33	a	825	C
33	a	836	A
33	a	881	A
33	a	883	G
33	a	893	U
33	a	894	G
33	a	923	A
33	a	924	A
33	a	936	G
33	a	940	C
33	a	943	C
33	a	969	U
33	a	978	A
33	a	980	G
33	a	981	C
33	a	984	A
33	a	985	G
33	a	986	A
33	a	992	A
33	a	1000	U
33	a	1001	U
33	a	1002	G
33	a	1013	A
33	a	1014	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	a	1015	A
33	a	1016	A
33	a	1018	U
33	a	1019	C
33	a	1022	G
33	a	1030	G
33	a	1031	C
33	a	1035	C
33	a	1036	C
33	a	1046	G
33	a	1047	A
33	a	1048	C
33	a	1056	C
33	a	1066	A
33	a	1076	U
33	a	1081	U
33	a	1096	U
33	a	1105	G
33	a	1106	U
33	a	1111	C
33	a	1112	A
33	a	1135	G
33	a	1136	U
33	a	1141	A
33	a	1149	G
33	a	1151	U
33	a	1152	G
33	a	1155	C
33	a	1156	A
33	a	1169	U
33	a	1170	G
33	a	1174	G
33	a	1175	U
33	a	1177	A
33	a	1178	C
33	a	1194	G
33	a	1206	A
33	a	1207	A
33	a	1221	U
33	a	1222	U
33	a	1223	A
33	a	1235	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	a	1236	C
33	a	1237	A
33	a	1267	A
33	a	1270	G
33	a	1289	A
33	a	1290	A
33	a	1296	U
33	a	1297	A
33	a	1310	G
33	a	1312	U
33	a	1330	C
33	a	1348	G
33	a	1356	A
33	a	1363	G
33	a	1374	U
33	a	1388	C
33	a	1408	A
33	a	1429	G
33	a	1452	G
33	a	1456	A
33	a	1464	A
33	a	1503	A
33	a	1513	A
33	a	1514	A
33	a	1516	G
33	a	1517	U
33	a	1528	G
33	a	1540	G
33	a	1541	G
33	a	1544	C
34	b	10	G
34	b	12	A
34	b	19	G
34	b	20	C
34	b	21	A
34	b	22	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	90	A
10	A	130	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	176	A
10	A	202	A
10	A	232	U
10	A	258	A
10	A	298	U
10	A	299	U
10	A	388	A
10	A	449	U
10	A	548	A
10	A	598	G
10	A	614	U
10	A	661	U
10	A	809	A
10	A	903	G
10	A	923	A
10	A	969	A
10	A	988	C
10	A	1028	G
10	A	1069	G
10	A	1135	G
10	A	1176	U
10	A	1177	A
10	A	1186	A
10	A	1221	C
10	A	1291	A
10	A	1347	G
10	A	1357	G
10	A	1407	C
10	A	1496	G
10	A	1510	U
10	A	1633	A
10	A	1691	G
10	A	1789	A
10	A	1874	A
10	A	1940	A
10	A	2062	G
10	A	2313	A
10	A	2347	A
10	A	2457	A
10	A	2501	U
10	A	2508	G
10	A	2783	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	2791	A
10	A	2805	A
10	A	2887	G
11	B	19	G
11	B	32	U
11	B	63	U
11	B	64	A
11	B	105	C
13	D	7	G
13	D	27	U
13	F	7	G
13	F	17(A)	U

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
10	2MG	A	2472	10	23,26,27	0.18	0	33,38,41	0.31	0
33	2MG	a	975	33	23,26,27	0.20	0	33,38,41	0.29	0
33	UR3	a	1509	33	19,22,23	0.16	0	26,32,35	0.22	0
10	5MU	A	792	10	19,22,23	0.15	0	27,32,35	0.33	0
33	G7M	a	535	33	23,26,27	0.19	0	34,39,42	0.39	0
10	H2U	A	2476	10	18,21,22	0.20	0	19,30,33	0.51	0
33	5MC	a	976	33	19,22,23	0.15	0	26,32,35	0.36	0
10	5MU	A	1966	10	19,22,23	0.19	0	27,32,35	0.33	0
10	OMG	A	2278	10,13	23,26,27	0.18	0	32,38,41	0.31	0
10	2MA	A	2530	10,56	22,25,26	0.93	2 (9%)	32,37,40	1.30	3 (9%)
33	4OC	a	1412	33,56	20,23,24	0.21	0	25,32,35	0.42	0
33	MA6	a	1530	33	23,26,27	0.20	0	33,38,41	0.58	1 (3%)
10	3TD	A	1942	10	19,22,23	0.19	0	23,32,35	0.36	0
33	MA6	a	1529	33	23,26,27	0.17	0	33,38,41	0.57	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	2MG	A	2472	10	-	0/9/27/28	0/3/3/3
33	2MG	a	975	33	-	0/9/27/28	0/3/3/3
33	UR3	a	1509	33	-	0/7/25/26	0/2/2/2
10	5MU	A	792	10	-	0/7/25/26	0/2/2/2
33	G7M	a	535	33	-	3/7/25/26	0/3/3/3
10	H2U	A	2476	10	-	1/7/38/39	0/2/2/2
33	5MC	a	976	33	-	0/7/25/26	0/2/2/2
10	5MU	A	1966	10	-	0/7/25/26	0/2/2/2
10	OMG	A	2278	10,13	-	1/9/27/28	0/3/3/3
10	2MA	A	2530	10,56	-	0/7/25/26	0/3/3/3
33	4OC	a	1412	33,56	-	0/9/29/30	0/2/2/2
33	MA6	a	1530	33	-	2/11/29/30	0/3/3/3
10	3TD	A	1942	10	-	0/7/25/26	0/2/2/2
33	MA6	a	1529	33	-	0/11/29/30	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2530	2MA	C6-N6	-2.69	1.27	1.34
10	A	2530	2MA	C6-N1	2.19	1.37	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2530	2MA	N6-C6-N1	4.55	123.17	117.03
10	A	2530	2MA	C5-C6-N1	-3.74	113.09	118.90
10	A	2530	2MA	C2-N1-C6	3.67	123.75	118.10
33	a	1529	MA6	C2-N1-C6	2.34	117.53	111.83
33	a	1530	MA6	C2-N1-C6	2.30	117.46	111.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2278	OMG	C1'-C2'-O2'-CM2
33	a	535	G7M	C3'-C4'-C5'-O5'
33	a	1530	MA6	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	a	535	G7M	O4'-C4'-C5'-O5'
33	a	1530	MA6	C3'-C4'-C5'-O5'
33	a	535	G7M	C4'-C5'-O5'-P
10	A	2476	H2U	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	792	5MU	2	0
10	A	2530	2MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 151 ligands modelled in this entry, 149 are monoatomic - leaving 2 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	PUT	A	3101	-	5,5,5	0.09	0	4,4,4	0.18	0
57	PUT	A	3102	-	5,5,5	0.14	0	4,4,4	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PUT	A	3101	-	-	0/3/3/3	-
57	PUT	A	3102	-	-	1/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	3102	PUT	C2-C3-C4-N2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	A	3101	PUT	1	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.

