



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:50 PM UTC

PDB ID : 7ST2 / pdb_00007st2
EMDB ID : EMD-25418
Title : Post translocation, non-rotated 70S ribosome with EF-G dissociated (Structure VII)
Authors : Carbone, C.E.; Korostelev, A.A.
Deposited on : 2021-11-11
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

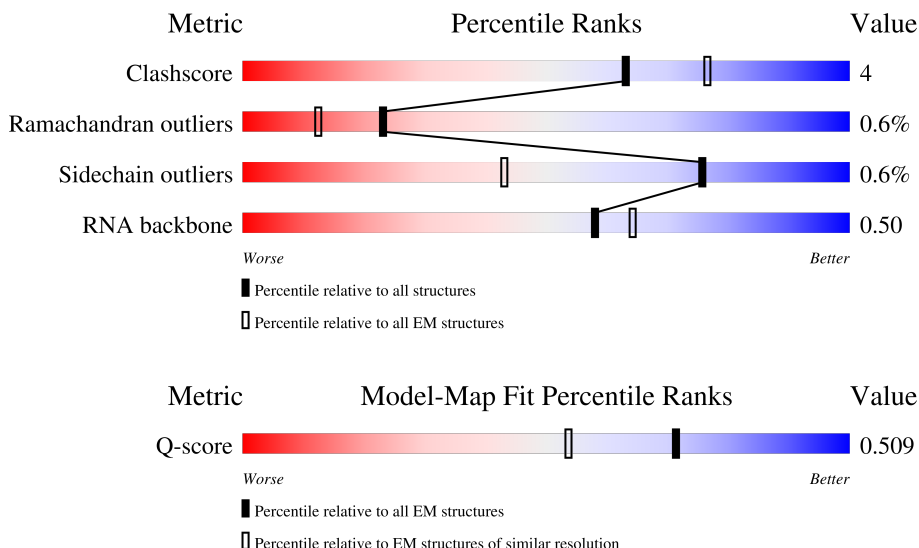
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	3	1539	
2	1	2903	
3	2	120	

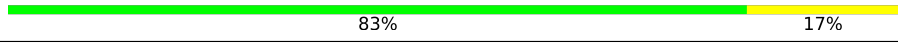
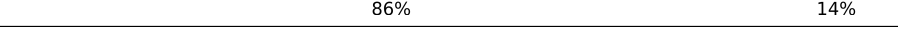
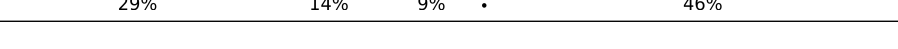
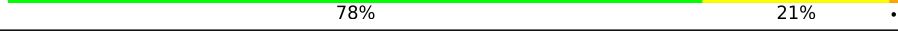
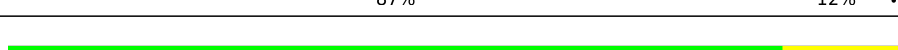
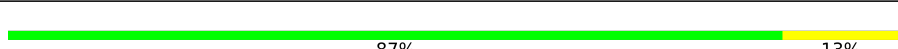
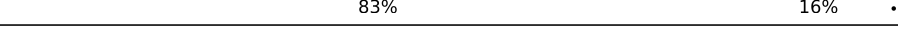
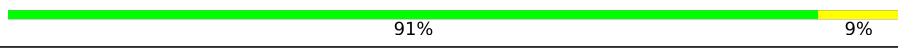
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Mol	Chain	Length	Quality of chain
4	6	77	
5	b	271	
6	c	209	
7	d	201	
8	e	177	
9	f	176	
10	g	149	
11	a	234	
12	h	131	
13	i	142	
14	j	142	
15	k	122	
16	l	143	
17	m	136	
18	n	120	
19	o	116	
20	p	114	
21	q	117	
22	r	103	
23	s	110	
24	t	93	
25	u	102	
26	v	94	
27	w	75	
28	x	77	

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Mol	Chain	Length	Quality of chain
29	y	63	
30	z	58	
31	A	66	
32	B	56	
33	C	50	
34	D	46	
35	E	64	
36	F	38	
37	4	35	
38	5	77	
39	G	225	
40	H	206	
41	I	205	
42	J	157	
43	K	100	
44	L	151	
45	M	129	
46	N	127	
47	O	98	
48	P	116	
49	Q	123	
50	R	114	
51	S	100	
52	T	88	
53	U	82	

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Mol	Chain	Length	Quality of chain
54	V	80	79% 20%
55	W	65	86% 14%
56	X	79	86% 14%
57	Y	85	85% 15%
58	Z	65	60% 38%

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 149087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 4 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	g	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 11 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	h	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	i	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 14 is a protein called 50S ribosomal protein L13.

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

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	l	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	n	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 19 is a protein called 50S ribosomal protein L18.

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

- Molecule 20 is a protein called 50S ribosomal protein L19.

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

- Molecule 21 is a protein called 50S ribosomal protein L20.

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

- Molecule 22 is a protein called 50S ribosomal protein L21.

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

- Molecule 23 is a protein called 50S ribosomal protein L22.

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

- Molecule 24 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	t	93	Total	C	N	O	S	0
			739	466	139	132	2	0

- Molecule 25 is a protein called 50S ribosomal protein L24.

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

- Molecule 26 is a protein called 50S ribosomal protein L25.

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

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	w	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 28 is a protein called 50S ribosomal protein L28.

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

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 32 is a protein called 50S ribosomal protein L32.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	C	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 34 is a protein called 50S ribosomal protein L34.

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

- Molecule 35 is a protein called 50S ribosomal protein L35.

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

- Molecule 36 is a protein called 50S ribosomal protein L36.

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

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	19	Total	C	N	O	P	0	0
			416	186	85	126	19		

- Molecule 38 is a RNA chain called tRNA Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5	77	Total	C	N	O	P	0	0
			1647	733	295	542	77		

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	G	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	J	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	O	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 48 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	P	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Q	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	R	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	U	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	V	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	W	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Y	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

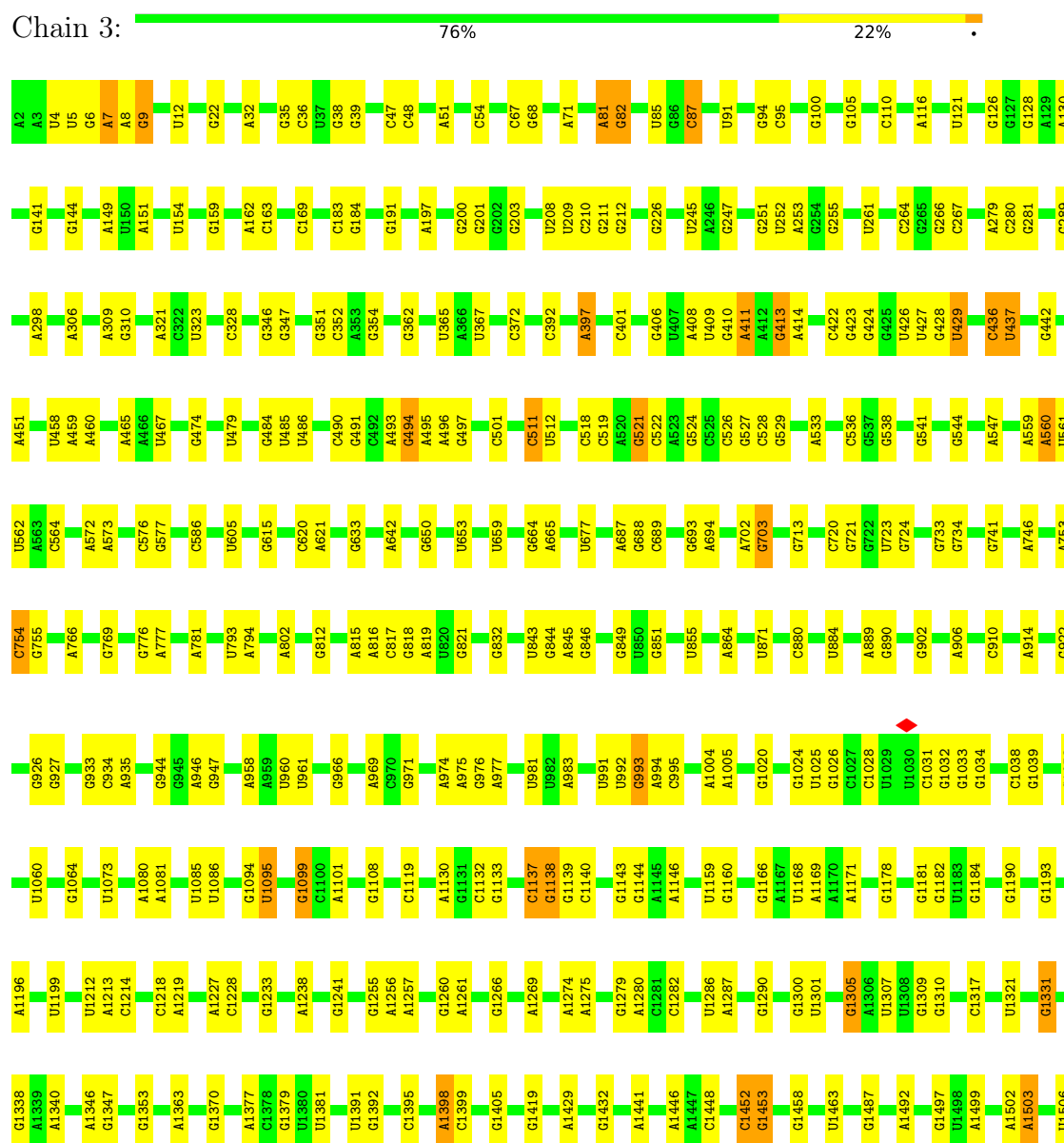
- Molecule 58 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

3 Residue-property plots

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

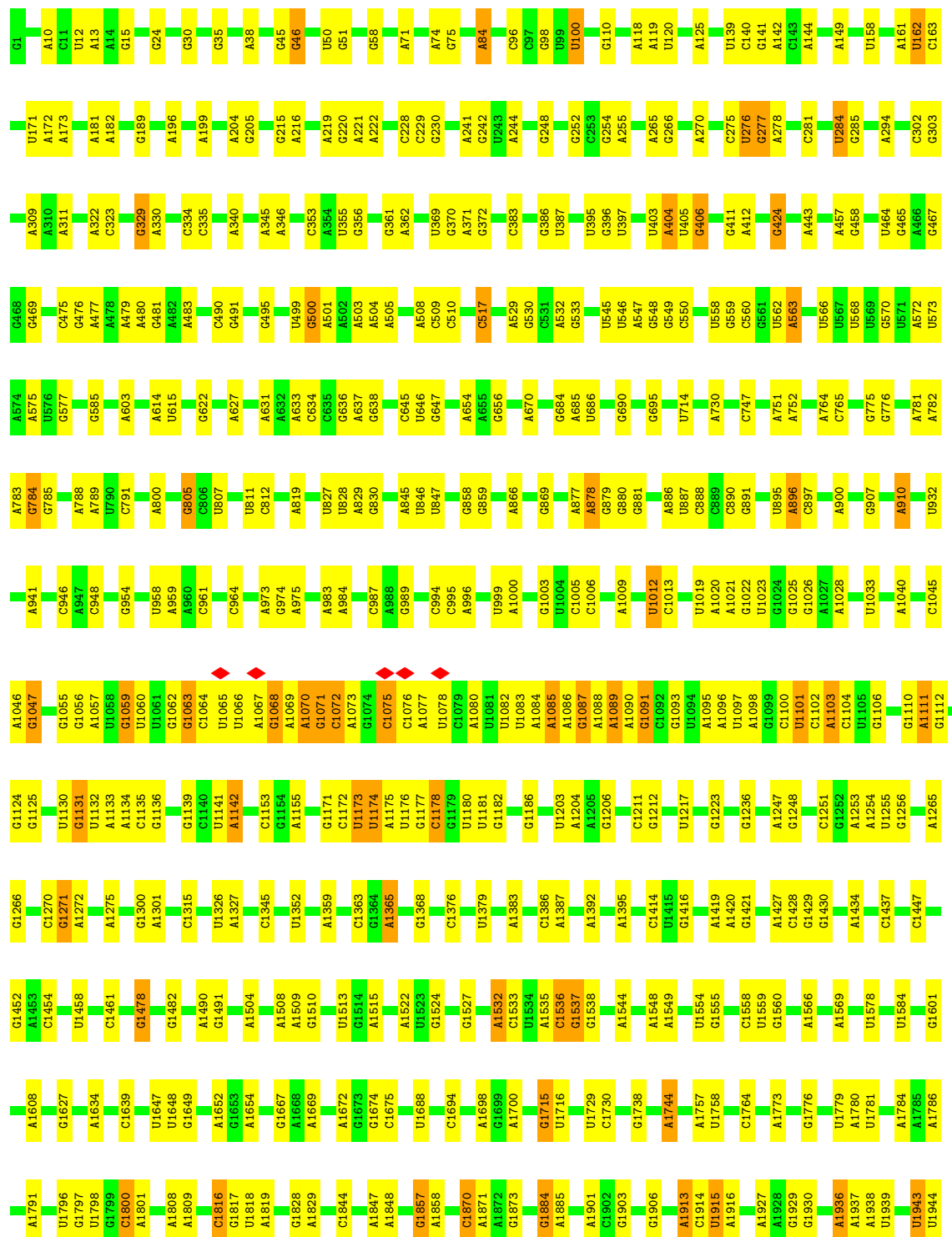
• Molecule 1: 16S rRNA

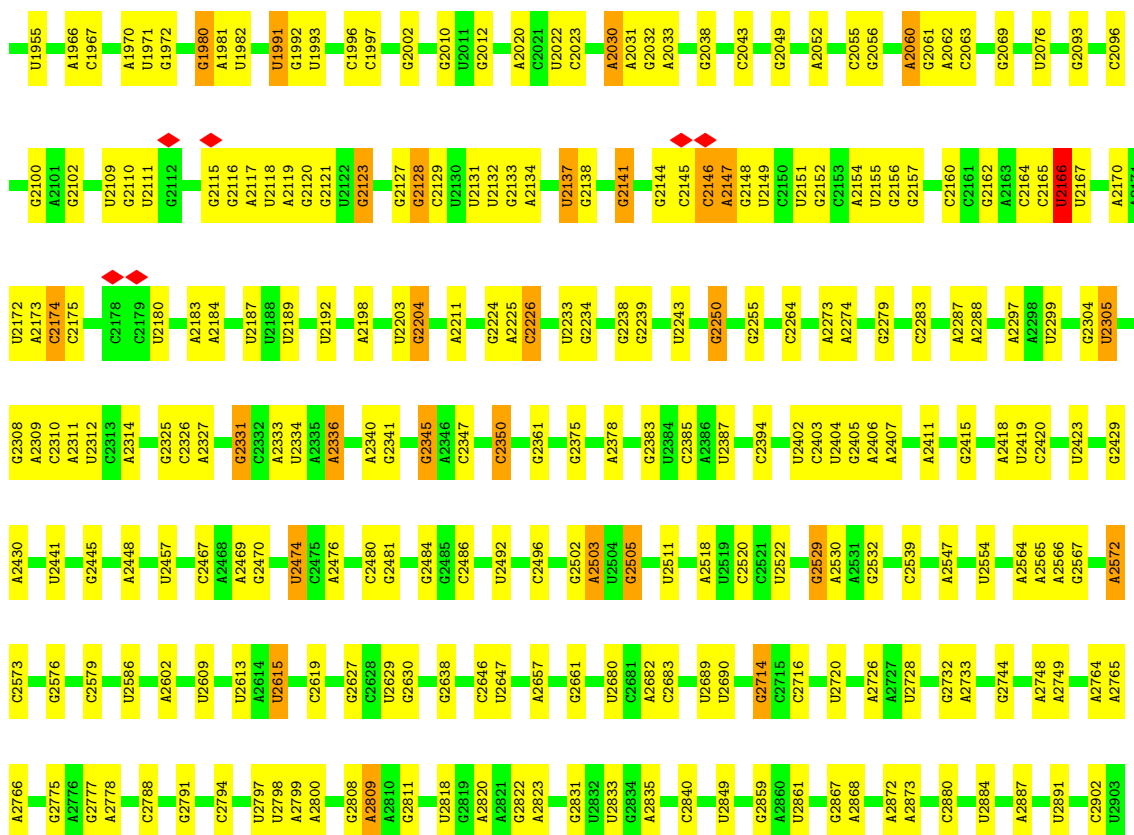




• Molecule 2: 23S rRNA

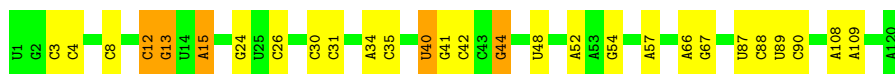
Chain 1: 74% 23%





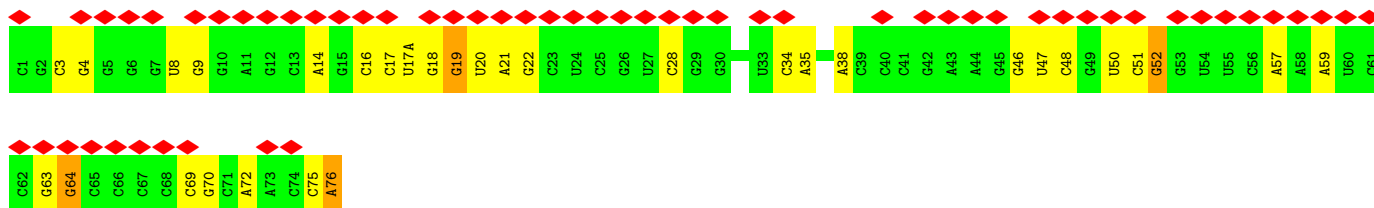
• Molecule 3: 5S rRNA

Chain 2: 77% 19%



• Molecule 4: tRNA fMet

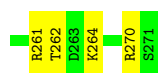
Chain 6: 58% 75% 36% 5%



• Molecule 5: 50S ribosomal protein L2

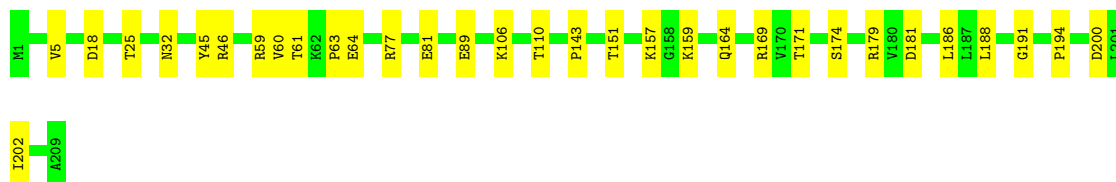
Chain b: 87% 13%





• Molecule 6: 50S ribosomal protein L3

Chain c: 85% 15%



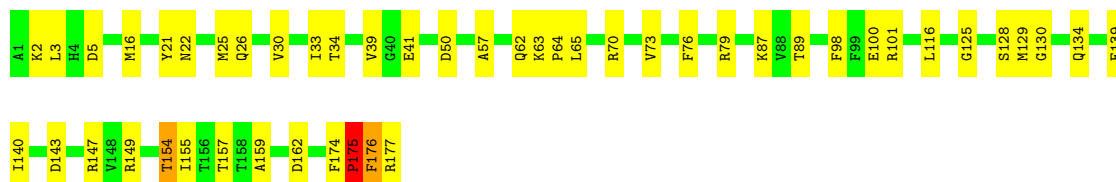
• Molecule 7: 50S ribosomal protein L4

Chain d: 87% 13%



• Molecule 8: 50S ribosomal protein L5

Chain e: 73% 25% ::