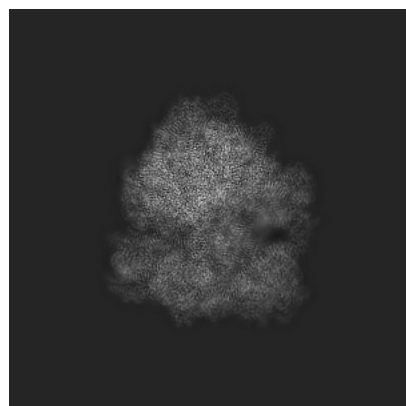
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51356. These allow visual inspection of the internal detail of the map and identification of artifacts.

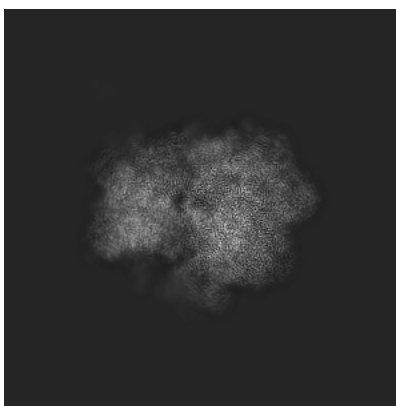
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

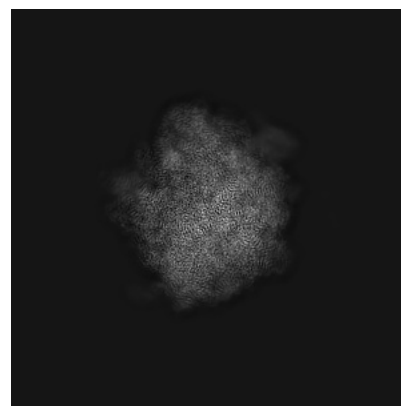
6.1.1 Primary map



X

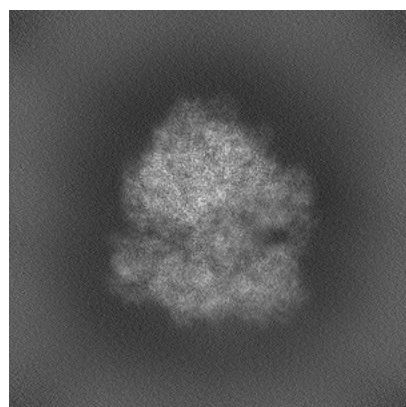


Y

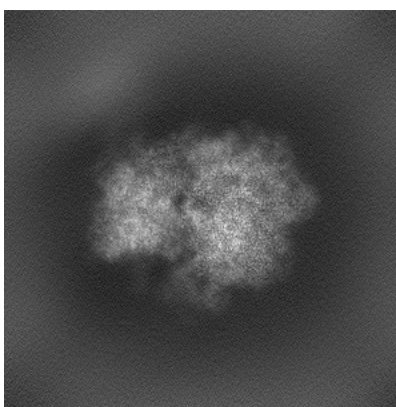


Z

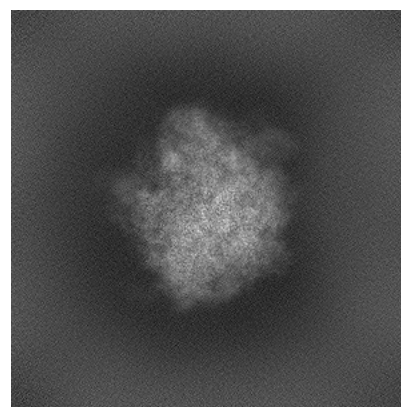
6.1.2 Raw map



X



Y

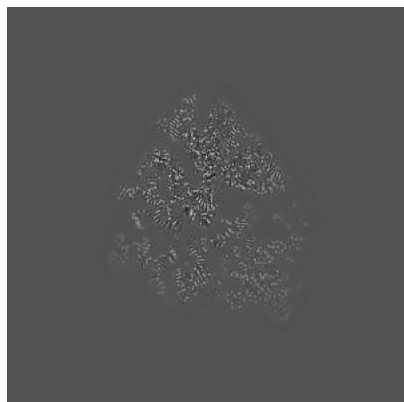


Z

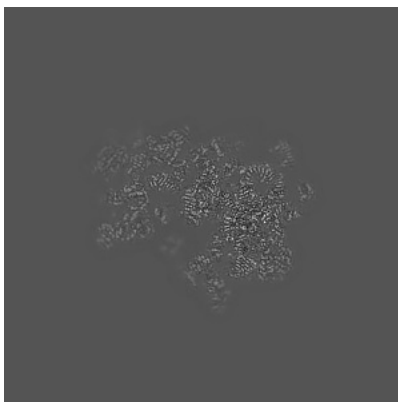
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