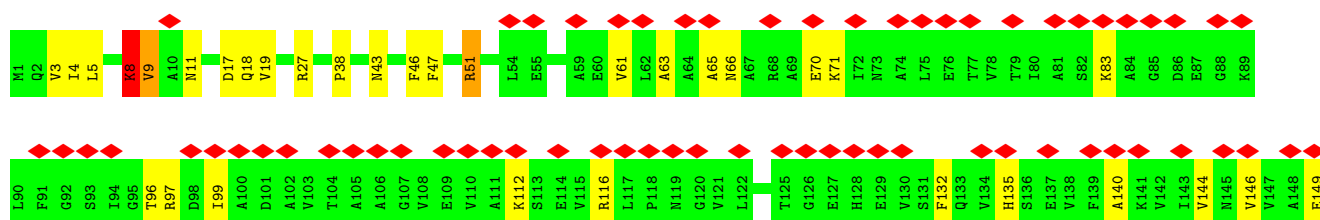
• Molecule 9: 50S ribosomal protein L6

Chain f: 85% 15%

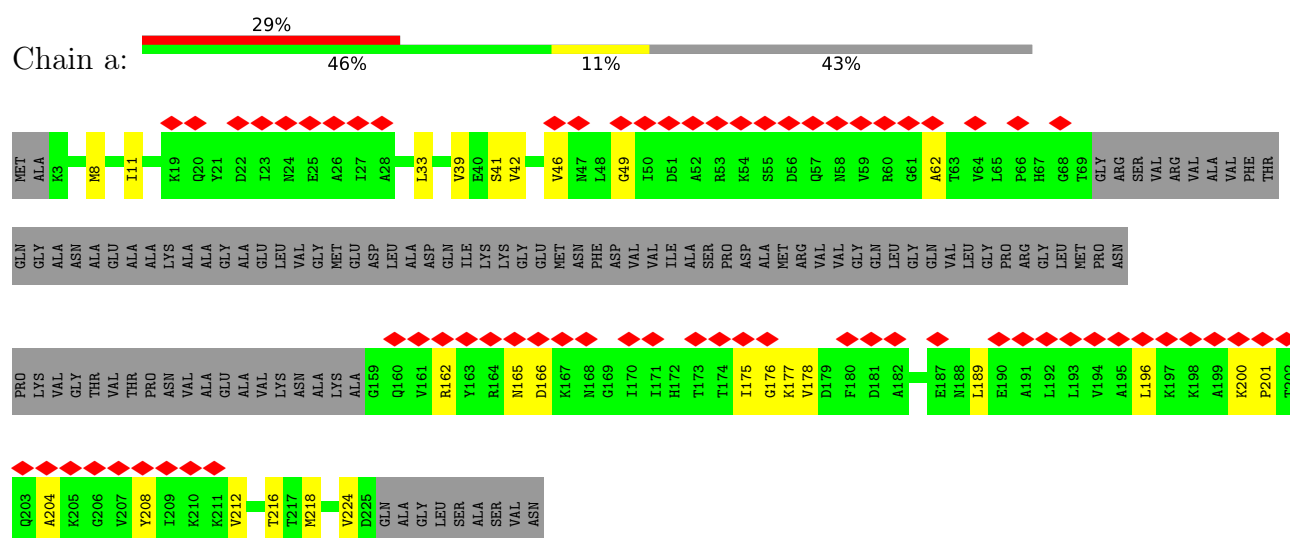


• Molecule 10: 50S ribosomal protein L9

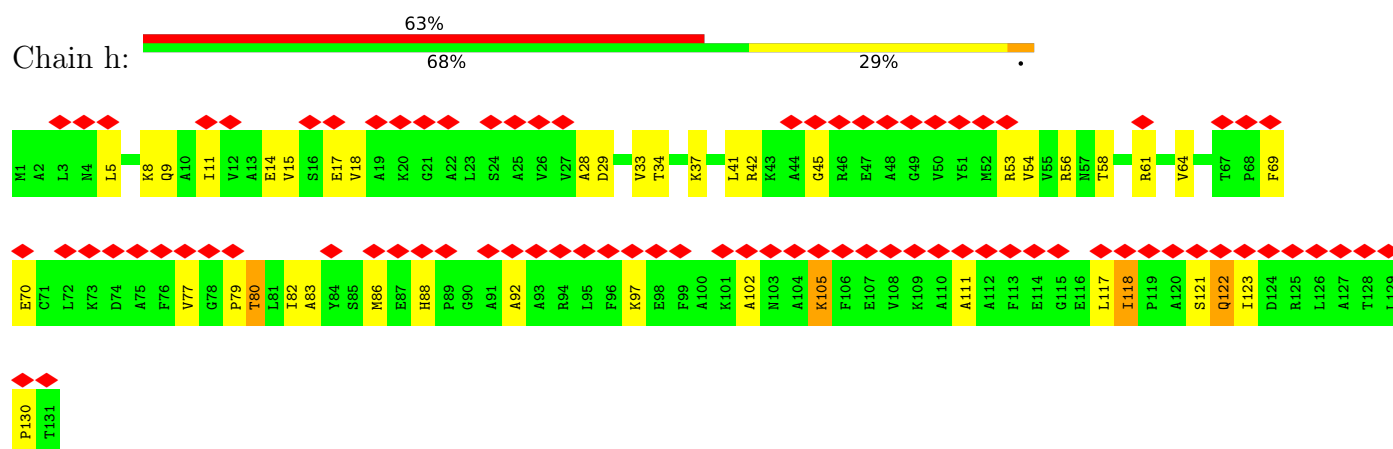
Chain g: 44% 78% 20% ::



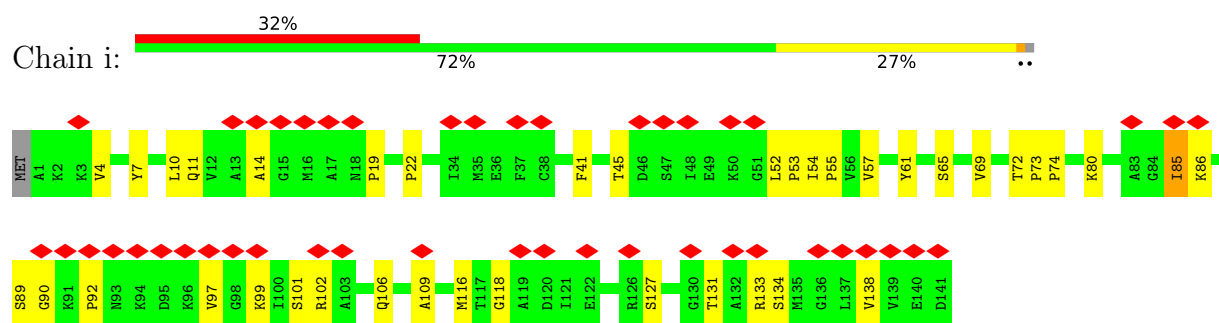
• Molecule 11: 50S ribosomal protein L1



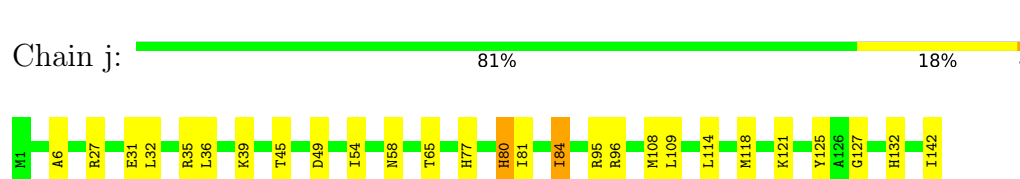
• Molecule 12: 50S ribosomal protein L10



• Molecule 13: 50S ribosomal protein L11



• Molecule 14: 50S ribosomal protein L13



• Molecule 15: 50S ribosomal protein L14

Chain k:  80% 20% .



- Molecule 16: 50S ribosomal protein L15

Chain l:  85% 13% ..



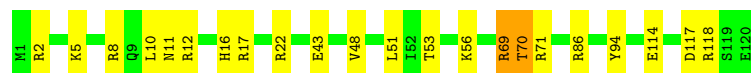
- Molecule 17: 50S ribosomal protein L16

Chain m:  93% 7% .



- Molecule 18: 50S ribosomal protein L17

Chain n:  82% 17% .



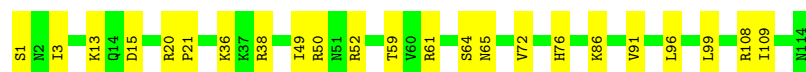
- Molecule 19: 50S ribosomal protein L18

Chain o:  74% 26%



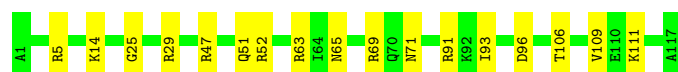
- Molecule 20: 50S ribosomal protein L19

Chain p:  80% 20%



- Molecule 21: 50S ribosomal protein L20

Chain q:  85% 15%



- Molecule 22: 50S ribosomal protein L21

Chain r:  85% 15%



- Molecule 23: 50S ribosomal protein L22

Chain s:  90% 10%



- Molecule 24: 50S ribosomal protein L23

Chain t:  76% 23% .



- Molecule 25: 50S ribosomal protein L24

Chain u:  86% 14%

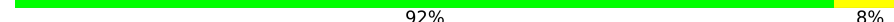


- Molecule 26: 50S ribosomal protein L25

Chain v:  78% 22%



- Molecule 27: 50S ribosomal protein L27

Chain w:  92% 8%



- Molecule 28: 50S ribosomal protein L28

Chain x:  78% 21% .



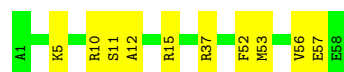
- Molecule 29: 50S ribosomal protein L29

Chain y:  68% 29%



- Molecule 30: 50S ribosomal protein L30

Chain z:  83% 17%



- Molecule 31: 50S ribosomal protein L31

Chain A:  86% 14%



- Molecule 32: 50S ribosomal protein L32

Chain B:  82% 18%



- Molecule 33: 50S ribosomal protein L33

Chain C:  88% 12%



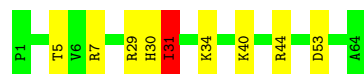
- Molecule 34: 50S ribosomal protein L34

Chain D:  80% 20%



- Molecule 35: 50S ribosomal protein L35

Chain E:  86% 12%



- Molecule 36: 50S ribosomal protein L36

Category	Count
M1	1
K2	1
V3	1
S6	1
C11	1
C14	1
K15	1
I16	1
V25	1
E30	1
P31	1
K32	1
R36	1
Q37	1
G38	1

[illegible]

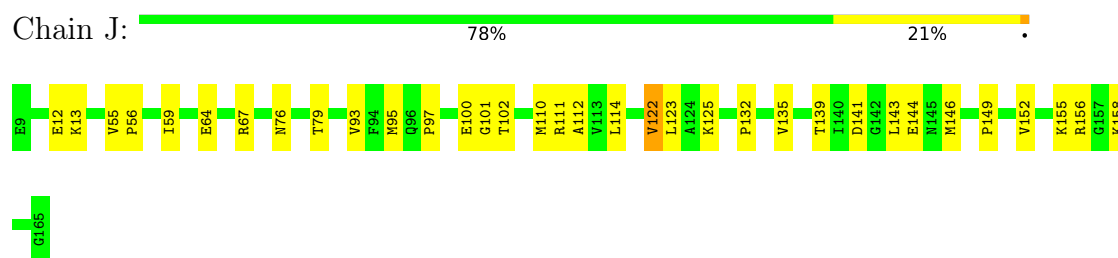
Item	Category
C1	C1
G2	G2
G3	G3
C4	C4
G5	G5
G10	G10
U17	U17
U17A	U17A
G18	G18
G19	G19
U20	U20
A21	A21
G22	G22
G31	G31
U32	U32
U33	U33
A41	A41
G42	G42
G46	G46
U47	U47
C48	C48
G49	G49
G57	G57
U60	U60
C61	C61
C62	C62
U65	U65
A73	A73
A76	A76

L116	L143	L160	I163	V182	L213	R224	S225	ALA	THR	VAL	SER	MET	ARG	ASP	MB	V13	H14	F15	G16	H17	Q18	T19	R20	Y21	M26	I30	F31	I39	L40	N41	L42	F43	K44	T45	V46	N50	I59	R62	K63	G70	T71	K72	S76	A82	V91	N92	W95	M99	M102	V106	L112
------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------

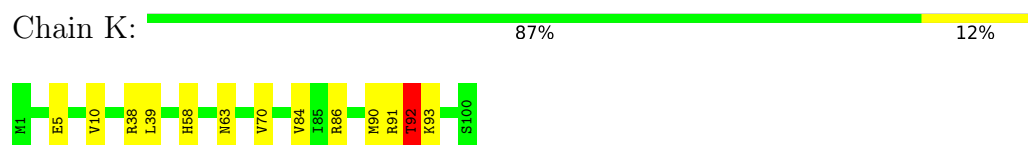
A horizontal bar chart showing the distribution of 1206 samples across 26 categories. The categories are labeled with codes: G1, Q2, K3, V4, H5, I9, T20, A23, E27, D30, D85, L46, A49, S82, V85, I56, E57, R58, R64, V85, T66, I67, H68, T89, A70, R71, I74, G77, K78, K79, L86, K107, P108, E109, E124, L143, V150, F151, V152. The bars are colored in a repeating pattern of green, yellow, and orange. A red arrow points to the G77 category.

A1	R2	K7	L8	K9	L10	S11	T16	V24	R25	A26	I27	D28	L29	K30	C31	K32	I33	E34	Q35	A36	H40	G41	K44	R55	E56	K57	R62	E68	R69	R72	L81	L97	T98	N99	V100	M104	A108	T109	R110	A111	E112	A113	R114	H119
V124	V128	V129	N130	V141	R145	E146	K147	Q151	S152	R153	A156	A157	L170	T180	R187	L190	S191	A192	E201	K206																								

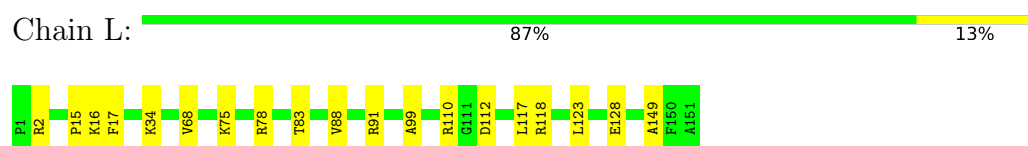
- Molecule 42: 30S ribosomal protein S5



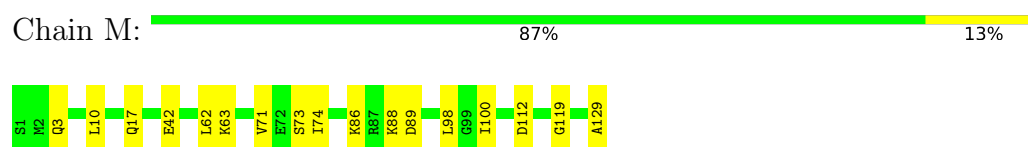
- Molecule 43: 30S ribosomal protein S6



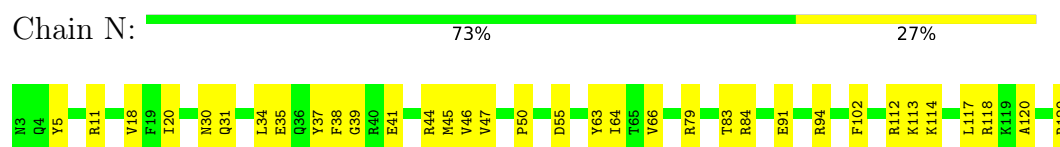
- Molecule 44: 30S ribosomal protein S7



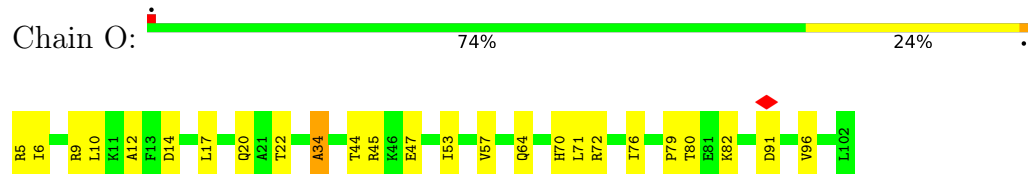
- Molecule 45: 30S ribosomal protein S8



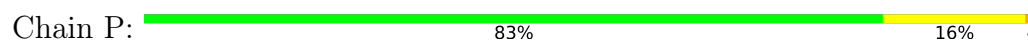
- Molecule 46: 30S ribosomal protein S9



- Molecule 47: 30S ribosomal protein S10

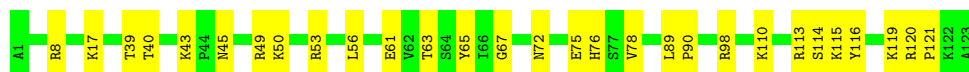
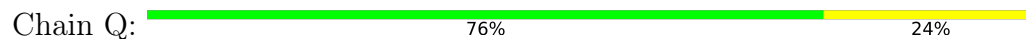


- Molecule 48: 30S ribosomal protein S11

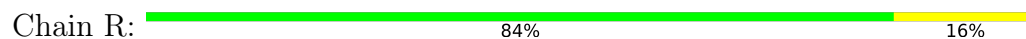




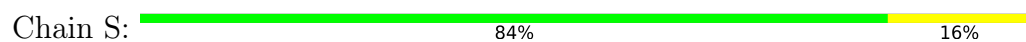
- Molecule 49: 30S ribosomal protein S12