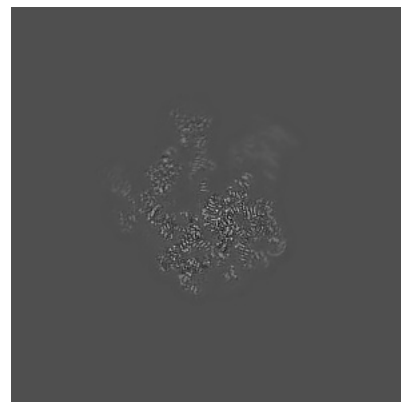
6.2.1 Primary map



X Index: 300

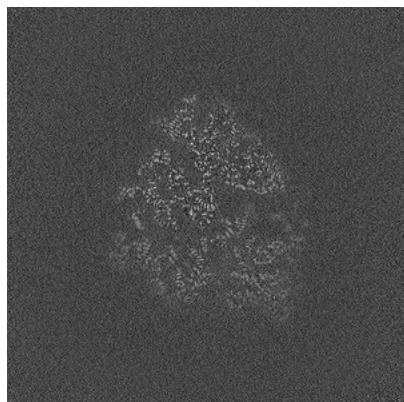


Y Index: 300

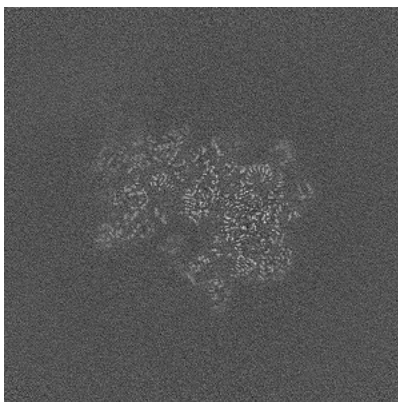


Z Index: 300

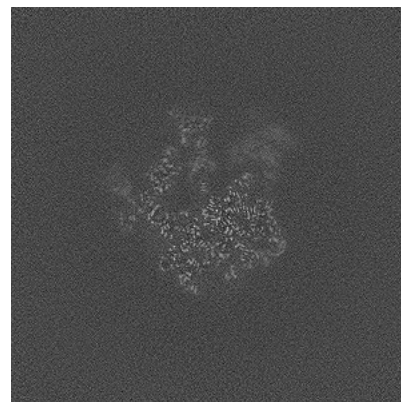
6.2.2 Raw map



X Index: 300



Y Index: 300

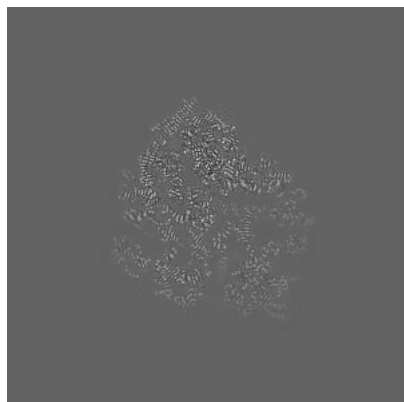


Z Index: 300

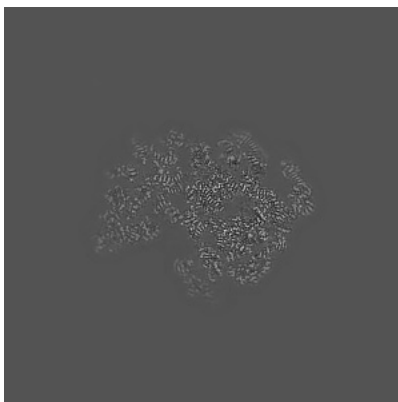
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

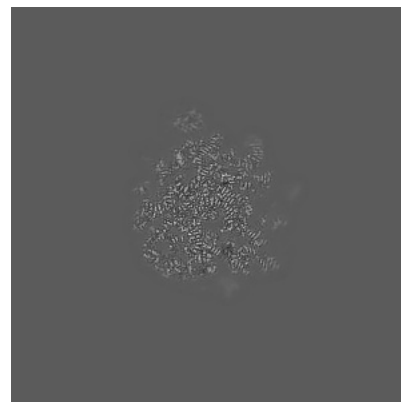
6.3.1 Primary map



X Index: 292

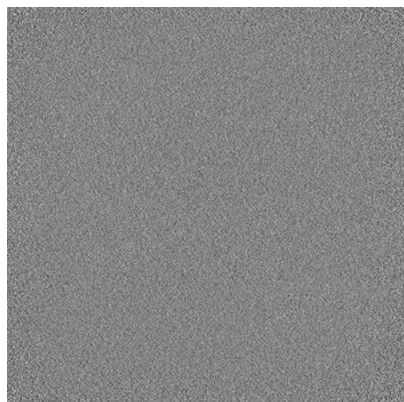


Y Index: 278

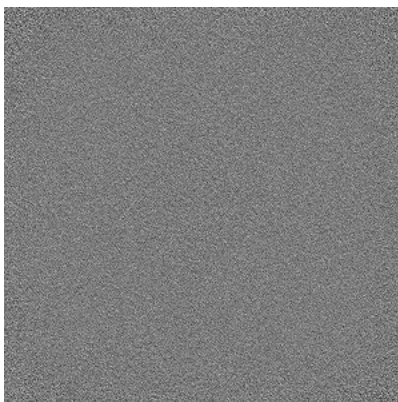


Z Index: 360

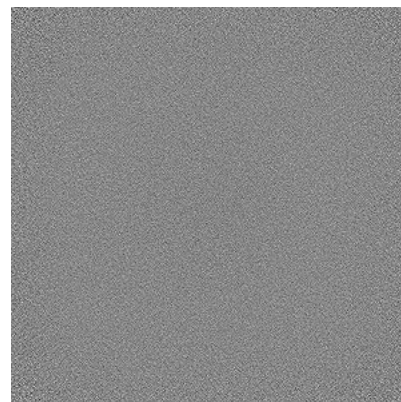
6.3.2 Raw map



X Index: 0



Y Index: 0

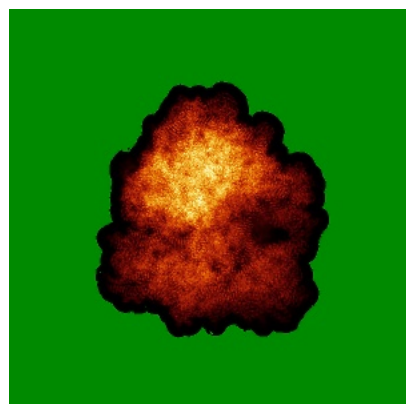


Z Index: 0

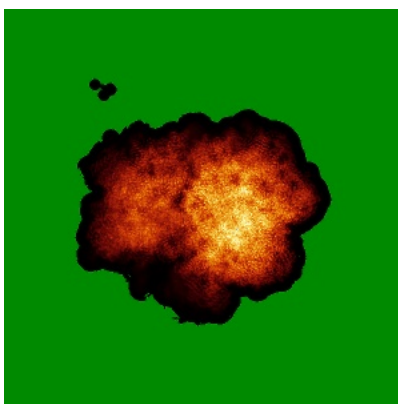
The images above show the largest variance slices of the map in three orthogonal directions.