- Molecule 50: 30S ribosomal protein S13



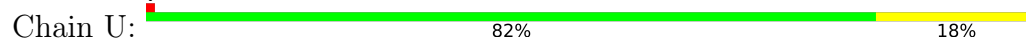
- Molecule 51: 30S ribosomal protein S14



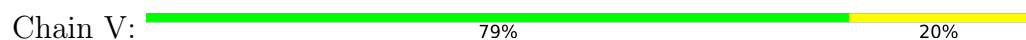
- Molecule 52: 30S ribosomal protein S15



- Molecule 53: 30S ribosomal protein S16



- Molecule 54: 30S ribosomal protein S17

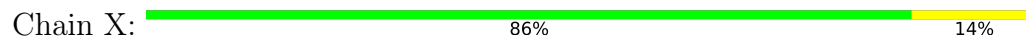


- Molecule 55: 30S ribosomal protein S18

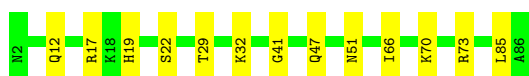
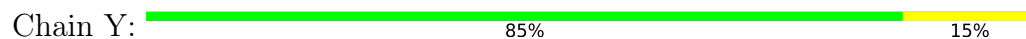




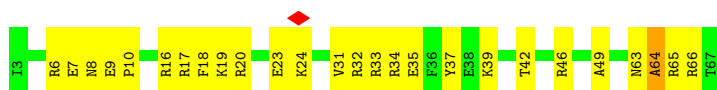
- Molecule 56: 30S ribosomal protein S19



- Molecule 57: 30S ribosomal protein S20



- Molecule 58: 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	55457	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	20.855	Depositor
Minimum map value	-7.489	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.005	Depositor
Recommended contour level	1.35	Depositor
Map size (Å)	389.76, 389.76, 389.76	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	3	0.57	0/36963	0.39	0/57662
2	1	0.62	0/69796	0.41	2/108888 (0.0%)
3	2	0.47	0/2872	0.40	0/4479
4	6	0.26	0/1832	0.36	0/2855
5	b	0.65	0/2122	0.63	0/2852
6	c	0.57	0/1586	0.60	0/2134
7	d	0.44	0/1571	0.58	0/2113
8	e	0.41	0/1435	0.67	2/1926 (0.1%)
9	f	0.35	0/1343	0.49	0/1816
10	g	0.30	0/1122	0.72	2/1515 (0.1%)
11	a	0.24	0/1033	0.57	0/1387
12	h	0.30	0/1002	0.83	0/1350
13	i	0.27	0/1046	0.63	0/1410
14	j	0.52	0/1152	0.52	2/1551 (0.1%)
15	k	0.61	0/948	0.71	2/1268 (0.2%)
16	l	0.54	0/1054	0.64	1/1403 (0.1%)
17	m	0.59	0/1093	0.64	2/1460 (0.1%)
18	n	0.57	0/974	0.67	0/1301
19	o	0.40	0/902	0.49	0/1209
20	p	0.56	0/929	0.63	0/1242
21	q	0.60	0/960	0.52	0/1278
22	r	0.47	0/829	0.60	0/1107
23	s	0.52	0/864	0.60	0/1156
24	t	0.42	0/745	0.51	0/994
25	u	0.39	0/788	0.69	2/1051 (0.2%)
26	v	0.43	0/766	0.47	0/1025
27	w	0.57	0/582	0.57	0/769
28	x	0.55	0/635	0.60	0/848
29	y	0.36	0/510	0.63	0/677
30	z	0.50	0/453	0.48	0/605
31	A	0.30	0/532	0.59	0/709
32	B	0.52	0/450	0.64	0/599
33	C	0.28	0/417	0.49	0/554
34	D	0.63	0/380	0.60	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	E	0.58	0/513	0.57	0/676
36	F	0.56	0/303	0.69	0/397
37	4	0.44	0/468	0.83	3/729 (0.4%)
38	5	0.45	0/1840	0.40	0/2868
39	G	0.39	0/1736	0.67	3/2338 (0.1%)
40	H	0.43	0/1652	0.53	0/2225
41	I	0.42	0/1665	0.65	0/2227
42	J	0.58	1/1170 (0.1%)	0.69	0/1573
43	K	0.40	0/836	0.73	4/1128 (0.4%)
44	L	0.39	0/1196	0.65	2/1602 (0.1%)
45	M	0.48	0/989	0.58	0/1326
46	N	0.39	0/1034	0.65	0/1375
47	O	0.43	0/797	0.77	1/1077 (0.1%)
48	P	0.51	0/886	0.76	3/1195 (0.3%)
49	Q	0.58	0/969	0.75	0/1300
50	R	0.43	0/893	0.67	0/1193
51	S	0.44	0/817	0.58	0/1088
52	T	0.48	0/722	0.60	0/964
53	U	0.46	0/659	0.63	0/884
54	V	0.45	0/658	0.59	0/881
55	W	0.47	0/545	0.74	0/731
56	X	0.39	0/653	0.55	0/877
57	Y	0.41	0/671	0.50	0/888
58	Z	0.42	0/551	1.22	9/728 (1.2%)
All	All	0.56	1/161909 (0.0%)	0.48	40/241961 (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
2	l	0	1
6	c	0	1
8	e	0	2
10	g	0	2
12	h	0	4
15	k	0	2
18	n	0	1
22	r	0	1
23	s	0	1
29	y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	A	0	1
35	E	0	1
36	F	0	1
39	G	0	2
41	I	0	2
42	J	0	2
47	O	0	1
48	P	0	2
50	R	0	1
51	S	0	1
54	V	0	2
55	W	0	1
58	Z	0	1
All	All	0	34

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	J	55	VAL	CA-CB	-7.56	1.50	1.54

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Z	7	GLU	CA-C-N	8.22	137.25	121.54
58	Z	7	GLU	C-N-CA	8.22	137.25	121.54
37	4	13	A	O4'-C1'-N9	7.90	120.35	108.50
17	m	69	PRO	CA-C-N	7.03	134.97	121.54
17	m	69	PRO	C-N-CA	7.03	134.97	121.54
37	4	13	A	C5'-C4'-O4'	6.52	119.58	109.80
10	g	8	LYS	CA-C-N	6.37	133.44	121.97
10	g	8	LYS	C-N-CA	6.37	133.44	121.97
16	l	29	LYS	N-CA-C	-6.34	97.28	110.80
25	u	97	SER	CA-C-N	6.34	133.65	121.54
25	u	97	SER	C-N-CA	6.34	133.65	121.54
58	Z	23	GLU	CA-C-N	6.23	133.44	121.54
58	Z	23	GLU	C-N-CA	6.23	133.44	121.54
48	P	119	GLY	CA-C-N	6.10	133.20	121.54
48	P	119	GLY	C-N-CA	6.10	133.20	121.54
2	1	2572	A	P-O3'-C3'	6.05	129.27	120.20
58	Z	35	GLU	CA-C-N	5.95	132.90	121.54
58	Z	35	GLU	C-N-CA	5.95	132.90	121.54
47	O	34	ALA	N-CA-C	5.94	117.55	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	17	HIS	CA-C-N	5.94	132.88	121.54
39	G	17	HIS	C-N-CA	5.94	132.88	121.54
8	e	175	PRO	CA-C-N	5.86	132.74	121.54
8	e	175	PRO	C-N-CA	5.86	132.74	121.54
43	K	92	THR	CA-C-N	5.84	136.03	126.86
43	K	92	THR	C-N-CA	5.84	136.03	126.86
58	Z	31	VAL	N-CA-C	-5.78	106.77	111.91
58	Z	64	ALA	CA-C-N	5.47	131.98	121.54
58	Z	64	ALA	C-N-CA	5.47	131.98	121.54
39	G	19	THR	N-CA-CB	5.43	119.67	110.49
15	k	107	LEU	CA-C-N	5.43	131.90	121.54
15	k	107	LEU	C-N-CA	5.43	131.90	121.54
43	K	91	ARG	CA-C-N	5.40	131.86	121.54
43	K	91	ARG	C-N-CA	5.40	131.86	121.54
2	1	2572	A	C2'-C3'-O3'	5.32	117.48	109.50
48	P	125	LYS	N-CA-C	5.24	116.86	110.41
37	4	13	A	C1'-O4'-C4'	-5.22	104.68	109.90
44	L	128	GLU	CA-C-N	5.15	131.37	121.54
44	L	128	GLU	C-N-CA	5.15	131.37	121.54
14	j	80	HIS	CA-C-N	5.05	128.90	120.62
14	j	80	HIS	C-N-CA	5.05	128.90	120.62

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	2166	U	Sidechain
31	A	29	GLY	Peptide
35	E	30	HIS	Peptide
36	F	36	ARG	Peptide
39	G	18	GLN	Peptide
39	G	21	TYR	Peptide
41	I	151	GLN	Peptide
41	I	190	LEU	Peptide
42	J	101	GLY	Peptide
42	J	158	LYS	Peptide
47	O	34	ALA	Peptide
48	P	118	ASN	Peptide
48	P	124	LYS	Peptide
50	R	8	ILE	Peptide
51	S	33	VAL	Peptide
54	V	16	MET	Peptide