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

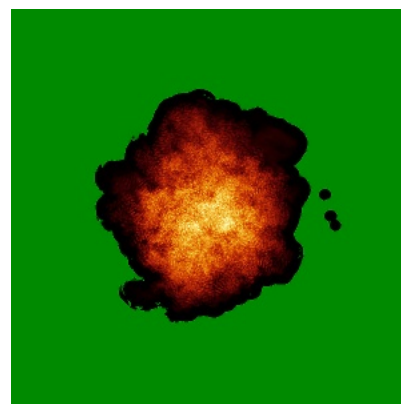
6.4.1 Primary map



X

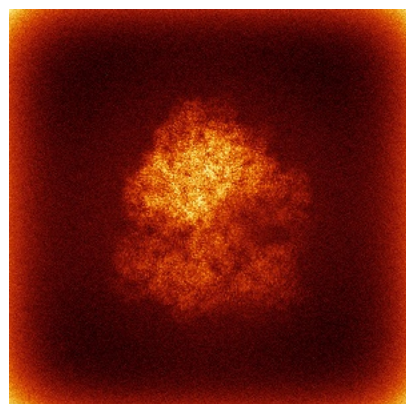


Y

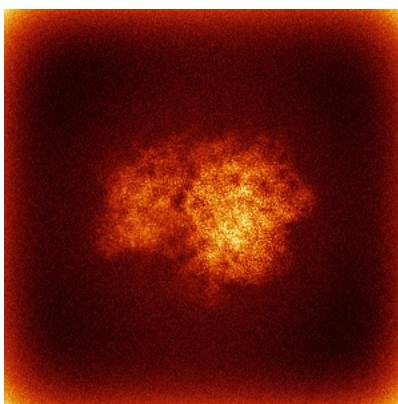


Z

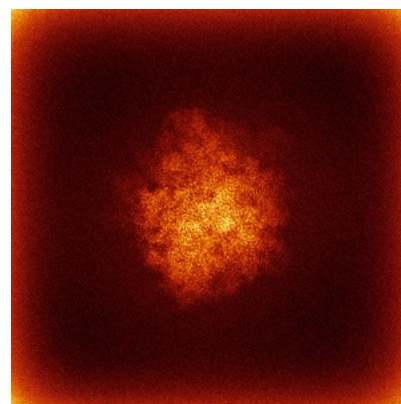
6.4.2 Raw map



X



Y

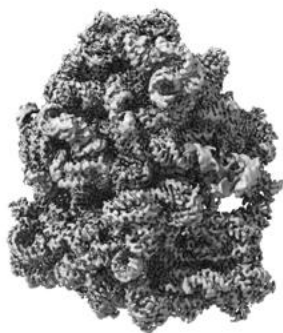


Z

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

6.5 Orthogonal surface views [i](#)

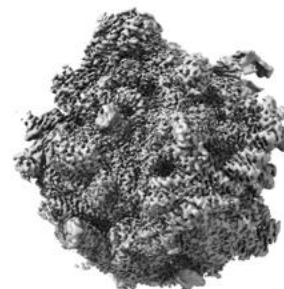
6.5.1 Primary map



X



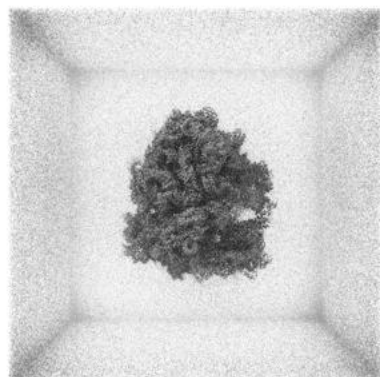
Y



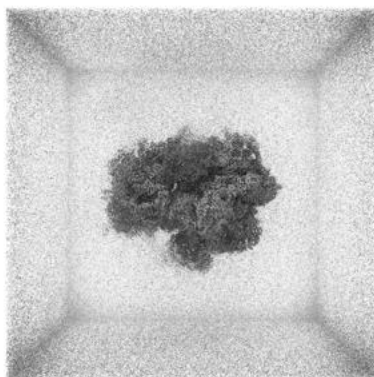
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

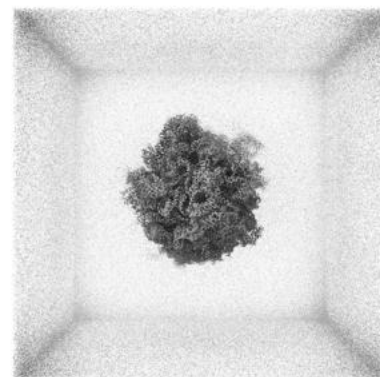
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

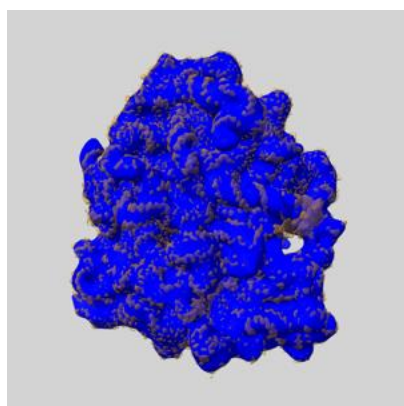
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

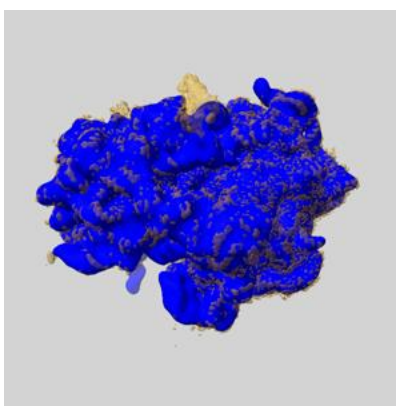
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

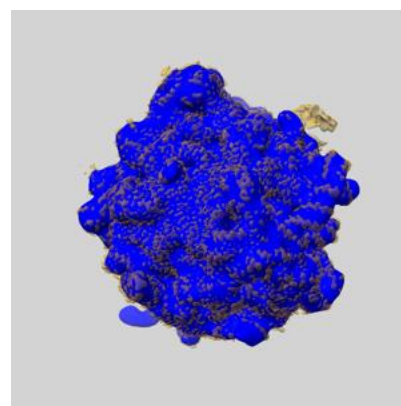
6.6.1 emd_51356_msk_1.map [i](#)