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Mol	Chain	Res	Type	Group
54	V	49	ASN	Peptide
55	W	19	GLU	Peptide
58	Z	63	ASN	Peptide
6	c	159	LYS	Peptide
8	e	174	PHE	Peptide
8	e	175	PRO	Peptide
10	g	51	ARG	Peptide
10	g	8	LYS	Peptide
12	h	105	LYS	Peptide
12	h	118	ILE	Peptide
12	h	122	GLN	Peptide
12	h	80	THR	Peptide
15	k	91	SER	Peptide
15	k	93	GLN	Peptide
18	n	10	LEU	Peptide
22	r	53	PHE	Peptide
23	s	8	ARG	Peptide
29	y	23	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	33012	0	16618	123	0
2	1	62317	0	31346	238	0
3	2	2568	0	1303	11	0
4	6	1640	0	837	9	0
5	b	2083	0	2157	23	0
6	c	1565	0	1616	21	0
7	d	1552	0	1619	19	0
8	e	1411	0	1447	32	0
9	f	1323	0	1374	16	0
10	g	1111	0	1148	19	0
11	a	1026	0	1092	16	0
12	h	989	0	1025	34	0
13	i	1032	0	1088	25	0
14	j	1129	0	1162	20	0
15	k	939	0	1012	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	l	1045	0	1117	21	0
17	m	1074	0	1157	6	0
18	n	961	0	1000	13	0
19	o	892	0	923	18	0
20	p	917	0	965	17	0
21	q	947	0	1022	17	0
22	r	816	0	839	11	0
23	s	857	0	922	8	0
24	t	739	0	807	14	0
25	u	780	0	834	8	0
26	v	753	0	780	14	0
27	w	575	0	592	5	0
28	x	625	0	655	11	0
29	y	509	0	543	11	0
30	z	449	0	491	5	0
31	A	523	0	522	5	0
32	B	444	0	461	8	0
33	C	410	0	440	5	0
34	D	377	0	418	6	0
35	E	504	0	574	8	0
36	F	302	0	340	9	0
37	4	416	0	208	5	0
38	5	1647	0	832	12	0
39	G	1705	0	1732	23	0
40	H	1625	0	1699	21	0
41	I	1643	0	1710	39	0
42	J	1157	0	1199	22	0
43	K	818	0	808	6	0
44	L	1182	0	1240	13	0
45	M	979	0	1034	13	0
46	N	1022	0	1070	22	0
47	O	787	0	828	16	0
48	P	870	0	878	13	0
49	Q	955	0	1019	22	0
50	R	884	0	944	14	0
51	S	805	0	847	10	0
52	T	714	0	737	6	0
53	U	649	0	666	10	0
54	V	649	0	691	10	0
55	W	536	0	552	5	0
56	X	638	0	665	8	0
57	Y	665	0	714	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	Z	545	0	579	11	0
All	All	149087	0	100898	948	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 (948) 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)
2:1:2166:U:H2'	2:1:2167:U:H5'	1.45	0.98
1:3:664:G:H22	1:3:741:G:H1	1.32	0.74
2:1:1652:A:H62	18:n:11:ASN:HD21	1.37	0.73
14:j:31:GLU:HG2	14:j:142:ILE:HG12	1.70	0.73
2:1:1936:A:H2	2:1:1943:U:H3	1.37	0.72
22:r:58:VAL:H	22:r:102:SER:HB3	1.55	0.72
19:o:7:ARG:HA	19:o:10:ARG:HE	1.55	0.71
12:h:117:LEU:HG	12:h:118:ILE:HG13	1.73	0.70
16:l:102:GLY:H	16:l:105:ILE:HD12	1.56	0.70
2:1:636:G:HO2'	2:1:638:G:HO2'	1.38	0.69
2:1:585:G:N7	21:q:5:ARG:NH1	2.41	0.68
1:3:38:G:H22	1:3:397:A:H5'	1.60	0.67
1:3:1534:A:N6	37:4:13:A:N7	2.42	0.67
39:G:91:VAL:HG21	39:G:95:TRP:HD1	1.58	0.67
2:1:2683:C:OP1	20:p:50:ARG:NH2	2.28	0.66
1:3:310:G:H5''	53:U:31:ARG:HB2	1.77	0.65
46:N:91:GLU:HA	46:N:94:ARG:HB2	1.79	0.65
15:k:110:GLU:H	15:k:113:MET:HE2	1.63	0.64
43:K:92:THR:OG1	43:K:93:LYS:N	2.31	0.64
2:1:1798:U:OP2	5:b:270:ARG:NH2	2.29	0.64
4:6:34:C:H42	37:4:18:G:H1	1.45	0.64
39:G:16:GLY:HA3	39:G:39:ILE:HA	1.80	0.64
1:3:437:U:O2	41:I:119:HIS:NE2	2.30	0.64
44:L:110:ARG:HB3	44:L:118:ARG:HG2	1.80	0.64
46:N:50:PRO:HD3	46:N:79:ARG:HG3	1.80	0.63
2:1:2032:G:N2	6:c:151:THR:OG1	2.31	0.63
2:1:2720:U:H5''	20:p:52:ARG:HH22	1.64	0.63
11:a:178:VAL:HG21	11:a:216:THR:HG23	1.81	0.63
1:3:1305:G:N2	1:3:1331:G:O2'	2.30	0.62
2:1:1055:G:H4'	12:h:33:VAL:HA	1.81	0.62
2:1:2530:A:N7	9:f:171:LYS:NZ	2.47	0.62
2:1:1365:A:OP1	28:x:2:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:F:11:CYS:SG	36:F:14:CYS:N	2.71	0.62
2:1:2165:C:H2'	2:1:2166:U:C2	2.35	0.62
13:i:55:PRO:HD3	13:i:74:PRO:HD3	1.82	0.62
42:J:110:MET:HG3	42:J:139:THR:HG21	1.82	0.62
2:1:2529:G:H4'	9:f:174:LYS:HG3	1.81	0.62
41:I:32:LYS:HB3	41:I:35:GLN:HE21	1.65	0.62
42:J:114:LEU:HD13	42:J:122:VAL:HG21	1.82	0.62
56:X:18:VAL:HG21	56:X:43:MET:HG2	1.82	0.62
8:e:3:LEU:HD13	8:e:100:GLU:HB3	1.82	0.61
1:3:501:C:OP1	49:Q:113:ARG:NH2	2.33	0.61
9:f:83:THR:HG22	9:f:133:LYS:HG2	1.81	0.61
11:a:8:MET:HA	11:a:11:ILE:HB	1.82	0.61
1:3:413:G:O2'	1:3:428:G:N2	2.33	0.61
1:3:1307:U:H5''	50:R:99:GLN:HE22	1.66	0.61
2:1:2305:U:H5''	8:e:130:GLY:HA3	1.81	0.61
2:1:1072:C:H41	2:1:1097:U:H5''	1.66	0.61
29:y:24:GLU:HA	29:y:27:ASN:HB2	1.81	0.61
31:A:37:CYS:H	31:A:40:CYS:HB3	1.66	0.60
42:J:12:GLU:OE2	42:J:67:ARG:NH2	2.35	0.60
51:S:36:SER:HA	51:S:40:ARG:HE	1.65	0.60
1:3:910:C:OP2	49:Q:17:LYS:NZ	2.34	0.60
53:U:4:ILE:HG12	53:U:21:VAL:HG22	1.83	0.60
16:l:2:ARG:O	16:l:2:ARG:NH1	2.35	0.60
16:l:75:ALA:HB2	16:l:105:ILE:HD13	1.83	0.60
41:I:8:LEU:HD21	41:I:31:CYS:HB2	1.83	0.60
41:I:120:LYS:HE2	41:I:130:ASN:HD21	1.67	0.59
2:1:1270:C:H5''	2:1:1271:G:H5'	1.83	0.59
2:1:309:A:N3	2:1:329:G:O2'	2.34	0.59
2:1:2144:G:N2	2:1:2146:C:O2'	2.35	0.59
15:k:17:ARG:HH21	15:k:47:ILE:HG22	1.67	0.59
17:m:20:LEU:HD13	26:v:81:PRO:HG2	1.84	0.59
42:J:93:VAL:HG11	42:J:139:THR:HG22	1.82	0.59
57:Y:47:GLN:O	57:Y:51:ASN:ND2	2.36	0.59
1:3:1086:U:H3	1:3:1099:G:H22	1.49	0.59
2:1:1478:G:H1	2:1:1513:U:H3	1.51	0.59
1:3:687:A:N6	1:3:703:G:O2'	2.36	0.59
1:3:1193:G:O6	40:H:2:GLN:NE2	2.36	0.59
20:p:59:THR:HB	20:p:72:VAL:HG22	1.85	0.59
1:3:890:G:O2'	1:3:906:A:N6	2.36	0.59
2:1:2002:G:OP1	18:n:17:ARG:NH2	2.36	0.59
36:F:11:CYS:N	36:F:14:CYS:SG	2.74	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1009:A:OP2	14:j:39:LYS:NZ	2.34	0.59
1:3:693:G:OP1	48:P:126:ARG:NH2	2.35	0.58
1:3:880:C:OP1	49:Q:8:ARG:NH2	2.36	0.58
1:3:1005:A:N6	1:3:1024:G:O2'	2.36	0.58
2:1:1715:G:N2	2:1:1744:A:OP2	2.34	0.58
56:X:10:ILE:HD12	56:X:37:SER:HB2	1.85	0.58
2:1:1816:C:N4	5:b:34:GLU:OE2	2.35	0.58
41:I:99:ASN:OD1	41:I:110:ARG:NH1	2.35	0.58
2:1:886:A:O2'	2:1:890:C:N4	2.37	0.58
2:1:2170:A:O5'	2:1:2170:A:H8	1.86	0.58
13:i:72:THR:HG22	13:i:116:MET:HE3	1.85	0.58
15:k:121:GLU:HG2	15:k:122:VAL:HG23	1.85	0.58
39:G:116:LEU:HB3	39:G:140:LEU:HD12	1.86	0.58
42:J:64:GLU:OE2	42:J:67:ARG:NH1	2.36	0.58
19:o:43:ASN:ND2	19:o:45:SER:OG	2.37	0.58
21:q:65:ASN:OD1	21:q:69:ARG:NH2	2.35	0.58
41:I:104:MET:HG2	41:I:170:LEU:HD13	1.85	0.58
2:1:495:G:N3	23:s:61:ASN:ND2	2.48	0.58
24:t:28:ASN:ND2	24:t:88:LYS:O	2.36	0.58
15:k:65:THR:HG23	15:k:68:GLY:H	1.69	0.58
34:D:24:THR:HG23	34:D:27:GLY:H	1.68	0.58
2:1:1082:U:H5'	13:i:118:GLY:HA2	1.86	0.57
1:3:1340:A:HO2'	38:5:31:G:HO2'	1.50	0.57
42:J:100:GLU:OE2	42:J:102:THR:OG1	2.23	0.57
2:1:2137:U:H2'	2:1:2138:G:H8	1.69	0.57
6:c:179:ARG:HB3	6:c:188:LEU:HD12	1.86	0.57
54:V:8:GLN:HG2	54:V:59:GLU:HG3	1.85	0.57
2:1:244:A:OP2	35:E:7:ARG:NH2	2.38	0.57
7:d:119:ILE:HB	7:d:187:VAL:HG12	1.87	0.57
1:3:1005:A:OP2	1:3:1024:G:N2	2.36	0.57
2:1:1326:U:HO2'	2:1:2010:G:HO2'	1.52	0.57
29:y:49:ASP:OD1	29:y:52:ARG:NH2	2.38	0.57
40:H:109:GLU:HB2	40:H:143:LEU:HD22	1.87	0.57
7:d:45:ALA:HB2	7:d:89:PRO:HD3	1.85	0.57
7:d:87:ALA:O	7:d:88:ARG:NH2	2.36	0.57
12:h:8:LYS:HG2	12:h:11:ILE:HD12	1.85	0.57
40:H:35:ASP:OD1	40:H:58:ARG:NH2	2.37	0.57
41:I:201:GLU:OE2	42:J:111:ARG:NH1	2.37	0.57
16:l:81:ASP:OD1	16:l:81:ASP:N	2.34	0.57
21:q:71:ASN:HD21	21:q:106:THR:HG22	1.69	0.57
1:3:1535:C:N4	37:4:9:G:O6	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:y:16:THR:HA	29:y:19:LEU:HD22	1.87	0.57
39:G:224:ARG:NH2	39:G:225:SER:OG	2.37	0.57
41:I:25:ARG:HH12	41:I:27:ILE:HG22	1.70	0.57
44:L:149:ALA:HB1	48:P:58:THR:HG21	1.85	0.57
57:Y:66:ILE:HD12	57:Y:70:LYS:HD3	1.86	0.57
4:6:50:U:H3	4:6:64:G:H1	1.51	0.57
8:e:147:ARG:HB3	8:e:149:ARG:HE	1.70	0.57
12:h:15:VAL:HG11	12:h:69:PHE:HB2	1.87	0.56
19:o:40:ILE:HG12	19:o:47:VAL:HG12	1.86	0.56
1:3:1492:A:O4'	2:1:1913:A:N6	2.37	0.56
47:O:47:GLU:OE1	51:S:75:LYS:NZ	2.38	0.56
1:3:1178:G:N2	1:3:1181:G:OP2	2.38	0.56
2:1:284:U:H3	2:1:356:G:H1	1.53	0.56
2:1:1980:G:O2'	2:1:1982:U:OP2	2.23	0.56
41:I:36:ALA:HA	41:I:41:GLY:HA3	1.86	0.56
2:1:340:A:O2'	7:d:162:ARG:NH1	2.38	0.56
30:z:15:ARG:HE	30:z:52:PHE:HE2	1.52	0.56
2:1:1072:C:N4	2:1:1098:A:OP2	2.38	0.56
9:f:27:GLY:HA3	9:f:78:VAL:HB	1.88	0.56
39:G:124:THR:HA	39:G:127:LYS:HD3	1.86	0.56
2:1:1056:G:N1	2:1:1102:C:OP2	2.39	0.56
1:3:689:C:OP2	48:P:52:ARG:NH2	2.34	0.56
1:3:1279:G:OP1	47:O:9:ARG:NH2	2.36	0.56
2:1:563:A:OP2	22:r:79:ARG:NH2	2.36	0.56
2:1:781:A:OP1	5:b:216:ARG:NH2	2.39	0.56
16:l:110:VAL:HB	16:l:127:VAL:HG23	1.87	0.56
29:y:16:THR:O	29:y:20:ASN:ND2	2.39	0.56
13:i:57:VAL:HB	13:i:69:VAL:HB	1.88	0.56
2:1:2680:U:H5'	6:c:194:PRO:HA	1.88	0.55
1:3:933:G:O6	44:L:2:ARG:NH2	2.39	0.55
2:1:1080:A:N3	13:i:127:SER:OG	2.40	0.55
28:x:71:ARG:NH2	28:x:77:TYR:OH	2.35	0.55
1:3:8:A:N6	41:I:201:GLU:O	2.36	0.55
1:3:490:C:OP1	41:I:145:ARG:NH2	2.39	0.55
13:i:85:ILE:HD12	13:i:97:VAL:HG12	1.87	0.55
1:3:255:G:OP1	54:V:70:LYS:NZ	2.39	0.55
52:T:17:ASP:N	52:T:17:ASP:OD1	2.37	0.55
1:3:105:G:OP2	57:Y:12:GLN:NE2	2.40	0.55
2:1:2788:C:O2'	2:1:2809:A:N3	2.38	0.55
2:1:2811:G:OP1	6:c:61:THR:OG1	2.24	0.55
8:e:116:LEU:O	8:e:177:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:346:G:OP1	20:p:38:ARG:NH1	2.37	0.55
2:1:948:C:O2	2:1:984:A:O2'	2.24	0.55
11:a:196:LEU:HB3	11:a:208:TYR:HE2	1.71	0.55
14:j:45:THR:HG22	21:q:63:ARG:HH21	1.71	0.55
39:G:70:GLY:HA3	39:G:163:ILE:HG12	1.88	0.55
2:1:2387:U:OP1	27:w:51:ARG:NH1	2.40	0.55
11:a:165:ASN:ND2	11:a:166:ASP:O	2.40	0.55
2:1:1063:G:H1	2:1:1075:C:H42	1.55	0.55
2:1:1070:A:N6	2:1:1096:A:O2'	2.40	0.55
42:J:13:LYS:HG2	42:J:112:ALA:HB1	1.89	0.55
42:J:56:PRO:HA	42:J:59:ILE:HG12	1.89	0.55
45:M:88:LYS:HE2	45:M:119:GLY:HA2	1.87	0.55
2:1:1055:G:H5''	12:h:33:VAL:HG12	1.89	0.55
5:b:144:GLU:HB2	5:b:187:CYS:HB3	1.87	0.55
6:c:77:ARG:NH2	6:c:200:ASP:OD1	2.40	0.55
8:e:34:THR:HG23	8:e:154:THR:HG23	1.88	0.55
10:g:9:VAL:HG23	10:g:11:ASN:H	1.72	0.55
45:M:17:GLN:HG2	45:M:62:LEU:HD13	1.89	0.55
2:1:2469:A:N6	2:1:2481:G:O2'	2.40	0.54
5:b:106:PRO:HD2	5:b:109:LEU:HD22	1.88	0.54
37:4:11:U:H3'	37:4:12:A:H4'	1.89	0.54
48:P:71:ASP:HA	48:P:74:LYS:HG3	1.90	0.54
2:1:566:U:OP1	16:l:29:LYS:NZ	2.39	0.54
40:H:152:VAL:HG12	40:H:197:VAL:HG22	1.89	0.54
47:O:71:LEU:O	47:O:72:ARG:NH1	2.36	0.54
1:3:521:G:OP2	49:Q:50:LYS:NZ	2.39	0.54
10:g:99:ILE:HD11	10:g:144:VAL:HG21	1.88	0.54
26:v:80:HIS:HD2	26:v:83:LYS:H	1.56	0.54
2:1:1068:G:N2	2:1:1095:A:O2'	2.40	0.54
6:c:5:VAL:H	6:c:32:ASN:HD21	1.56	0.54
41:I:187:ARG:O	41:I:187:ARG:NH1	2.36	0.54
48:P:125:LYS:HB3	48:P:126:ARG:HG3	1.89	0.54
2:1:1019:U:H3	2:1:1142:A:H62	1.55	0.54
2:1:1844:C:O3'	5:b:255:LYS:NZ	2.40	0.54
28:x:73:ARG:HH21	28:x:75:GLU:HG3	1.72	0.54
2:1:370:G:O2'	2:1:424:G:OP1	2.25	0.54
2:1:1086:A:H1'	2:1:1103:A:H61	1.72	0.54
50:R:53:ASP:OD1	50:R:53:ASP:N	2.40	0.54
7:d:143:LEU:HD22	7:d:185:LYS:HG3	1.89	0.54
48:P:112:VAL:HG12	55:W:72:ARG:HD2	1.88	0.54
2:1:2749:A:OP1	9:f:1:SER:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:g:61:VAL:O	10:g:65:ALA:N	2.41	0.54
1:3:203:G:O2'	1:3:465:A:N1	2.41	0.53
2:1:270:A:N1	2:1:369:U:O2'	2.36	0.53
2:1:1858:A:N6	2:1:1884:G:O2'	2.41	0.53
2:1:2166:U:C2'	2:1:2167:U:H5'	2.27	0.53
7:d:125:SER:O	7:d:137:LYS:NZ	2.40	0.53
2:1:1059:G:O2'	13:i:116:MET:SD	2.62	0.53
8:e:62:GLN:NE2	8:e:89:THR:O	2.40	0.53
10:g:4:ILE:HG22	10:g:18:GLN:HB3	1.90	0.53
24:t:36:LYS:NZ	24:t:79:ASP:OD2	2.42	0.53
41:l:11:SER:OG	41:l:16:THR:O	2.26	0.53
15:k:71:ARG:HH22	15:k:105:ARG:HG3	1.73	0.53
46:N:34:LEU:HD11	46:N:47:VAL:HG21	1.90	0.53
2:1:1080:A:H1'	13:i:127:SER:HA	1.90	0.53
19:o:94:ARG:NH2	19:o:97:PHE:O	2.41	0.53
28:x:17:ARG:HE	28:x:23:ALA:HB2	1.74	0.53
46:N:30:ASN:HD21	46:N:66:VAL:H	1.57	0.53
2:1:807:U:OP2	16:l:41:ARG:NH1	2.40	0.53
11:a:11:ILE:HG23	11:a:33:LEU:HD22	1.91	0.53
38:5:21:A:N6	38:5:47:U:O2'	2.42	0.53
54:V:67:SER:OG	54:V:68:LYS:N	2.41	0.53
5:b:48:ILE:HD11	5:b:51:ARG:HA	1.89	0.53
8:e:79:ARG:NH1	38:5:19:G:O6	2.42	0.53
46:N:31:GLN:NE2	46:N:63:TYR:OH	2.42	0.53
51:S:38:GLU:O	51:S:42:ASN:ND2	2.42	0.53
2:1:1136:G:HO2'	2:1:2038:G:HO2'	1.55	0.53
4:6:51:C:H2'	4:6:52:G:H8	1.73	0.53
9:f:104:LEU:HB2	9:f:112:VAL:HG23	1.90	0.53
44:L:78:ARG:HB3	44:L:83:THR:HB	1.90	0.53
45:M:89:ASP:OD1	45:M:89:ASP:N	2.35	0.53
14:j:49:ASP:OD1	14:j:121:LYS:NZ	2.42	0.53
17:m:66:ARG:NH1	17:m:104:GLU:OE2	2.42	0.53
46:N:55:ASP:OD1	46:N:55:ASP:N	2.40	0.53
2:1:1057:A:H1'	12:h:34:THR:HG21	1.89	0.52
2:1:2539:C:H5'	36:F:3:VAL:HG11	1.90	0.52
6:c:61:THR:HG23	6:c:63:PRO:HD2	1.90	0.52
10:g:66:ASN:O	10:g:70:GLU:N	2.42	0.52
1:3:677:U:H3	1:3:713:G:H22	1.57	0.52
1:3:1038:C:H2'	1:3:1039:G:H8	1.74	0.52
2:1:1223:G:OP1	22:r:68:ARG:NH2	2.43	0.52
2:1:2619:C:OP1	6:c:157:LYS:NZ	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:2831:G:OP2	6:c:59:ARG:NH1	2.40	0.52
3:2:54:G:H21	8:e:25:MET:HE3	1.74	0.52
15:k:80:ASP:OD2	20:p:61:ARG:NH1	2.39	0.52
31:A:44:PHE:HD2	31:A:45:THR:HG23	1.74	0.52
1:3:560:A:H8	1:3:560:A:H5''	1.74	0.52
2:1:572:A:OP2	22:r:80:ARG:NH2	2.42	0.52
12:h:102:ALA:HA	12:h:105:LYS:HB3	1.91	0.52
31:A:58:ASP:OD1	31:A:58:ASP:N	2.40	0.52
34:D:31:LEU:HG	34:D:42:LEU:HD21	1.92	0.52
40:H:30:ASP:OD1	40:H:30:ASP:N	2.43	0.52
55:W:10:CYS:SG	55:W:11:ARG:N	2.76	0.52
2:1:1045:C:O2'	12:h:61:ARG:NH1	2.43	0.52
47:O:12:ALA:HB2	47:O:96:VAL:HG23	1.90	0.52
8:e:98:PHE:HD1	8:e:101:ARG:HH11	1.58	0.52
11:a:189:LEU:HD13	11:a:224:VAL:HG11	1.90	0.52
12:h:53:ARG:NE	12:h:86:MET:SD	2.83	0.52
11:a:200:LYS:HD2	11:a:201:PRO:HD2	1.92	0.52
1:3:1025:U:H5''	1:3:1026:G:H5'	1.92	0.52
15:k:7:MET:HE2	15:k:44:LYS:HG3	1.92	0.52
13:i:61:TYR:HB2	13:i:65:SER:HB2	1.91	0.52
44:L:15:PRO:HA	46:N:45:MET:HE3	1.92	0.52
2:1:1091:G:N2	2:1:1100:C:O2	2.39	0.51
2:1:1153:C:OP1	21:q:91:ARG:NH2	2.34	0.51
2:1:1203:U:O2'	16:l:4:ASN:ND2	2.39	0.51
2:1:1800:C:H5'	5:b:145:MET:HE1	1.92	0.51
58:Z:39:LYS:HA	58:Z:42:THR:HG22	1.91	0.51
2:1:1012:U:OP2	21:q:69:ARG:NH1	2.42	0.51
2:1:1217:U:OP2	21:q:14:LYS:NZ	2.43	0.51
19:o:15:ARG:NH2	19:o:95:SER:OG	2.43	0.51
45:M:73:SER:OG	45:M:129:ALA:O	2.25	0.51
2:1:13:A:O2'	2:1:15:G:N7	2.36	0.51
47:O:14:ASP:OD1	47:O:14:ASP:N	2.42	0.51
6:c:106:LYS:HD3	6:c:174:SER:HB3	1.93	0.51
13:i:7:TYR:HE1	13:i:57:VAL:HG13	1.76	0.51
7:d:176:ASP:OD1	7:d:176:ASP:N	2.42	0.51
10:g:96:THR:HG23	10:g:112:LYS:HD2	1.93	0.51
38:5:1:C:N4	38:5:2:G:O6	2.43	0.51
1:3:126:G:OP1	1:3:605:U:O2'	2.26	0.51
1:3:1347:G:O6	46:N:11:ARG:NH2	2.42	0.51
2:1:1251:C:OP2	21:q:5:ARG:NH2	2.42	0.51
12:h:18:VAL:HG13	12:h:70:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:i:52:LEU:HD12	13:i:53:PRO:HD2	1.93	0.51
26:v:1:MET:HE1	26:v:59:GLU:HG2	1.92	0.51
37:4:12:A:H3'	37:4:13:A:H5''	1.93	0.51
46:N:35:GLU:HA	46:N:39:GLY:HA3	1.92	0.51
1:3:538:G:H5'	49:Q:110:LYS:HB2	1.92	0.51
2:1:500:G:N1	2:1:503:A:OP2	2.43	0.51
11:a:201:PRO:HG2	11:a:204:ALA:HB2	1.91	0.51
13:i:99:LYS:HB3	13:i:138:VAL:HB	1.93	0.51
41:I:97:LEU:HA	41:I:100:VAL:HB	1.92	0.51
1:3:261:U:OP2	57:Y:73:ARG:NH2	2.40	0.51
1:3:1119:C:OP1	46:N:84:ARG:NH2	2.43	0.51
2:1:2314:A:OP1	8:e:87:LYS:NZ	2.39	0.51
10:g:63:ALA:HB1	10:g:135:HIS:HE1	1.75	0.51
48:P:51:PHE:HE2	48:P:64:VAL:HG11	1.75	0.51
1:3:7:A:H2'	42:J:123:LEU:HD22	1.93	0.51
2:1:517:C:OP1	32:B:12:ARG:NH2	2.44	0.51
2:1:1057:A:O2'	12:h:34:THR:OG1	2.23	0.51
8:e:73:VAL:HG12	8:e:76:PHE:H	1.76	0.51
42:J:79:THR:OG1	42:J:97:PRO:O	2.26	0.51
1:3:422:C:O2'	1:3:423:G:N2	2.44	0.50
1:3:1539:C:O2'	58:Z:17:ARG:NH2	2.44	0.50
12:h:28:ALA:HB3	12:h:111:ALA:HB2	1.93	0.50
26:v:45:ASP:OD1	26:v:45:ASP:N	2.42	0.50
29:y:51:ALA:O	29:y:55:THR:OG1	2.28	0.50
50:R:78:ARG:NH1	56:X:64:GLU:OE2	2.42	0.50
1:3:927:G:O2'	1:3:1503:A:N7	2.39	0.50
1:3:1266:G:N2	1:3:1269:A:OP2	2.40	0.50
1:3:1538:C:O2	58:Z:20:ARG:NH2	2.44	0.50
22:r:1:MET:HE2	22:r:43:ASN:HD22	1.76	0.50
39:G:82:ALA:HB2	39:G:213:LEU:HD13	1.93	0.50