X



Y

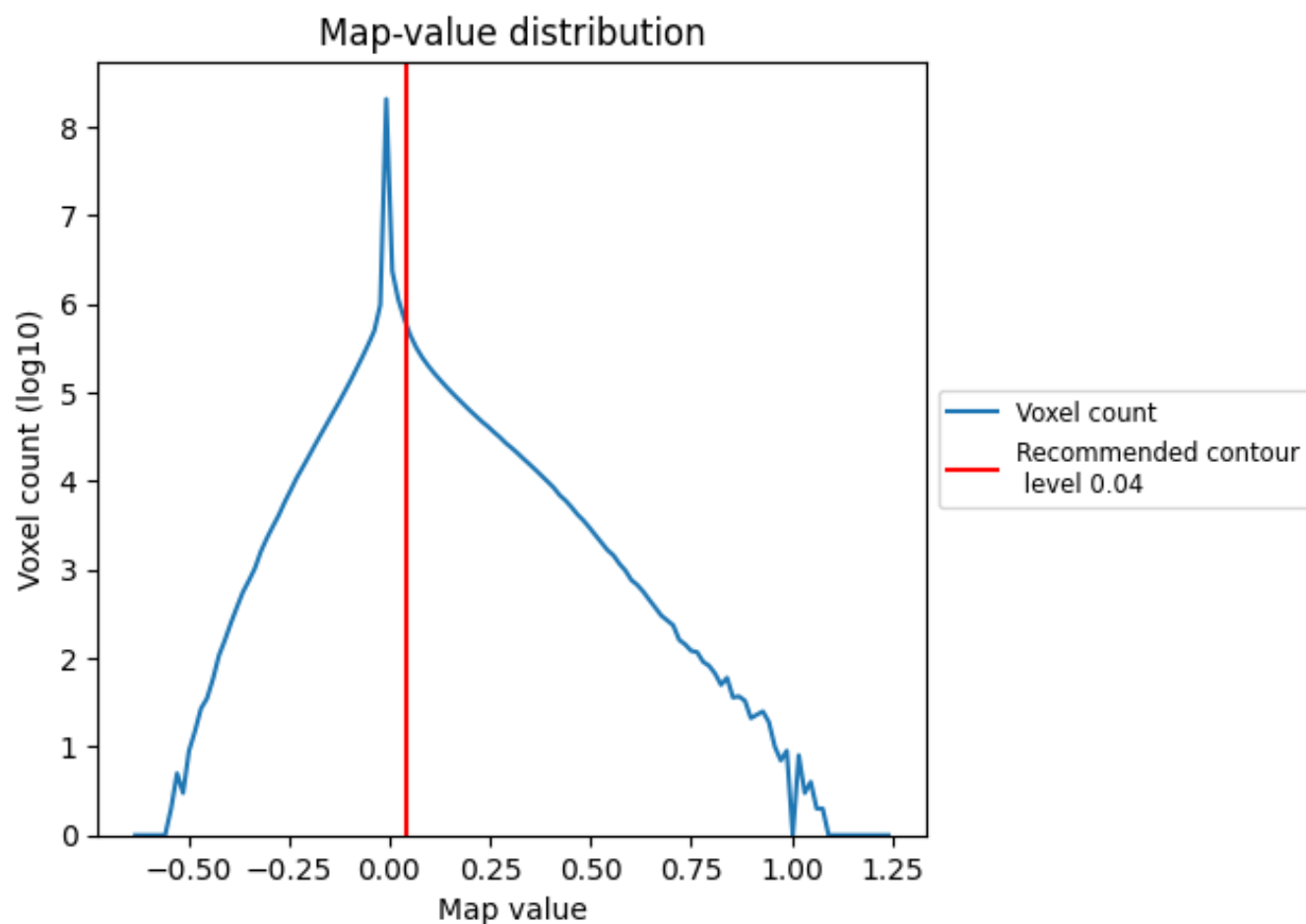


Z

7 Map analysis [i](#)

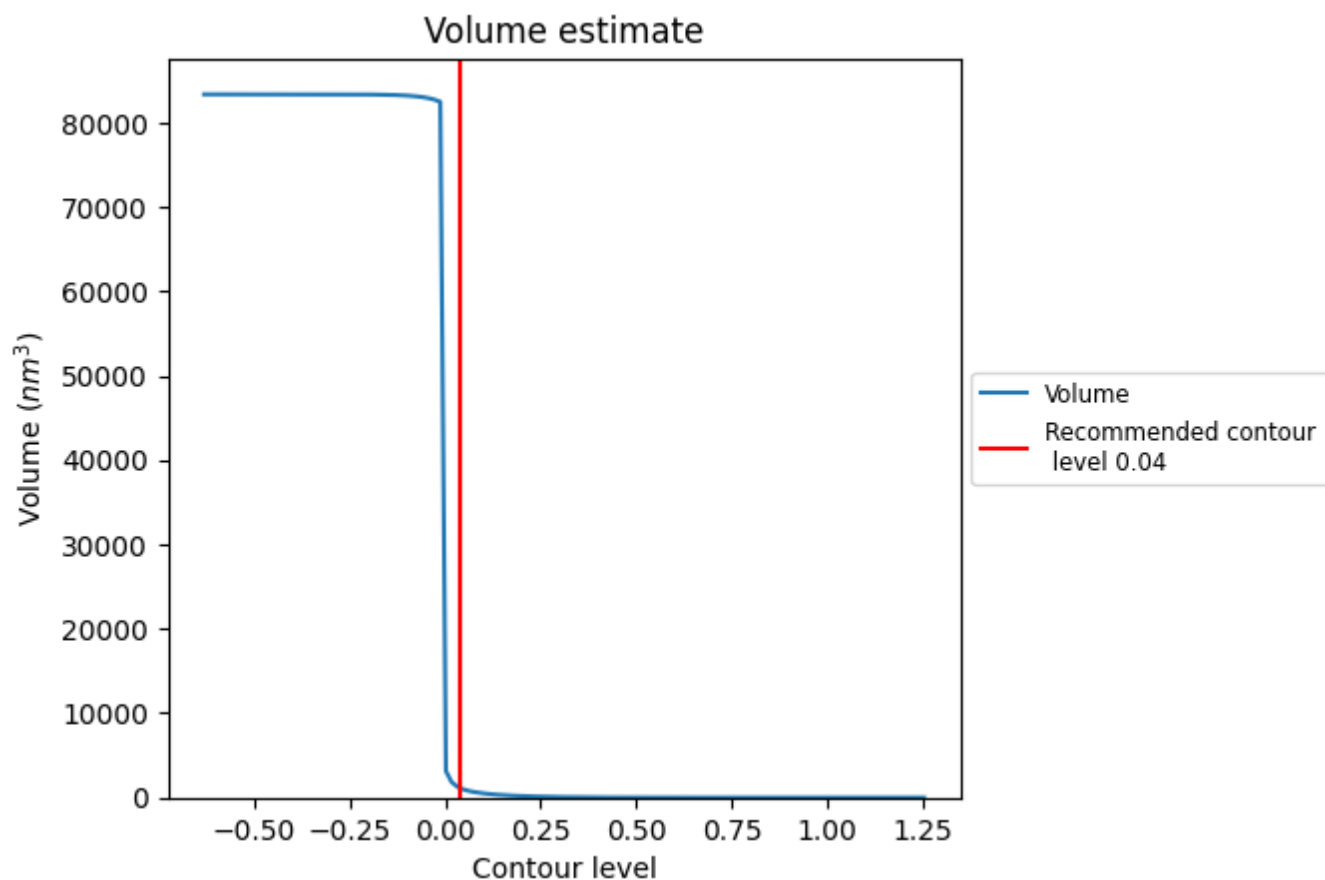
This section contains the results of statistical analysis of the map.