2:1:1266:G:O2'	2:1:2012:G:O6	2.26	0.50
46:N:112:ARG:NH2	47:O:64:GLN:OE1	2.44	0.50
49:Q:49:ARG:HG3	49:Q:89:LEU:HD21	1.93	0.50
3:2:30:C:H1'	3:2:57:A:H61	1.77	0.50
18:n:114:GLU:OE1	18:n:118:ARG:NH2	2.44	0.50
25:u:39:ASN:HB3	25:u:62:ALA:HB3	1.93	0.50
26:v:77:VAL:HG12	26:v:89:ILE:HG12	1.92	0.50
26:v:80:HIS:CD2	26:v:83:LYS:H	2.30	0.50
53:U:46:LYS:HG3	53:U:47:GLU:H	1.75	0.50
2:1:2419:U:OP1	35:E:40:LYS:NZ	2.40	0.50
2:1:2576:G:O2'	2:1:2579:C:OP2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:f:23:ILE:HD13	9:f:36:LEU:HG	1.92	0.50
18:n:69:ARG:O	18:n:71:ARG:N	2.44	0.50
33:C:7:LYS:HA	33:C:23:THR:HA	1.93	0.50
40:H:56:ILE:HG12	40:H:65:VAL:HG12	1.94	0.50
2:1:560:C:O2'	21:q:47:ARG:NH2	2.45	0.50
2:1:647:G:N2	2:1:2350:C:O2'	2.41	0.50
14:j:125:TYR:OH	14:j:132:HIS:NE2	2.40	0.50
32:B:27:LEU:HD23	32:B:36:LYS:HB3	1.93	0.50
1:3:544:G:OP1	41:I:55:ARG:NH2	2.42	0.50
9:f:59:ASP:HB2	9:f:62:ALA:HB3	1.94	0.50
9:f:136:ASP:HB3	9:f:139:VAL:HG12	1.93	0.50
10:g:132:PHE:O	10:g:140:ALA:N	2.41	0.50
23:s:18:ARG:NH1	23:s:76:VAL:O	2.45	0.50
1:3:36:C:H5''	49:Q:119:LYS:HG2	1.94	0.50
1:3:401:C:O2'	1:3:621:A:N3	2.42	0.50
1:3:1144:G:H21	1:3:1146:A:H62	1.59	0.50
2:1:1857:G:O2'	2:1:1885:A:N6	2.44	0.50
10:g:17:ASP:OD1	10:g:17:ASP:N	2.43	0.50
11:a:49:GLY:N	11:a:208:TYR:O	2.45	0.50
2:1:2683:C:O2	15:k:70:ARG:NH2	2.39	0.50
5:b:36:ASN:HB2	5:b:61:TYR:HB2	1.94	0.50
24:t:8:LEU:O	29:y:29:ARG:NH1	2.42	0.50
29:y:1:MET:HA	29:y:4:LYS:HE2	1.94	0.50
43:K:38:ARG:HB3	43:K:63:ASN:HB2	1.93	0.50
50:R:78:ARG:HH22	56:X:68:HIS:HE1	1.60	0.50
1:3:754:C:H5'	52:T:71:ARG:HH22	1.77	0.49
2:1:636:G:H5''	16:l:128:THR:HB	1.93	0.49
45:M:42:GLU:HG2	45:M:100:ILE:HD13	1.92	0.49
2:1:335:C:O2	25:u:67:SER:OG	2.31	0.49
42:J:155:LYS:O	45:M:63:LYS:NZ	2.45	0.49
2:1:788:A:OP1	2:1:791:C:N4	2.38	0.49
5:b:44:ASN:OD1	5:b:44:ASN:N	2.45	0.49
2:1:886:A:H1'	2:1:890:C:H41	1.77	0.49
2:1:2420:C:OP1	33:C:7:LYS:NZ	2.45	0.49
2:1:2532:G:O2'	2:1:2657:A:N1	2.45	0.49
16:l:109:LYS:HE2	16:l:128:THR:HG22	1.93	0.49
41:I:69:ARG:HG2	41:I:72:ARG:HH21	1.78	0.49
24:t:13:ALA:HB3	24:t:33:LYS:HD3	1.95	0.49
26:v:75:GLN:HB2	26:v:92:VAL:HG23	1.95	0.49
33:C:28:THR:HG23	33:C:29:LYS:HG2	1.95	0.49
36:F:36:ARG:NH2	36:F:37:GLN:OE1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:I:120:LYS:HG3	41:I:128:VAL:HG11	1.94	0.49
2:1:2255:G:O2'	38:5:3:G:OP1	2.30	0.49
2:1:2840:C:H5''	18:n:53:THR:HG21	1.94	0.49
41:I:108:ALA:N	41:I:112:GLU:OE1	2.43	0.49
1:3:944:G:N1	1:3:1338:G:OP2	2.40	0.49
2:1:752:A:OP1	34:D:3:ARG:NH1	2.44	0.49
3:2:48:U:H4'	19:o:100:HIS:HD2	1.77	0.49
1:3:1405:G:H21	1:3:1518:A:H8	1.61	0.49
2:1:2638:G:O2'	2:1:2775:G:N2	2.44	0.49
3:2:40:U:N3	3:2:44:G:OP2	2.40	0.49
7:d:106:LYS:HG3	7:d:200:LEU:HD13	1.93	0.49
48:P:17:ASP:OD2	48:P:36:ARG:NH2	2.41	0.49
53:U:20:VAL:HG23	53:U:35:ARG:HA	1.95	0.49
2:1:483:A:O2'	25:u:56:GLY:N	2.46	0.49
2:1:1171:G:N2	2:1:1178:C:N3	2.57	0.49
12:h:15:VAL:HA	12:h:18:VAL:HG12	1.95	0.49
18:n:56:LYS:NZ	18:n:94:TYR:OH	2.46	0.49
28:x:39:VAL:HG22	28:x:42:GLU:H	1.78	0.49
52:T:1:SER:OG	52:T:2:LEU:N	2.45	0.49
2:1:2418:A:OP1	35:E:44:ARG:NH1	2.39	0.48
41:I:187:ARG:HH22	41:I:192:ALA:HA	1.78	0.48
51:S:22:LYS:HD2	51:S:23:ARG:HG3	1.93	0.48
1:3:1255:G:OP2	47:O:45:ARG:NH2	2.45	0.48
2:1:476:G:N1	2:1:479:A:OP2	2.44	0.48
39:G:76:SER:HB2	39:G:92:ASN:HB2	1.95	0.48
41:I:141:VAL:HA	41:I:180:THR:HA	1.94	0.48
44:L:112:ASP:HB2	44:L:118:ARG:HG3	1.94	0.48
2:1:2204:G:OP2	5:b:146:LYS:NZ	2.39	0.48
6:c:60:VAL:HG23	6:c:64:GLU:HG3	1.95	0.48
12:h:61:ARG:HA	12:h:64:VAL:HB	1.95	0.48
14:j:32:LEU:HD22	14:j:54:ILE:HG21	1.94	0.48
19:o:67:ASN:ND2	19:o:69:ASP:OD1	2.45	0.48
26:v:64:VAL:HG12	26:v:69:GLU:HG3	1.94	0.48
27:w:55:LEU:HD12	27:w:76:ILE:HD12	1.95	0.48
43:K:5:GLU:HB3	43:K:90:MET:HB2	1.95	0.48
2:1:2141:G:H1	2:1:2151:U:H3	1.59	0.48
1:3:427:U:O2'	1:3:541:G:OP1	2.32	0.48
1:3:1073:U:O2	39:G:102:ASN:ND2	2.43	0.48
6:c:181:ASP:HB3	6:c:186:LEU:HB2	1.96	0.48
12:h:14:GLU:HA	12:h:53:ARG:HH12	1.79	0.48
18:n:86:ARG:NH1	18:n:117:ASP:OD2	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:96:ASP:OD2	22:r:13:ARG:NE	2.40	0.48
1:3:586:C:O2'	45:M:3:GLN:NE2	2.46	0.48
9:f:17:LYS:HB2	9:f:24:THR:HB	1.94	0.48
13:i:89:SER:HB3	13:i:92:PRO:HD3	1.94	0.48
23:s:108:SER:OG	23:s:110:ARG:OXT	2.32	0.48
29:y:9:LYS:HG2	29:y:12:GLU:HG2	1.95	0.48
2:1:878:A:H3'	2:1:879:G:H8	1.79	0.48
2:1:1009:A:N3	2:1:1153:C:O2'	2.47	0.48
2:1:1326:U:H2'	2:1:1327:A:H8	1.79	0.48
2:1:1667:G:O2'	2:1:1991:U:O4	2.28	0.48
8:e:33:ILE:HG12	8:e:155:ILE:HG12	1.96	0.48
13:i:127:SER:O	13:i:131:THR:OG1	2.26	0.48
40:H:46:LEU:HD21	40:H:86:LEU:HD11	1.96	0.48
58:Z:64:ALA:HB1	58:Z:66:ARG:HH11	1.78	0.48
2:1:577:G:O2'	2:1:1254:A:OP1	2.31	0.48
2:1:954:G:OP2	17:m:16:ARG:NH1	2.47	0.48
8:e:5:ASP:OD1	8:e:5:ASP:N	2.47	0.48
8:e:143:ASP:OD1	8:e:143:ASP:N	2.43	0.48
12:h:56:ARG:HG2	12:h:83:ALA:HB2	1.96	0.48
15:k:40:LYS:NZ	15:k:89:ASN:OD1	2.47	0.48
28:x:1:SER:OG	28:x:2:ARG:N	2.47	0.48
28:x:5:GLN:HE21	28:x:49:ARG:H	1.62	0.48
35:E:5:THR:HG23	35:E:7:ARG:HD2	1.96	0.48
39:G:46:VAL:O	39:G:50:ASN:ND2	2.47	0.48
1:3:323:U:H5'	57:Y:17:ARG:HB3	1.95	0.48
1:3:409:U:H5'	41:I:24:VAL:HB	1.96	0.48
1:3:511:C:O2'	41:I:40:HIS:NE2	2.47	0.48
28:x:64:ASP:OD1	28:x:64:ASP:N	2.45	0.48
40:H:4:VAL:HG13	40:H:5:HIS:H	1.79	0.48
55:W:40:PRO:HG2	55:W:43:ILE:HG12	1.96	0.48
2:1:910:A:N3	2:1:2264:C:O2'	2.43	0.48
2:1:1028:A:N3	2:1:2486:C:O2'	2.47	0.48
12:h:92:ALA:HB3	12:h:130:PRO:HD2	1.96	0.48
16:l:62:PRO:HB3	35:E:29:ARG:HE	1.78	0.48
36:F:30:GLU:HG3	36:F:32:LYS:H	1.78	0.48
40:H:71:ARG:HD3	40:H:74:ILE:HD12	1.96	0.48
2:1:2394:C:N3	4:6:76:A:O2'	2.41	0.47
8:e:134:GLN:HE21	8:e:140:ILE:HG21	1.79	0.47
25:u:24:VAL:HA	25:u:35:VAL:HG12	1.96	0.47
1:3:426:U:OP1	41:I:35:GLN:NE2	2.42	0.47
2:1:397:U:OP2	28:x:9:LYS:NZ	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:45:TYR:OH	6:c:81:GLU:OE2	2.32	0.47
23:s:86:MET:HE3	23:s:88:ARG:HD3	1.96	0.47
25:u:73:ASN:HD22	25:u:76:THR:H	1.59	0.47
29:y:15:ASN:OD1	29:y:15:ASN:N	2.46	0.47
1:3:974:A:OP1	51:S:68:ARG:NH1	2.42	0.47
2:1:277:G:H4'	2:1:278:A:C8	2.50	0.47
2:1:2299:U:OP2	8:e:70:ARG:NH1	2.47	0.47
11:a:62:ALA:HA	11:a:162:ARG:HA	1.96	0.47
13:i:133:ARG:NH1	13:i:134:SER:OG	2.48	0.47
44:L:110:ARG:O	44:L:118:ARG:NE	2.47	0.47
6:c:18:ASP:OD1	6:c:18:ASP:N	2.46	0.47
38:5:17:U:OP1	38:5:60:U:O2'	2.32	0.47
50:R:74:MET:O	50:R:78:ARG:N	2.45	0.47
2:1:355:U:H2'	2:1:356:G:H8	1.80	0.47
2:1:1527:G:N1	2:1:1544:A:OP2	2.40	0.47
2:1:2405:G:O2'	2:1:2411:A:N6	2.47	0.47
12:h:17:GLU:O	12:h:88:HIS:NE2	2.45	0.47
20:p:64:SER:OG	20:p:65:ASN:N	2.45	0.47
41:I:44:LYS:HA	41:I:44:LYS:HD3	1.75	0.47
1:3:35:G:O2'	49:Q:114:SER:O	2.29	0.47
14:j:58:ASN:ND2	14:j:127:GLY:O	2.48	0.47
17:m:17:ASN:O	17:m:38:ARG:NH1	2.46	0.47
18:n:2:ARG:NH1	18:n:5:LYS:O	2.48	0.47
18:n:8:ARG:NH2	18:n:43:GLU:OE2	2.47	0.47
18:n:22:ARG:HG3	18:n:70:THR:HA	1.95	0.47
19:o:100:HIS:O	19:o:104:GLN:NE2	2.48	0.47
26:v:28:ALA:N	26:v:40:ILE:O	2.43	0.47
34:D:43:THR:OG1	34:D:44:VAL:N	2.47	0.47
42:J:139:THR:O	42:J:143:LEU:N	2.47	0.47
1:3:494:G:H2'	1:3:496:A:H8	1.80	0.47
2:1:2174:C:H1'	11:a:218:MET:HG3	1.96	0.47
2:1:2345:G:H5'	2:1:2347:C:H5'	1.97	0.47
2:1:2375:G:N2	2:1:2378:A:OP2	2.39	0.47
16:l:127:VAL:HG11	16:l:142:ILE:HD13	1.97	0.47
2:1:100:U:O2'	25:u:90:LYS:NZ	2.47	0.47
2:1:1106:G:H4'	12:h:56:ARG:HB2	1.96	0.47
10:g:5:LEU:HD11	10:g:19:VAL:HG22	1.96	0.47
45:M:17:GLN:HE21	45:M:71:VAL:HG22	1.80	0.47
55:W:33:THR:OG1	55:W:34:GLU:N	2.48	0.47
8:e:39:VAL:HG12	8:e:41:GLU:H	1.80	0.47
12:h:86:MET:HE3	12:h:88:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:t:67:VAL:HG22	24:t:76:ARG:HG3	1.97	0.47
26:v:51:GLN:OE1	26:v:57:TYR:OH	2.31	0.47
30:z:11:SER:OG	30:z:12:ALA:N	2.48	0.47
42:J:149:PRO:HA	42:J:152:VAL:HG12	1.96	0.47
39:G:31:PHE:HB2	39:G:39:ILE:HG13	1.97	0.46
2:1:1131:G:O2'	2:1:1133:A:N7	2.47	0.46
2:1:2394:C:H5''	16:l:63:LYS:HD3	1.97	0.46
3:2:13:G:O2'	3:2:15:A:OP2	2.33	0.46
8:e:162:ASP:OD1	8:e:162:ASP:N	2.38	0.46
39:G:26:MET:HB3	39:G:26:MET:HE2	1.77	0.46
43:K:38:ARG:HE	43:K:39:LEU:H	1.63	0.46
2:1:1091:G:N2	2:1:1101:U:O2	2.48	0.46
39:G:91:VAL:HG21	39:G:95:TRP:CD1	2.45	0.46
53:U:75:ILE:O	53:U:80:LYS:NZ	2.43	0.46
58:Z:46:ARG:HD2	58:Z:49:ALA:HB3	1.96	0.46
1:3:110:C:O2'	53:U:25:ARG:O	2.28	0.46
1:3:151:A:OP2	1:3:169:C:N4	2.47	0.46
2:1:499:U:H5''	25:u:42:LYS:HD2	1.96	0.46
13:i:19:PRO:HB2	13:i:22:PRO:HB2	1.97	0.46
18:n:53:THR:HA	18:n:56:LYS:HG2	1.96	0.46
45:M:112:ASP:OD1	45:M:112:ASP:N	2.45	0.46
1:3:159:G:N2	1:3:162:A:OP2	2.47	0.46
1:3:993:G:H2'	1:3:995:C:H41	1.80	0.46
3:2:12:C:H3'	27:w:72:ASN:HD21	1.81	0.46
40:H:78:LYS:HG3	40:H:79:LYS:HG2	1.97	0.46
1:3:1095:U:OP1	1:3:1108:G:N2	2.41	0.46
12:h:41:LEU:HD11	12:h:54:VAL:HG11	1.96	0.46
41:I:33:ILE:HG23	41:I:34:GLU:HG3	1.97	0.46
47:O:6:ILE:HB	47:O:76:ILE:HB	1.97	0.46
50:R:49:GLU:HA	50:R:52:ILE:HD12	1.97	0.46
1:3:766:A:OP2	1:3:812:G:N2	2.48	0.46
2:1:189:G:O6	2:1:205:G:O2'	2.31	0.46
2:1:1047:G:O2'	2:1:1111:A:N6	2.49	0.46
2:1:2109:U:O2'	2:1:2180:U:O2	2.33	0.46
8:e:139:GLU:HG3	31:A:28:VAL:HG22	1.98	0.46
25:u:12:VAL:HG21	25:u:38:ILE:HG21	1.98	0.46
39:G:160:LEU:HB2	39:G:182:VAL:HG12	1.96	0.46
48:P:93:GLU:OE2	58:Z:19:LYS:NZ	2.46	0.46
58:Z:32:ARG:HG2	58:Z:33:ARG:HG2	1.97	0.46
2:1:684:G:OP1	34:D:21:ARG:NH2	2.47	0.46
2:1:1870:C:O2'	2:1:1871:A:O4'	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:g:27:ARG:NH1	28:x:59:ASP:OD2	2.49	0.46
26:v:80:HIS:HD2	26:v:82:TYR:H	1.64	0.46
38:5:18:G:O2'	38:5:57:G:N2	2.43	0.46
2:1:877:A:O2'	2:1:900:A:N6	2.49	0.46
2:1:1509:A:H2'	2:1:1510:G:C8	2.51	0.46
2:1:2123:G:N2	2:1:2175:C:O2	2.48	0.46
52:T:19:ASN:OD1	52:T:19:ASN:N	2.41	0.46
54:V:30:HIS:HD2	54:V:33:TYR:H	1.62	0.46
2:1:275:C:H2'	2:1:276:U:H4'	1.97	0.46
8:e:128:SER:HA	8:e:154:THR:HA	1.98	0.46
46:N:37:TYR:HD2	46:N:38:PHE:HD1	1.65	0.46
2:1:2467:C:O2	17:m:123:LYS:NZ	2.43	0.45
8:e:22:ASN:HB2	8:e:26:GLN:HE22	1.81	0.45
13:i:80:LYS:HB3	13:i:86:LYS:HA	1.98	0.45
43:K:86:ARG:NH1	55:W:63:TYR:O	2.44	0.45
2:1:2102:G:H1	2:1:2187:U:H3	1.64	0.45
2:1:2340:A:H2'	2:1:2341:G:H8	1.82	0.45
4:6:3:C:H42	4:6:70:G:H1	1.64	0.45
24:t:38:ALA:O	24:t:81:LYS:NZ	2.43	0.45
24:t:62:VAL:HA	24:t:81:LYS:HA	1.97	0.45
42:J:152:VAL:HG11	45:M:98:LEU:HD13	1.97	0.45
1:3:981:U:OP1	51:S:8:ARG:NH1	2.47	0.45
51:S:42:ASN:O	51:S:46:LYS:N	2.41	0.45
51:S:73:LEU:HD12	51:S:83:VAL:HG21	1.97	0.45
15:k:40:LYS:HE3	15:k:57:VAL:HG12	1.98	0.45
21:q:93:ILE:HD12	22:r:13:ARG:HB2	1.97	0.45
27:w:21:ARG:HD3	27:w:21:ARG:HA	1.85	0.45
35:E:53:ASP:OD1	35:E:53:ASP:N	2.48	0.45
39:G:71:THR:OG1	39:G:72:LYS:N	2.49	0.45
49:Q:98:ARG:HB2	49:Q:116:TYR:HA	1.98	0.45
2:1:1266:G:OP2	32:B:15:ARG:NH2	2.50	0.45
8:e:50:ASP:OD1	8:e:50:ASP:N	2.35	0.45
15:k:7:MET:HB3	15:k:18:ARG:HH21	1.82	0.45
24:t:39:THR:HG23	24:t:42:GLU:H	1.80	0.45
41:I:153:ARG:HA	41:I:156:ALA:HB3	1.99	0.45
50:R:57:ASP:OD1	50:R:57:ASP:N	2.43	0.45
54:V:47:ASP:OD1	54:V:47:ASP:N	2.50	0.45
2:1:1363:C:O2'	2:1:1809:A:N3	2.47	0.45
10:g:83:LYS:HA	10:g:149:GLU:H	1.81	0.45
14:j:35:ARG:HB2	14:j:54:ILE:HD11	1.99	0.45
18:n:48:VAL:HA	18:n:51:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:E:31:ILE:HG21	35:E:34:LYS:HE3	1.99	0.45
46:N:114:LYS:HB2	46:N:117:LEU:HD12	1.98	0.45
2:1:1124:G:O2'	36:F:37:GLN:NE2	2.49	0.45
2:1:1386:C:H2'	2:1:1387:A:C8	2.51	0.45
39:G:59:ILE:HD13	39:G:62:ARG:HH11	1.82	0.45
2:1:1125:G:H5'	36:F:37:GLN:HE21	1.82	0.45
26:v:86:LEU:HD13	26:v:89:ILE:HD11	1.99	0.45
2:1:1915:U:H3'	2:1:1916:A:H8	1.81	0.45
7:d:176:ASP:OD1	7:d:179:SER:OG	2.35	0.45
58:Z:16:ARG:HA	58:Z:18:PHE:HD2	1.81	0.45
1:3:82:G:O6	1:3:87:C:N4	2.50	0.45
2:1:964:C:O2'	2:1:2273:A:N3	2.46	0.45
2:1:987:C:O2'	2:1:1000:A:N3	2.47	0.45
6:c:25:THR:OG1	6:c:191:GLY:O	2.34	0.45
8:e:125:GLY:O	8:e:157:THR:OG1	2.35	0.45
14:j:77:HIS:HD2	14:j:84:ILE:HB	1.81	0.45
21:q:111:LYS:HG2	22:r:48:LYS:HZ1	1.82	0.45
38:5:3:G:H1'	38:5:4:C:H5'	1.99	0.45
44:L:68:VAL:HG23	44:L:99:ALA:HB1	1.99	0.45
1:3:1522:U:OP1	48:P:127:ARG:NH1	2.50	0.44
2:1:2174:C:O2'	11:a:218:MET:O	2.34	0.44
2:1:2682:A:H61	2:1:2728:U:H1'	1.82	0.44
58:Z:46:ARG:HD2	58:Z:46:ARG:HA	1.80	0.44
2:1:161:A:N6	2:1:162:U:O4	2.50	0.44
2:1:458:G:O2'	2:1:469:G:O6	2.28	0.44
2:1:495:G:N2	23:s:61:ASN:OD1	2.44	0.44
2:1:1082:U:H4'	12:h:42:ARG:HH21	1.82	0.44
7:d:88:ARG:HD3	7:d:88:ARG:HA	1.75	0.44
14:j:114:LEU:HG	14:j:118:MET:HE3	1.99	0.44
16:l:63:LYS:O	35:E:29:ARG:NH1	2.50	0.44
19:o:33:ARG:O	19:o:65:THR:OG1	2.28	0.44
20:p:99:LEU:HD21	20:p:109:ILE:HD11	2.00	0.44
41:I:2:ARG:HE	41:I:114:ARG:HD3	1.83	0.44
53:U:67:ILE:HG13	53:U:71:VAL:HG13	1.98	0.44
1:3:1218:C:H2'	1:3:1219:A:C8	2.52	0.44
1:3:1463:U:OP1	20:p:108:ARG:NH2	2.50	0.44
2:1:1817:G:OP1	5:b:86:ARG:NH2	2.46	0.44
2:1:2522:U:O2'	2:1:2647:U:OP1	2.26	0.44
6:c:5:VAL:HG22	6:c:202:ILE:HG12	1.99	0.44
9:f:86:LEU:HB2	9:f:130:ILE:HB	1.99	0.44
13:i:55:PRO:HD3	13:i:73:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:z:37:ARG:HA	30:z:37:ARG:HD3	1.78	0.44
43:K:10:VAL:HB	43:K:58:HIS:HB3	2.00	0.44
51:S:83:VAL:O	51:S:87:ALA:N	2.50	0.44
1:3:411:A:C4	1:3:413:G:H1'	2.51	0.44
1:3:458:U:H3	1:3:474:G:H1	1.65	0.44
1:3:491:G:OP2	41:I:147:LYS:NZ	2.50	0.44
1:3:816:A:OP1	1:3:1526:G:O2'	2.32	0.44
12:h:121:SER:OG	12:h:122:GLN:O	2.32	0.44
16:l:122:VAL:HG22	16:l:142:ILE:HG12	2.00	0.44
20:p:86:LYS:HD3	20:p:86:LYS:HA	1.75	0.44
46:N:83:THR:HG21	46:N:102:PHE:HB3	2.00	0.44
49:Q:67:GLY:O	49:Q:98:ARG:NH1	2.47	0.44
2:1:1072:C:N4	2:1:1093:G:H22	2.16	0.44
2:1:2155:U:H3'	2:1:2156:G:H8	1.82	0.44
2:1:2308:G:H2'	2:1:2310:C:H5	1.83	0.44
10:g:3:VAL:HG23	10:g:38:PRO:HA	2.00	0.44
10:g:132:PHE:N	10:g:140:ALA:O	2.47	0.44
19:o:31:THR:HG23	19:o:34:HIS:H	1.82	0.44
39:G:99:MET:HA	39:G:106:VAL:HG21	1.98	0.44
40:H:55:VAL:HG13	40:H:66:THR:HB	2.00	0.44
41:I:25:ARG:HE	41:I:30:LYS:HZ1	1.64	0.44
44:L:112:ASP:HB3	44:L:117:LEU:HD23	1.98	0.44
1:3:659:U:O4	1:3:746:A:N6	2.50	0.44
2:1:2120:G:H2'	2:1:2121:G:C8	2.52	0.44
2:1:2311:A:O2'	2:1:2312:U:O4'	2.33	0.44
24:t:15:HIS:H	24:t:32:LEU:HA	1.82	0.44
51:S:25:GLU:HA	51:S:28:ALA:HB3	2.00	0.44
2:1:479:A:H1'	2:1:480:A:H5''	2.00	0.44
8:e:2:LYS:HE3	8:e:2:LYS:HB3	1.90	0.44
10:g:43:ASN:HA	10:g:46:PHE:HB2	2.00	0.44
11:a:46:VAL:HG13	11:a:212:VAL:HG22	1.99	0.44
46:N:41:GLU:O	46:N:44:ARG:NH2	2.50	0.44
53:U:47:GLU:HG2	53:U:48:GLU:HB2	2.00	0.44
1:3:769:G:H4'	1:3:1513:A:H4'	2.00	0.44
1:3:776:G:N2	1:3:802:A:OP2	2.47	0.44
2:1:404:A:H1'	2:1:406:G:C4	2.53	0.44
2:1:2060:A:H62	7:d:69:ARG:HH12	1.66	0.44
2:1:2615:U:C2	32:B:3:GLN:HA	2.52	0.44
15:k:76:VAL:HG12	20:p:72:VAL:HB	2.00	0.44
20:p:1:SER:OG	20:p:3:ILE:N	2.49	0.44
54:V:57:VAL:HB	54:V:79:GLU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:12:U:H4'	1:3:526:C:H4'	1.99	0.44
1:3:993:G:O2'	1:3:994:A:N7	2.50	0.44
1:3:1166:G:O2'	1:3:1169:A:N6	2.50	0.44
2:1:2849:U:O4	20:p:20:ARG:NH2	2.47	0.44
12:h:5:LEU:O	12:h:9:GLN:N	2.51	0.44
14:j:36:LEU:O	14:j:121:LYS:NZ	2.51	0.44
20:p:91:VAL:HG11	20:p:96:LEU:HD11	1.99	0.44
29:y:17:GLU:HB2	29:y:53:VAL:HG11	1.99	0.44
47:O:10:LEU:HD21	47:O:22:THR:HG22	1.99	0.44
1:3:442:G:N3	1:3:493:A:N6	2.66	0.43
1:3:1060:U:H4'	47:O:53:ILE:HG23	2.00	0.43
2:1:1071:G:H1'	2:1:1089:A:C8	2.52	0.43
5:b:57:HIS:O	5:b:57:HIS:ND1	2.50	0.43
13:i:4:VAL:HA	13:i:7:TYR:HB3	2.00	0.43
40:H:150:VAL:HG22	40:H:199:VAL:HG22	1.98	0.43
1:3:1241:G:OP1	44:L:34:LYS:NZ	2.49	0.43
2:1:181:A:H2'	2:1:182:A:C8	2.54	0.43
16:l:2:ARG:HA	16:l:2:ARG:HD2	1.84	0.43
20:p:21:PRO:HD3	20:p:49:ILE:HD12	2.00	0.43
24:t:34:VAL:HG21	24:t:43:ILE:HD11	2.00	0.43
49:Q:72:ASN:N	49:Q:72:ASN:OD1	2.49	0.43
52:T:52:ARG:HE	52:T:52:ARG:HB2	1.62	0.43
1:3:922:G:H21	1:3:1398:A:H8	1.65	0.43
2:1:895:U:O2'	2:1:896:A:N7	2.50	0.43
2:1:959:A:N3	2:1:2457:U:O2'	2.50	0.43
19:o:75:GLY:HA2	19:o:78:VAL:HG12	1.99	0.43
30:z:5:LYS:HB2	30:z:57:GLU:HB3	1.99	0.43
32:B:11:LYS:HE3	32:B:11:LYS:HB3	1.86	0.43
41:I:153:ARG:O	41:I:157:ALA:N	2.51	0.43
42:J:76:ASN:N	42:J:79:THR:O	2.44	0.43
1:3:855:U:OP2	1:3:871:U:N3	2.48	0.43
2:1:1142:A:H4'	14:j:27:ARG:HH22	1.82	0.43
2:1:1791:A:N6	2:1:1828:G:O2'	2.48	0.43
10:g:47:PHE:HA	10:g:51:ARG:HB2	1.99	0.43
16:l:132:ARG:HG3	16:l:142:ILE:HD12	1.99	0.43
20:p:15:ASP:OD1	20:p:15:ASP:N	2.49	0.43
42:J:146:MET:HE2	42:J:146:MET:HB3	1.84	0.43
2:1:690:G:H21	5:b:42:ARG:HH12	1.66	0.43
6:c:59:ARG:HA	6:c:59:ARG:HD3	1.83	0.43
36:F:6:SER:O	36:F:6:SER:OG	2.36	0.43
38:5:33:U:OP2	46:N:129:ARG:NH1	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:J:95:MET:HE2	42:J:114:LEU:HD11	1.99	0.43
46:N:18:VAL:HG12	46:N:64:ILE:HG12	2.00	0.43
5:b:132:ARG:NH1	5:b:186:ASP:OD1	2.51	0.43
13:i:41:PHE:O	13:i:45:THR:OG1	2.32	0.43
1:3:511:C:O2'	1:3:512:U:O4'	2.36	0.43
1:3:1321:U:O2'	56:X:77:ARG:NH2	2.51	0.43
2:1:45:G:H5''	2:1:46:G:H5'	2.01	0.43
2:1:1085:A:N7	12:h:37:LYS:HE2	2.33	0.43
9:f:17:LYS:HE2	9:f:24:THR:HB	2.00	0.43
24:t:10:VAL:HG12	24:t:11:LEU:HD12	2.00	0.43
39:G:63:LYS:HA	39:G:63:LYS:HD3	1.77	0.43
40:H:20:THR:O	40:H:20:THR:OG1	2.35	0.43
47:O:80:THR:HG23	47:O:82:LYS:H	1.83	0.43
48:P:86:LYS:HB2	48:P:112:VAL:HG23	2.01	0.43
1:3:200:G:H2'	1:3:201:G:H8	1.83	0.43
1:3:436:C:H2'	1:3:437:U:C6	2.54	0.43
1:3:694:A:HO2'	4:6:38:A:HO2'	1.57	0.43
2:1:805:G:N2	2:1:829:A:OP1	2.51	0.43
2:1:1173:U:C2	2:1:1174:U:H1'	2.54	0.43
2:1:2714:G:H5''	2:1:2714:G:H8	1.83	0.43
5:b:134:ILE:O	5:b:166:ARG:NH2	2.52	0.43
8:e:175:PRO:HB2	8:e:176:PHE:H	1.69	0.43
24:t:79:ASP:OD1	24:t:79:ASP:N	2.39	0.43
29:y:34:SER:O	29:y:36:GLN:NE2	2.50	0.43
39:G:42:LEU:HA	39:G:45:THR:HG22	2.00	0.43
40:H:124:GLU:OE1	40:H:189:HIS:N	2.52	0.43
1:3:1233:G:OP1	46:N:118:ARG:NH1	2.52	0.43
2:1:1365:A:OP1	28:x:27:ARG:NH2	2.52	0.43
2:1:1601:G:OP1	24:t:64:LYS:NZ	2.47	0.43
2:1:2484:G:OP1	17:m:44:ARG:NH2	2.51	0.43
2:1:2511:U:O2'	6:c:143:PRO:O	2.34	0.43
8:e:125:GLY:HA3	8:e:159:ALA:HB3	1.99	0.43
13:i:101:SER:OG	13:i:102:ARG:N	2.52	0.43
14:j:6:ALA:H	14:j:45:THR:HG21	1.83	0.43
47:O:44:THR:HG22	47:O:70:HIS:HA	2.01	0.43
49:Q:75:GLU:O	49:Q:76:HIS:ND1	2.51	0.43
53:U:56:ARG:HD2	53:U:56:ARG:HA	1.73	0.43
1:3:1064:G:O2'	1:3:1190:G:N2	2.52	0.43
2:1:888:C:N4	50:R:81:ASP:OD1	2.51	0.43
3:2:52:A:N7	19:o:64:TYR:OH	2.44	0.43
19:o:52:SER:N	19:o:55:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:11:GLU:HA	31:A:25:ARG:HA	2.00	0.43
39:G:18:GLN:O	39:G:19:THR:OG1	2.28	0.43
1:3:1143:G:H2'	1:3:1144:G:H8	1.84	0.42
2:1:1141:U:H2'	14:j:65:THR:HG21	2.00	0.42
7:d:112:LEU:HD13	7:d:186:VAL:HG11	2.01	0.42
36:F:16:ILE:HD13	36:F:25:VAL:HG22	2.00	0.42
42:J:156:ARG:NH1	45:M:42:GLU:OE2	2.52	0.42
46:N:113:LYS:HA	46:N:120:ALA:HB2	2.01	0.42
1:3:459:A:H2'	1:3:460:A:H8	1.84	0.42
33:C:52:LYS:HE3	33:C:52:LYS:HB2	1.71	0.42
47:O:5:ARG:HG2	47:O:79:PRO:HB3	2.01	0.42
56:X:28:LYS:HE3	56:X:28:LYS:HB3	1.94	0.42
1:3:436:C:O2'	41:I:153:ARG:NH1	2.27	0.42
2:1:751:A:H5'	23:s:90:LYS:HA	2.01	0.42
2:1:2304:G:H22	2:1:2312:U:H3	1.66	0.42
9:f:44:HIS:HA	9:f:49:LEU:HD23	2.01	0.42
11:a:41:SER:OG	11:a:176:GLY:O	2.31	0.42
20:p:13:LYS:HE3	20:p:76:HIS:HA	2.01	0.42
54:V:16:MET:O	54:V:19:SER:OG	2.37	0.42
57:Y:19:HIS:O	57:Y:22:SER:OG	2.36	0.42
1:3:410:G:H2'	1:3:429:U:C4	2.55	0.42
2:1:631:A:N3	2:1:2415:G:O2'	2.49	0.42
2:1:811:U:H2'	16:l:21:ARG:HA	2.00	0.42
4:6:19:G:C4	4:6:57:A:C2	3.07	0.42
7:d:46:GLN:H	7:d:87:ALA:HB3	1.84	0.42
9:f:151:ARG:HD3	9:f:151:ARG:HA	1.81	0.42
16:l:82:LEU:HD12	16:l:82:LEU:HA	1.80	0.42
19:o:29:HIS:HB3	19:o:36:TYR:HB2	2.01	0.42
50:R:6:ILE:HG13	50:R:7:ASN:H	1.84	0.42
2:1:1536:C:H4'	2:1:1537:G:C2	2.54	0.42
2:1:2127:G:H2'	2:1:2128:G:C8	2.54	0.42
41:I:97:LEU:HD21	41:I:129:VAL:HG21	2.01	0.42
50:R:28:ARG:NH2	50:R:62:PHE:HB2	2.34	0.42
2:1:2063:C:O2'	38:5:76:A:O3'	2.31	0.42
8:e:57:ALA:HB2	8:e:64:PRO:HD3	2.02	0.42
12:h:37:LYS:HE3	12:h:37:LYS:HB3	1.92	0.42
12:h:41:LEU:O	12:h:45:GLY:N	2.53	0.42
18:n:12:ARG:HG2	18:n:16:HIS:ND1	2.35	0.42
21:q:47:ARG:NH2	21:q:51:GLN:OE1	2.52	0.42
34:D:3:ARG:O	34:D:6:GLN:NE2	2.47	0.42
40:H:52:SER:N	40:H:68:HIS:O	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:946:A:H2'	1:3:947:G:C8	2.54	0.42
13:i:10:LEU:HB3	13:i:11:GLN:H	1.60	0.42
40:H:49:ALA:O	40:H:69:THR:OG1	2.38	0.42
52:T:2:LEU:HD12	52:T:2:LEU:HA	1.86	0.42
2:1:994:C:OP1	21:q:52:ARG:NH2	2.53	0.42
9:f:70:LEU:HD23	9:f:70:LEU:HA	1.86	0.42
12:h:17:GLU:HB3	12:h:88:HIS:HE1	1.84	0.42
32:B:52:LYS:HE2	32:B:54:ILE:HG22	2.01	0.42
40:H:78:LYS:HZ3	40:H:79:LYS:HE3	1.85	0.42
40:H:107:LYS:HB3	40:H:143:LEU:HD23	2.01	0.42
49:Q:39:THR:OG1	49:Q:40:THR:N	2.53	0.42
53:U:43:ALA:O	53:U:46:LYS:NZ	2.39	0.42
1:3:522:C:OP2	49:Q:65:TYR:OH	2.33	0.42
1:3:958:A:C4	56:X:54:ARG:HD3	2.54	0.42
7:d:7:ASP:OD1	7:d:7:ASP:N	2.50	0.42
10:g:71:LYS:HA	10:g:71:LYS:HD2	1.85	0.42
14:j:95:ARG:HG2	14:j:96:ARG:HG2	2.02	0.42
40:H:23:ALA:HB1	40:H:27:GLU:HG2	2.01	0.42
47:O:17:LEU:HD12	47:O:20:GLN:HE21	1.83	0.42
56:X:38:THR:HA	56:X:69:LYS:HA	2.00	0.42
1:3:81:A:H2'	1:3:82:G:C8	2.55	0.42
1:3:1310:G:OP2	50:R:86:ARG:NH2	2.48	0.42
2:1:1548:A:H2'	2:1:1549:A:C8	2.55	0.42
2:1:1779:U:OP2	2:1:1784:A:N6	2.45	0.42
3:2:8:C:O3'	19:o:25:ARG:NH1	2.52	0.42
10:g:97:ARG:HG3	10:g:112:LYS:HD3	2.02	0.42
15:k:8:LEU:HD23	15:k:82:ASN:HB3	2.02	0.42
19:o:8:ILE:O	19:o:12:THR:OG1	2.37	0.42
41:I:10:LEU:HB3	41:I:62:ARG:HD3	2.01	0.42
49:Q:56:LEU:HD23	49:Q:56:LEU:HA	1.89	0.42
2:1:38:A:H4'	7:d:45:ALA:HB3	2.00	0.41
2:1:355:U:H2'	2:1:356:G:C8	2.55	0.41
2:1:2109:U:H1'	2:1:2180:U:H3	1.85	0.41
12:h:29:ASP:OD1	12:h:29:ASP:N	2.50	0.41
12:h:97:LYS:HD3	12:h:97:LYS:HA	1.87	0.41
39:G:113:LEU:HB2	39:G:143:LEU:HD23	2.02	0.41
41:I:28:ASP:OD1	41:I:28:ASP:N	2.52	0.41
41:I:187:ARG:HA	41:I:187:ARG:HD2	1.86	0.41
1:3:1038:C:H2'	1:3:1039:G:C8	2.53	0.41
2:1:144:A:H4'	24:t:2:ILE:HG21	2.02	0.41
2:1:1047:G:H2'	2:1:1110:G:N1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:2503:A:O2'	2:1:2505:G:OP2	2.31	0.41
5:b:117:SER:OG	5:b:118:GLY:N	2.53	0.41
47:O:91:ASP:OD1	47:O:91:ASP:N	2.41	0.41
1:3:252:U:O4	1:3:253:A:N6	2.53	0.41
2:1:633:A:O2'	2:1:2404:U:OP1	2.32	0.41
2:1:2250:G:O2'	2:1:2496:C:OP1	2.31	0.41
5:b:68:ARG:NH1	5:b:126:GLY:O	2.41	0.41
13:i:54:ILE:HG12	13:i:73:PRO:HD3	2.02	0.41
21:q:25:GLY:O	21:q:29:ARG:NH1	2.50	0.41
49:Q:43:LYS:HA	49:Q:43:LYS:HD2	1.79	0.41
1:3:255:G:H4'	54:V:18:LYS:HD3	2.01	0.41
1:3:362:G:N2	1:3:365:U:OP2	2.51	0.41
2:1:2233:U:H2'	2:1:2234:G:C8	2.56	0.41
2:1:2331:G:O2'	2:1:2336:A:N1	2.49	0.41
2:1:2822:G:OP1	6:c:164:GLN:NE2	2.53	0.41
5:b:261:ARG:O	5:b:264:LYS:NZ	2.54	0.41
12:h:29:ASP:OD1	12:h:56:ARG:NH2	2.53	0.41
12:h:58:THR:HG21	12:h:82:ILE:HB	2.03	0.41
41:I:57:LYS:NZ	41:I:68:GLU:OE1	2.48	0.41
44:L:75:LYS:HE2	44:L:88:VAL:HG21	2.03	0.41
45:M:10:LEU:HD22	45:M:74:ILE:HD11	2.02	0.41
1:3:1452:C:H4'	1:3:1453:G:C2	2.56	0.41
2:1:24:G:O2'	23:s:78:GLU:O	2.37	0.41
2:1:880:G:H2'	2:1:881:G:C8	2.54	0.41
2:1:1315:C:O2'	2:1:1392:A:N3	2.53	0.41
2:1:2224:G:H4'	2:1:2226:C:C2	2.55	0.41
5:b:160:TYR:HB3	5:b:193:GLU:HB3	2.01	0.41
21:q:71:ASN:HB3	21:q:109:VAL:HG21	2.03	0.41
22:r:1:MET:HB2	22:r:43:ASN:HD22	1.84	0.41
39:G:41:ASN:HB3	39:G:44:LYS:HB2	2.02	0.41
1:3:408:A:OP2	41:I:7:LYS:NZ	2.49	0.41
1:3:1458:G:OP1	57:Y:29:THR:OG1	2.39	0.41
2:1:558:U:H2'	2:1:559:G:H8	1.85	0.41
2:1:2147:A:H62	2:1:2148:G:H21	1.68	0.41
2:1:2627:G:N2	2:1:2777:G:OP2	2.52	0.41
3:2:41:G:H21	8:e:65:LEU:HD11	1.85	0.41
3:2:42:C:OP1	8:e:63:LYS:NZ	2.37	0.41
7:d:58:LYS:NZ	7:d:62:GLN:OE1	2.54	0.41
22:r:60:LYS:O	22:r:99:THR:OG1	2.36	0.41
45:M:86:LYS:HA	45:M:86:LYS:HD3	1.85	0.41
46:N:46:VAL:HG23	46:N:79:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Z:6:ARG:HD2	58:Z:8:ASN:HB3	2.03	0.41
1:3:437:U:H5'	41:I:151:GLN:NE2	2.35	0.41
2:1:1006:C:O2'	14:j:108:MET:O	2.36	0.41
13:i:14:ALA:HB2	13:i:54:ILE:HB	2.02	0.41
40:H:57:GLU:OE2	40:H:64:ARG:NE	2.50	0.41
41:I:81:LEU:HD23	41:I:81:LEU:HA	1.87	0.41
44:L:16:LYS:HG3	44:L:17:PHE:HD1	1.86	0.41
48:P:34:THR:HG22	48:P:40:ALA:HA	2.03	0.41
49:Q:53:ARG:HG3	49:Q:63:THR:HG22	2.03	0.41
57:Y:32:LYS:HD2	57:Y:32:LYS:HA	1.88	0.41
1:3:264:C:O2'	54:V:65:PRO:O	2.31	0.41
1:3:528:C:H41	49:Q:45:ASN:ND2	2.19	0.41
2:1:783:A:H2'	2:1:784:G:H4'	2.03	0.41
5:b:154:ALA:HB2	5:b:161:VAL:HG23	2.02	0.41
14:j:142:ILE:HD12	14:j:142:ILE:HA	1.90	0.41
19:o:34:HIS:ND1	19:o:53:THR:OG1	2.43	0.41
22:r:55:ASP:OD1	22:r:56:GLY:N	2.54	0.41
23:s:86:MET:HE2	23:s:86:MET:HB3	1.87	0.41
40:H:9:ILE:HG23	40:H:10:ARG:HG3	2.03	0.41
50:R:47:LEU:HD23	50:R:47:LEU:HA	1.90	0.41
1:3:1137:C:H5'	1:3:1138:G:H5'	2.03	0.41
1:3:1377:A:OP1	44:L:91:ARG:NH2	2.47	0.41
2:1:171:U:H2'	2:1:172:A:H8	1.86	0.41
2:1:302:C:H2'	2:1:303:G:H8	1.85	0.41
2:1:1087:G:H2'	2:1:1089:A:C8	2.56	0.41
2:1:1181:U:H2'	2:1:1182:G:C8	2.56	0.41
2:1:2331:G:H4'	27:w:39:THR:H	1.85	0.41
3:2:34:A:N6	3:2:44:G:O2'	2.53	0.41
4:6:51:C:H2'	4:6:52:G:C8	2.54	0.41
13:i:106:GLN:HA	13:i:109:ALA:HB3	2.03	0.41
14:j:125:TYR:HH	14:j:132:HIS:CD2	2.37	0.41
26:v:51:GLN:OE1	26:v:79:ARG:NH2	2.54	0.41
30:z:10:ARG:HB2	30:z:53:MET:HB2	2.03	0.41
32:B:27:LEU:HB3	32:B:36:LYS:HD2	2.03	0.41
33:C:24:LYS:HE2	33:C:24:LYS:HB3	1.91	0.41
42:J:141:ASP:HA	42:J:144:GLU:HG2	2.03	0.41
49:Q:89:LEU:HA	49:Q:90:PRO:HD3	1.87	0.41
58:Z:33:ARG:HG3	58:Z:34:ARG:HB2	2.03	0.41
1:3:9:G:OP2	42:J:125:LYS:NZ	2.38	0.41
1:3:67:C:H2'	1:3:68:G:C8	2.56	0.41
2:1:242:G:O2'	2:1:254:G:O6	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:570:G:H2'	2:1:2030:A:N7	2.36	0.41
2:1:1818:U:O2'	5:b:152:GLN:O	2.33	0.41
6:c:46:ARG:NH2	6:c:89:GLU:OE2	2.44	0.41
7:d:148:ILE:HB	7:d:169:VAL:HG12	2.01	0.41
8:e:79:ARG:HH11	38:5:19:G:H1	1.69	0.41
8:e:129:MET:HE2	8:e:129:MET:HB3	1.83	0.41
57:Y:41:GLY:HA2	57:Y:85:LEU:HD11	2.03	0.41
2:1:84:A:N1	2:1:98:G:O2'	2.48	0.40
2:1:2117:A:N1	2:1:2170:A:N1	2.68	0.40
7:d:18:THR:HA	7:d:106:LYS:HG2	2.03	0.40
14:j:80:HIS:HB3	14:j:81:ILE:H	1.73	0.40
19:o:115:LEU:HD12	19:o:115:LEU:HA	1.94	0.40
49:Q:110:LYS:HD3	49:Q:121:PRO:HG3	2.03	0.40
2:1:171:U:H2'	2:1:172:A:C8	2.56	0.40
2:1:1429:G:H2'	2:1:1430:G:H8	1.86	0.40
4:6:48:C:C4	4:6:59:A:H1'	2.56	0.40
6:c:110:THR:HB	6:c:171:THR:HG23	2.03	0.40
7:d:44:ARG:HH11	7:d:46:GLN:HE22	1.68	0.40
11:a:42:VAL:HG21	11:a:175:ILE:HG12	2.03	0.40
12:h:77:VAL:HG12	12:h:82:ILE:HG13	2.03	0.40
38:5:4:C:H1'	38:5:5:G:H5'	2.03	0.40
42:J:132:PRO:HA	42:J:135:VAL:HG22	2.03	0.40
49:Q:53:ARG:NE	49:Q:61:GLU:OE2	2.42	0.40
2:1:1086:A:H62	12:h:34:THR:HB	1.87	0.40
2:1:1447:C:O2'	2:1:1544:A:N3	2.48	0.40
2:1:1532:A:N6	2:1:1538:G:O6	2.55	0.40
2:1:1688:U:O2'	2:1:1700:A:N7	2.47	0.40
5:b:257:ARG:HH22	5:b:262:THR:HG23	1.85	0.40
9:f:97:VAL:HG12	9:f:102:ILE:HG12	2.03	0.40
21:q:106:THR:HA	21:q:109:VAL:HG22	2.03	0.40
26:v:4:ILE:HB	26:v:63:ILE:HD13	2.03	0.40
46:N:5:TYR:HB2	46:N:20:ILE:HG12	2.03	0.40
47:O:76:ILE:HD13	47:O:76:ILE:HA	1.91	0.40
54:V:27:PHE:HD1	54:V:27:PHE:HA	1.76	0.40
1:3:1309:G:N7	50:R:97:ARG:NH2	2.70	0.40
2:1:636:G:H2'	16:l:111:ILE:HD11	2.03	0.40
2:1:2183:A:H2'	2:1:2184:A:C4	2.56	0.40
2:1:2273:A:H2'	2:1:2274:A:C8	2.57	0.40
2:1:2474:U:H6	2:1:2474:U:H2'	1.70	0.40
8:e:16:MET:HG3	8:e:21:TYR:HB2	2.03	0.40
10:g:116:ARG:HA	10:g:116:ARG:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:39:VAL:HG22	11:a:177:LYS:HD2	2.03	0.40
14:j:109:LEU:HD23	14:j:109:LEU:HA	1.90	0.40
16:l:111:ILE:HD12	16:l:111:ILE:HA	1.84	0.40
48:P:58:THR:HG23	48:P:60:PHE:H	1.85	0.40
49:Q:115:LYS:H	49:Q:115:LYS:HG3	1.70	0.40
1:3:1391:U:H2'	1:3:1392:G:C8	2.57	0.40
2:1:172:A:H2'	2:1:173:A:C8	2.57	0.40
2:1:1796:U:H2'	2:1:1797:G:C8	2.57	0.40
2:1:2151:U:H2'	2:1:2152:G:C8	2.57	0.40
20:p:36:LYS:HA	20:p:36:LYS:HD3	1.85	0.40
32:B:15:ARG:HH21	32:B:15:ARG:HD2	1.76	0.40
39:G:13:VAL:HG12	39:G:15:PHE:HE1	1.87	0.40
46:N:18:VAL:HG12	46:N:64:ILE:HG23	2.03	0.40
50:R:89:ARG:HB2	50:R:96:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	b	269/271 (99%)	251 (93%)	18 (7%)	0	100	100
6	c	207/209 (99%)	190 (92%)	16 (8%)	1 (0%)	24	54
7	d	199/201 (99%)	181 (91%)	17 (8%)	1 (0%)	24	54
8	e	175/177 (99%)	158 (90%)	15 (9%)	2 (1%)	11	36
9	f	174/176 (99%)	160 (92%)	14 (8%)	0	100	100
10	g	147/149 (99%)	125 (85%)	20 (14%)	2 (1%)	9	30
11	a	130/234 (56%)	115 (88%)	15 (12%)	0	100	100
12	h	129/131 (98%)	95 (74%)	31 (24%)	3 (2%)	5	19
13	i	139/142 (98%)	119 (86%)	19 (14%)	1 (1%)	18	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	j	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
15	k	120/122 (98%)	101 (84%)	18 (15%)	1 (1%)	16	44
16	l	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	18	48
17	m	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	8	28
18	n	118/120 (98%)	101 (86%)	15 (13%)	2 (2%)	7	26
19	o	114/116 (98%)	107 (94%)	7 (6%)	0	100	100
20	p	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
21	q	115/117 (98%)	115 (100%)	0	0	100	100
22	r	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	12	39
23	s	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
24	t	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
25	u	100/102 (98%)	87 (87%)	12 (12%)	1 (1%)	12	39
26	v	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
27	w	73/75 (97%)	63 (86%)	10 (14%)	0	100	100
28	x	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
29	y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	7	27
30	z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
31	A	64/66 (97%)	57 (89%)	7 (11%)	0	100	100
32	B	54/56 (96%)	48 (89%)	4 (7%)	2 (4%)	2	11
33	C	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
34	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
35	E	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	7	27
36	F	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
39	G	216/225 (96%)	193 (89%)	21 (10%)	2 (1%)	14	41
40	H	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
41	I	203/205 (99%)	177 (87%)	26 (13%)	0	100	100
42	J	155/157 (99%)	136 (88%)	19 (12%)	0	100	100
43	K	98/100 (98%)	84 (86%)	13 (13%)	1 (1%)	12	39
44	L	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
45	M	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
46	N	125/127 (98%)	110 (88%)	15 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	O	96/98 (98%)	81 (84%)	14 (15%)	1 (1%)	12	39
48	P	114/116 (98%)	105 (92%)	9 (8%)	0	100	100
49	Q	121/123 (98%)	100 (83%)	20 (16%)	1 (1%)	16	44
50	R	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
51	S	98/100 (98%)	81 (83%)	17 (17%)	0	100	100
52	T	86/88 (98%)	78 (91%)	6 (7%)	2 (2%)	5	19
53	U	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
54	V	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
55	W	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
56	X	77/79 (98%)	70 (91%)	7 (9%)	0	100	100
57	Y	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
58	Z	63/65 (97%)	39 (62%)	19 (30%)	5 (8%)	1	2
All	All	5976/6190 (96%)	5372 (90%)	570 (10%)	34 (1%)	23	51