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.

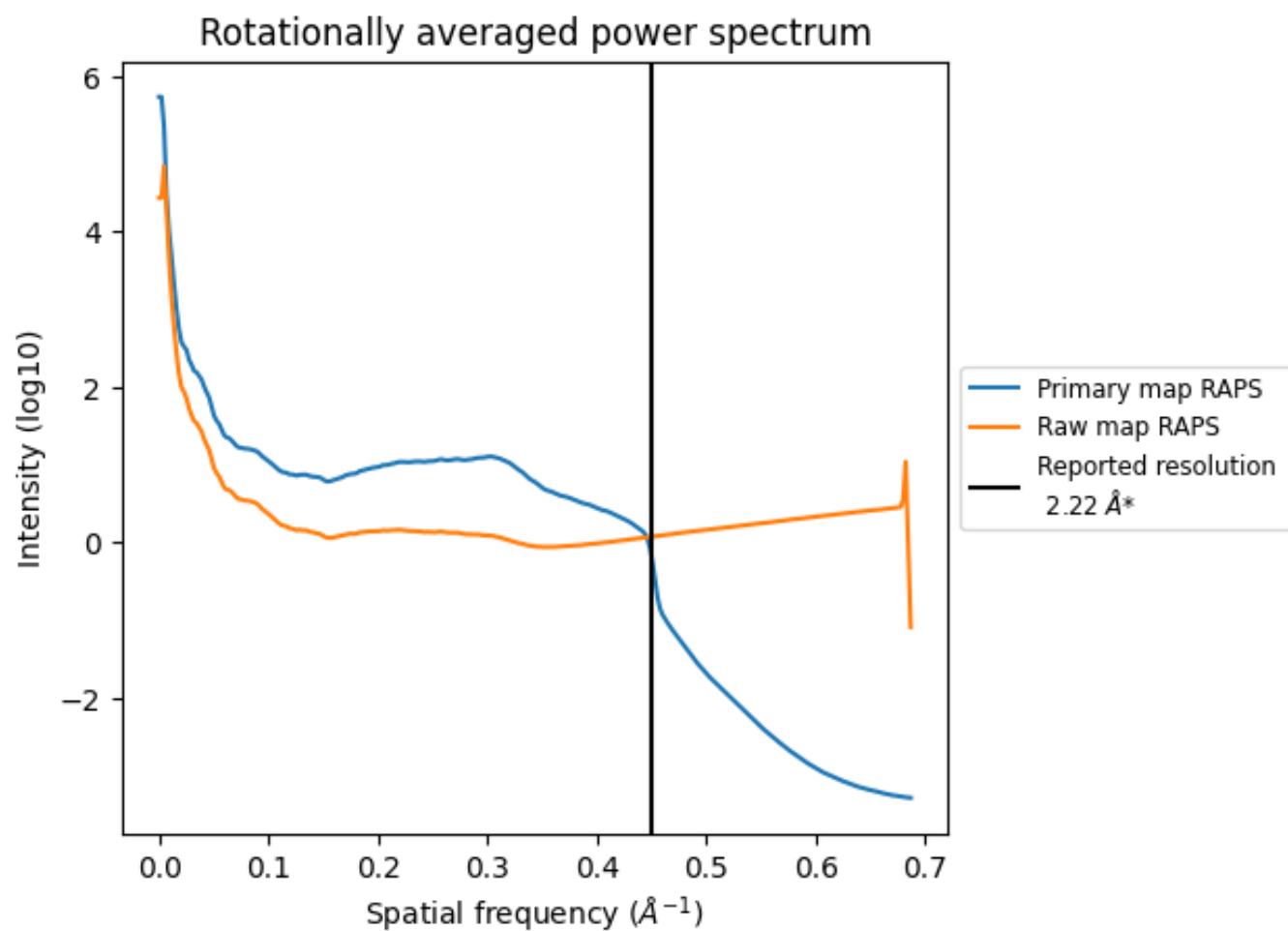
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1125 nm^3 ; this corresponds to an approximate mass of 1016 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 ⓘ

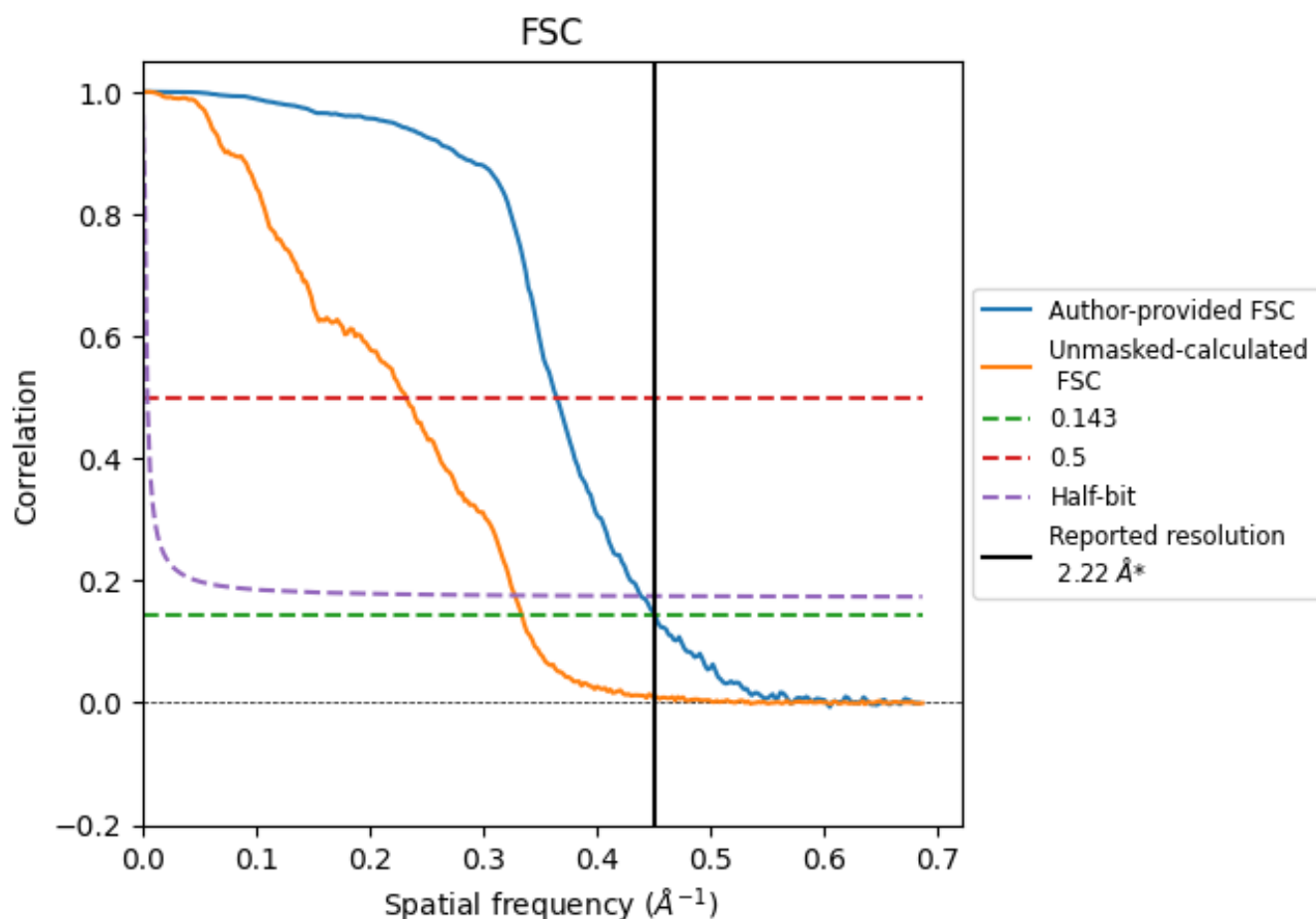


*Reported resolution corresponds to spatial frequency of 0.450 $\text{\AA}^{-1}$

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 0.450 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

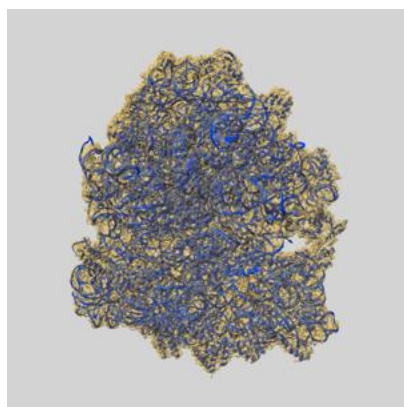
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.22	-	-
Author-provided FSC curve	2.22	2.74	2.28
Unmasked-calculated*	2.99	4.30	3.05

*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 2.99 differs from the reported value 2.22 by more than 10 %

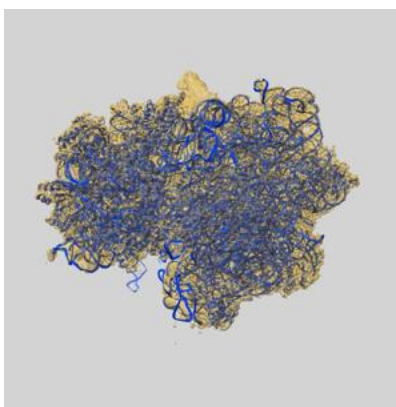
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51356 and PDB model 9GHG. Per-residue inclusion information can be found in section [3](#) on page [18](#).

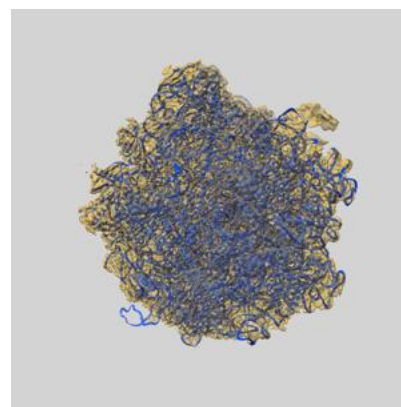
9.1 Map-model overlay [i](#)



X



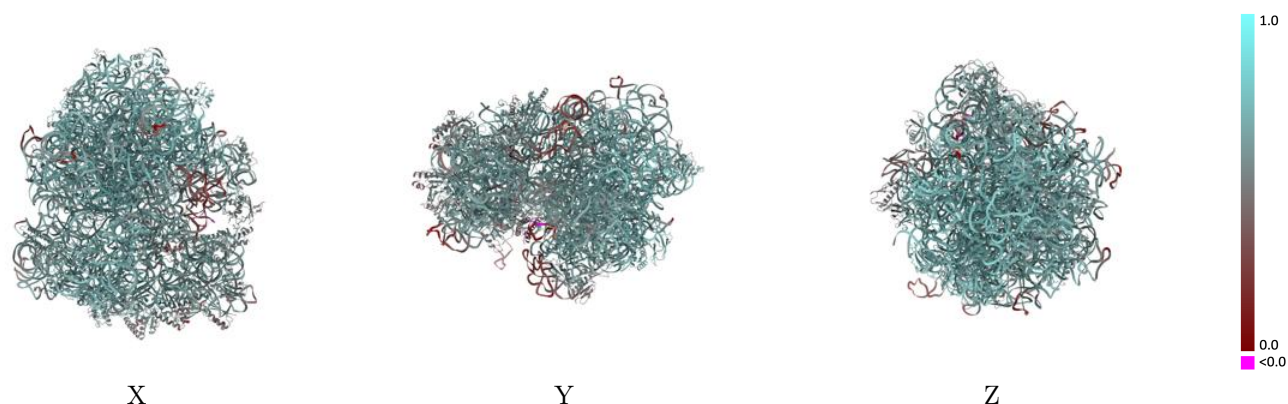
Y



Z

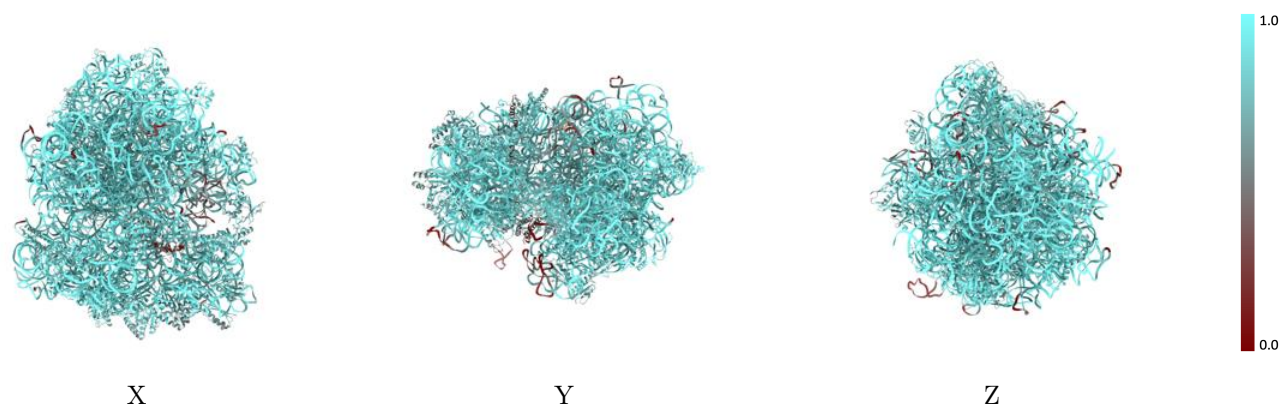
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