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	n	70	THR
8	e	175	PRO
8	e	176	PHE
10	g	9	VAL
16	l	29	LYS
17	m	70	ASP
29	y	24	GLU
35	E	31	ILE
39	G	19	THR
52	T	45	HIS
58	Z	24	LYS
58	Z	65	ARG
15	k	108	ARG
25	u	98	ASN
32	B	23	ALA
7	d	86	ALA
17	m	69	PRO
18	n	69	ARG
22	r	54	VAL
39	G	72	LYS
43	K	92	THR

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Mol	Chain	Res	Type
52	T	44	GLU
58	Z	37	TYR
12	h	80	THR
58	Z	9	GLU
6	c	169	ARG
10	g	8	LYS
47	O	57	VAL
58	Z	10	PRO
12	h	79	PRO
12	h	123	ILE
49	Q	120	ARG
32	B	24	VAL
13	i	90	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	b	216/216 (100%)	214 (99%)	2 (1%)	70	90
6	c	164/164 (100%)	164 (100%)	0	100	100
7	d	165/165 (100%)	164 (99%)	1 (1%)	78	93
8	e	148/148 (100%)	146 (99%)	2 (1%)	59	85
9	f	137/137 (100%)	136 (99%)	1 (1%)	76	92
10	g	114/114 (100%)	113 (99%)	1 (1%)	70	90
11	a	110/181 (61%)	110 (100%)	0	100	100
12	h	100/100 (100%)	100 (100%)	0	100	100
13	i	109/110 (99%)	108 (99%)	1 (1%)	70	90
14	j	116/116 (100%)	115 (99%)	1 (1%)	70	90
15	k	103/103 (100%)	102 (99%)	1 (1%)	68	89
16	l	102/102 (100%)	100 (98%)	2 (2%)	48	78
17	m	109/109 (100%)	109 (100%)	0	100	100
18	n	100/100 (100%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	o	86/86 (100%)	86 (100%)	0	100	100
20	p	99/99 (100%)	99 (100%)	0	100	100
21	q	89/89 (100%)	89 (100%)	0	100	100
22	r	84/84 (100%)	84 (100%)	0	100	100
23	s	93/93 (100%)	92 (99%)	1 (1%)	65	88
24	t	80/80 (100%)	79 (99%)	1 (1%)	61	86
25	u	83/83 (100%)	83 (100%)	0	100	100
26	v	78/78 (100%)	78 (100%)	0	100	100
27	w	57/57 (100%)	57 (100%)	0	100	100
28	x	67/67 (100%)	65 (97%)	2 (3%)	36	70
29	y	55/55 (100%)	54 (98%)	1 (2%)	51	80
30	z	48/48 (100%)	47 (98%)	1 (2%)	47	77
31	A	59/59 (100%)	59 (100%)	0	100	100
32	B	47/47 (100%)	47 (100%)	0	100	100
33	C	45/45 (100%)	45 (100%)	0	100	100
34	D	38/38 (100%)	38 (100%)	0	100	100
35	E	51/51 (100%)	50 (98%)	1 (2%)	48	78
36	F	34/34 (100%)	34 (100%)	0	100	100
39	G	180/186 (97%)	178 (99%)	2 (1%)	65	88
40	H	170/170 (100%)	169 (99%)	1 (1%)	78	93
41	I	172/172 (100%)	171 (99%)	1 (1%)	78	93
42	J	119/119 (100%)	118 (99%)	1 (1%)	73	90
43	K	87/87 (100%)	85 (98%)	2 (2%)	44	76
44	L	124/124 (100%)	123 (99%)	1 (1%)	73	90
45	M	104/104 (100%)	104 (100%)	0	100	100
46	N	105/105 (100%)	105 (100%)	0	100	100
47	O	86/86 (100%)	86 (100%)	0	100	100
48	P	89/89 (100%)	89 (100%)	0	100	100
49	Q	103/103 (100%)	102 (99%)	1 (1%)	68	89
50	R	92/92 (100%)	92 (100%)	0	100	100
51	S	83/83 (100%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	T	76/76 (100%)	76 (100%)	0	100	100
53	U	65/65 (100%)	65 (100%)	0	100	100
54	V	74/74 (100%)	73 (99%)	1 (1%)	59	85
55	W	56/56 (100%)	56 (100%)	0	100	100
56	X	70/70 (100%)	70 (100%)	0	100	100
57	Y	65/65 (100%)	65 (100%)	0	100	100
58	Z	55/55 (100%)	55 (100%)	0	100	100
All	All	4961/5039 (98%)	4932 (99%)	29 (1%)	76	93