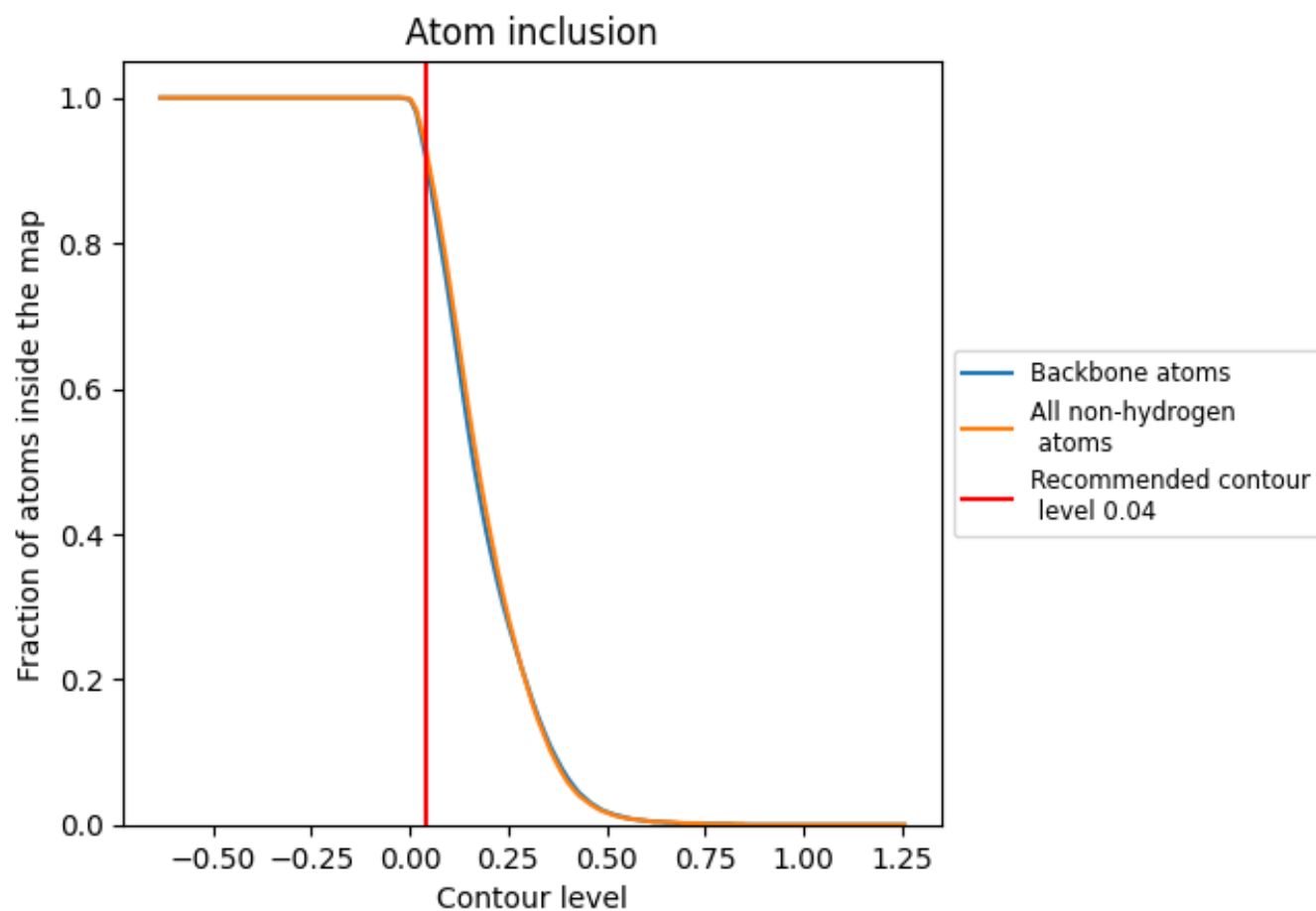
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.6390
1	 0.9420	 0.6520
2	 0.8960	 0.6110
3	 0.9630	 0.6760
4	 0.7520	 0.4910
5	 0.9610	 0.7050
6	 0.8860	 0.6100
7	 0.9880	 0.7370
8	 0.9940	 0.7330
9	 0.9550	 0.6550
A	 0.9630	 0.6700
B	 0.9790	 0.6110
C	 0.5710	 0.4130
D	 0.6060	 0.3400
F	 0.9500	 0.6220
G	 0.9740	 0.7100
H	 0.9670	 0.7040
I	 0.9420	 0.6840
J	 0.8400	 0.5430
K	 0.8020	 0.5130
M	 0.9620	 0.6940
N	 0.9720	 0.7030
O	 0.9520	 0.6770
P	 0.9560	 0.6580
Q	 0.9600	 0.6970
R	 0.8960	 0.5720
S	 0.9520	 0.6760
T	 0.9790	 0.7240
U	 0.9510	 0.6800
V	 0.9630	 0.7050
W	 0.9430	 0.6440
X	 0.8490	 0.5730
Y	 0.8350	 0.5450
Z	 0.9720	 0.6740
a	 0.9610	 0.6320



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.6730	 0.4460
c	 0.7900	 0.5230
d	 0.8240	 0.5510
e	 0.9160	 0.6050
f	 0.9390	 0.6530
g	 0.8840	 0.6060
h	 0.8420	 0.5630
i	 0.9500	 0.6470
j	 0.8570	 0.5700
k	 0.7830	 0.5250
l	 0.8660	 0.5900
m	 0.9380	 0.6470
n	 0.8610	 0.5650
o	 0.9520	 0.6330
p	 0.9210	 0.6380
q	 0.9060	 0.6180
r	 0.9210	 0.6240
s	 0.9160	 0.6360
t	 0.8420	 0.5500
u	 0.9160	 0.6320
v	 0.4470	 0.4540