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	b	18	VAL
5	b	44	ASN
7	d	186	VAL
8	e	30	VAL
8	e	154	THR
9	f	42	VAL
10	g	146	VAL
13	i	85	ILE
14	j	84	ILE
15	k	8	LEU
16	l	81	ASP
16	l	90	VAL
23	s	106	VAL
24	t	62	VAL
28	x	39	VAL
28	x	69	GLU
29	y	19	LEU
30	z	56	VAL
35	E	31	ILE
39	G	19	THR
39	G	30	ILE
40	H	4	VAL
41	I	124	VAL
42	J	122	VAL
43	K	70	VAL
43	K	84	VAL
44	L	123	LEU
49	Q	78	VAL

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Mol	Chain	Res	Type
54	V	77	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
5	b	52	HIS
5	b	85	ASN
5	b	116	GLN
5	b	238	ASN
7	d	9	GLN
7	d	46	GLN
8	e	26	GLN
8	e	134	GLN
9	f	47	ASN
9	f	103	ASN
9	f	138	GLN
10	g	28	ASN
11	a	165	ASN
11	a	188	ASN
13	i	110	GLN
14	j	40	HIS
14	j	58	ASN
16	l	4	ASN
16	l	35	HIS
17	m	13	HIS
18	n	3	HIS
18	n	11	ASN
18	n	81	ASN
19	o	43	ASN
19	o	104	GLN
20	p	55	HIS
21	q	19	GLN
21	q	71	ASN
22	r	43	ASN
23	s	40	ASN
24	t	48	GLN
24	t	59	ASN
25	u	68	ASN
25	u	73	ASN
26	v	80	HIS
27	w	8	ASN
27	w	72	ASN

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Mol	Chain	Res	Type
28	x	5	GLN
29	y	27	ASN
31	A	20	ASN
31	A	61	ASN
31	A	65	ASN
32	B	3	GLN
32	B	5	ASN
34	D	13	ASN
36	F	13	ASN
36	F	37	GLN
39	G	14	HIS
39	G	57	ASN
39	G	169	HIS
40	H	68	HIS
40	H	139	ASN
40	H	189	HIS
41	I	70	GLN
41	I	73	ASN
41	I	88	ASN
41	I	151	GLN
41	I	197	HIS
42	J	134	ASN
42	J	145	ASN
43	K	52	ASN
44	L	85	GLN
44	L	147	ASN
45	M	3	GLN
45	M	17	GLN
45	M	66	GLN
46	N	30	ASN
46	N	31	GLN
47	O	70	HIS
48	P	21	HIS
48	P	39	ASN
48	P	80	ASN
49	Q	45	ASN
50	R	13	HIS
51	S	42	ASN
52	T	34	GLN
53	U	9	HIS
53	U	26	ASN
53	U	79	ASN

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Mol	Chain	Res	Type
54	V	30	HIS
55	W	30	ASN
55	W	51	GLN
55	W	53	GLN
56	X	56	HIS
56	X	68	HIS
57	Y	19	HIS
57	Y	47	GLN
57	Y	51	ASN
57	Y	60	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	1538/1539 (99%)	234 (15%)	1 (0%)
2	1	2902/2903 (99%)	508 (17%)	11 (0%)
3	2	119/120 (99%)	17 (14%)	3 (2%)
37	4	18/35 (51%)	8 (44%)	2 (11%)
38	5	76/77 (98%)	19 (25%)	0
4	6	76/77 (98%)	23 (30%)	0
All	All	4729/4751 (99%)	809 (17%)	17 (0%)

All (809) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	4	U
1	3	5	U
1	3	6	G
1	3	7	A
1	3	9	G
1	3	22	G
1	3	32	A
1	3	39	G
1	3	47	C
1	3	48	C
1	3	51	A
1	3	54	C
1	3	71	A
1	3	81	A
1	3	82	G
1	3	85	U

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Mol	Chain	Res	Type
1	3	87	C
1	3	91	U
1	3	94	G
1	3	95	C
1	3	100	G
1	3	116	A
1	3	121	U
1	3	128	G
1	3	130	A
1	3	141	G
1	3	144	G
1	3	149	A
1	3	154	U
1	3	163	C
1	3	183	C
1	3	184	G
1	3	191	G
1	3	197	A
1	3	208	U
1	3	209	U
1	3	210	C
1	3	211	G
1	3	212	G
1	3	226	G
1	3	245	U
1	3	247	G
1	3	251	G
1	3	266	G
1	3	267	C
1	3	279	A
1	3	280	C
1	3	281	G
1	3	289	G
1	3	298	A
1	3	306	A
1	3	309	A
1	3	321	A
1	3	328	C
1	3	347	G
1	3	351	G
1	3	352	C
1	3	354	G

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Mol	Chain	Res	Type
1	3	367	U
1	3	372	C
1	3	392	C
1	3	397	A
1	3	406	G
1	3	411	A
1	3	413	G
1	3	414	A
1	3	424	G
1	3	429	U
1	3	436	C
1	3	437	U
1	3	451	A
1	3	467	U
1	3	479	U
1	3	484	G
1	3	485	U
1	3	486	U
1	3	494	G
1	3	495	A
1	3	497	G
1	3	511	C
1	3	518	C
1	3	519	C
1	3	521	G
1	3	524	G
1	3	527	G
1	3	529	G
1	3	533	A
1	3	536	C
1	3	547	A
1	3	559	A
1	3	560	A
1	3	561	U
1	3	562	U
1	3	564	C
1	3	572	A
1	3	573	A
1	3	576	C
1	3	577	G
1	3	615	G
1	3	620	C

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Mol	Chain	Res	Type
1	3	633	G
1	3	642	A
1	3	650	G
1	3	653	U
1	3	665	A
1	3	688	G
1	3	702	A
1	3	703	G
1	3	720	C
1	3	721	G
1	3	723	U
1	3	724	G
1	3	733	G
1	3	734	G
1	3	753	A
1	3	754	C
1	3	755	G
1	3	777	A
1	3	781	A
1	3	793	U
1	3	794	A
1	3	815	A
1	3	817	C
1	3	818	G
1	3	819	A
1	3	821	G
1	3	832	G
1	3	843	U
1	3	844	G
1	3	845	A
1	3	846	G
1	3	849	G
1	3	851	G
1	3	864	A
1	3	884	U
1	3	889	A
1	3	902	G
1	3	914	A
1	3	926	G
1	3	934	C
1	3	935	A
1	3	960	U

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Mol	Chain	Res	Type
1	3	961	U
1	3	966	G
1	3	969	A
1	3	971	G
1	3	975	A
1	3	976	G
1	3	977	A
1	3	983	A
1	3	991	U
1	3	992	U
1	3	993	G
1	3	1004	A
1	3	1020	G
1	3	1028	C
1	3	1031	C
1	3	1032	G
1	3	1033	G
1	3	1034	G
1	3	1053	G
1	3	1080	A
1	3	1081	A
1	3	1085	U
1	3	1094	G
1	3	1095	U
1	3	1099	G
1	3	1101	A
1	3	1130	A
1	3	1132	C
1	3	1133	G
1	3	1137	C
1	3	1138	G
1	3	1139	G
1	3	1140	C
1	3	1159	U
1	3	1160	G
1	3	1168	U
1	3	1171	A
1	3	1182	G
1	3	1184	G
1	3	1196	A
1	3	1199	U
1	3	1212	U

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Mol	Chain	Res	Type
1	3	1213	A
1	3	1214	C
1	3	1227	A
1	3	1228	C
1	3	1238	A
1	3	1257	A
1	3	1260	G
1	3	1261	A
1	3	1274	A
1	3	1275	A
1	3	1280	A
1	3	1282	C
1	3	1286	U
1	3	1287	A
1	3	1290	G
1	3	1300	G
1	3	1301	U
1	3	1305	G
1	3	1317	C
1	3	1331	G
1	3	1346	A
1	3	1353	G
1	3	1363	A
1	3	1370	G
1	3	1379	G
1	3	1381	U
1	3	1395	C
1	3	1398	A
1	3	1399	C
1	3	1419	G
1	3	1429	A
1	3	1432	G
1	3	1441	A
1	3	1446	A
1	3	1448	C
1	3	1452	C
1	3	1453	G
1	3	1487	G
1	3	1497	G
1	3	1499	A
1	3	1502	A
1	3	1503	A

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Mol	Chain	Res	Type
1	3	1506	U
1	3	1507	A
1	3	1517	G
1	3	1519	A
1	3	1529	G
1	3	1530	G
1	3	1534	A
1	3	1535	C
2	1	10	A
2	1	12	U
2	1	30	G
2	1	35	G
2	1	46	G
2	1	50	U
2	1	51	G
2	1	58	G
2	1	71	A
2	1	74	A
2	1	75	G
2	1	84	A
2	1	96	C
2	1	100	U
2	1	110	G
2	1	118	A
2	1	119	A
2	1	120	U
2	1	125	A
2	1	139	U
2	1	140	C
2	1	141	G
2	1	142	A
2	1	149	A
2	1	158	U
2	1	162	U
2	1	163	C
2	1	196	A
2	1	199	A
2	1	204	A
2	1	215	G
2	1	216	A
2	1	219	A
2	1	220	G

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Mol	Chain	Res	Type
2	1	221	A
2	1	222	A
2	1	228	C
2	1	229	C
2	1	230	G
2	1	241	A
2	1	248	G
2	1	252	G
2	1	255	A
2	1	265	A
2	1	266	G
2	1	276	U
2	1	277	G
2	1	281	C
2	1	284	U
2	1	285	G
2	1	294	A
2	1	311	A
2	1	322	A
2	1	323	C
2	1	329	G
2	1	330	A
2	1	334	C
2	1	345	A
2	1	346	A
2	1	353	C
2	1	361	G
2	1	362	A
2	1	371	A
2	1	372	G
2	1	383	C
2	1	386	G
2	1	387	U
2	1	395	U
2	1	396	G
2	1	403	U
2	1	404	A
2	1	405	U
2	1	406	G
2	1	411	G
2	1	412	A
2	1	424	G

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Mol	Chain	Res	Type
2	1	443	A
2	1	457	A
2	1	465	G
2	1	467	G
2	1	475	C
2	1	477	A
2	1	481	G
2	1	491	G
2	1	500	G
2	1	501	A
2	1	504	A
2	1	505	A
2	1	508	A
2	1	509	C
2	1	510	C
2	1	517	C
2	1	529	A
2	1	530	G
2	1	532	A
2	1	533	G
2	1	545	U
2	1	546	U
2	1	547	A
2	1	548	G
2	1	549	G
2	1	550	C
2	1	562	U
2	1	563	A
2	1	568	U
2	1	573	U
2	1	575	A
2	1	603	A
2	1	614	A
2	1	615	U
2	1	622	G
2	1	627	A
2	1	634	C
2	1	637	A
2	1	645	C
2	1	646	U
2	1	654	A
2	1	656	G

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Mol	Chain	Res	Type
2	1	670	A
2	1	685	A
2	1	686	U
2	1	695	G
2	1	714	U
2	1	730	A
2	1	747	C
2	1	764	A
2	1	765	C
2	1	775	G
2	1	776	G
2	1	782	A
2	1	784	G
2	1	785	G
2	1	789	A
2	1	800	A
2	1	805	G
2	1	812	C
2	1	819	A
2	1	827	U
2	1	828	U
2	1	830	G
2	1	845	A
2	1	846	U
2	1	847	U
2	1	858	G
2	1	859	G
2	1	866	A
2	1	869	G
2	1	878	A
2	1	887	U
2	1	891	G
2	1	896	A
2	1	897	C
2	1	907	G
2	1	910	A
2	1	932	U
2	1	941	A
2	1	946	C
2	1	958	U
2	1	961	C
2	1	973	A

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Mol	Chain	Res	Type
2	1	974	G
2	1	975	A
2	1	983	A
2	1	989	G
2	1	995	C
2	1	996	A
2	1	999	U
2	1	1003	G
2	1	1005	C
2	1	1012	U
2	1	1013	C
2	1	1021	A
2	1	1022	G
2	1	1023	U
2	1	1025	G
2	1	1026	G
2	1	1033	U
2	1	1040	A
2	1	1046	A
2	1	1047	G
2	1	1059	G
2	1	1060	U
2	1	1062	G
2	1	1063	G
2	1	1064	C
2	1	1065	U
2	1	1066	U
2	1	1067	A
2	1	1068	G
2	1	1069	A
2	1	1070	A
2	1	1071	G
2	1	1072	C
2	1	1073	A
2	1	1075	C
2	1	1076	C
2	1	1077	A
2	1	1078	U
2	1	1083	U
2	1	1084	A
2	1	1085	A
2	1	1087	G

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Mol	Chain	Res	Type
2	1	1088	A
2	1	1089	A
2	1	1090	A
2	1	1091	G
2	1	1101	U
2	1	1103	A
2	1	1104	C
2	1	1111	A
2	1	1112	G
2	1	1130	U
2	1	1131	G
2	1	1132	U
2	1	1134	A
2	1	1135	C
2	1	1139	G
2	1	1142	A
2	1	1155	A
2	1	1172	C
2	1	1173	U
2	1	1174	U
2	1	1175	A
2	1	1176	U
2	1	1177	G
2	1	1178	C
2	1	1180	U
2	1	1186	G
2	1	1204	A
2	1	1206	G
2	1	1211	C
2	1	1212	G
2	1	1236	G
2	1	1247	A
2	1	1248	G
2	1	1253	A
2	1	1255	U
2	1	1256	G
2	1	1265	A
2	1	1271	G
2	1	1272	A
2	1	1275	A
2	1	1300	G
2	1	1301	A

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Mol	Chain	Res	Type
2	1	1345	C
2	1	1352	U
2	1	1359	A
2	1	1365	A
2	1	1368	G
2	1	1376	C
2	1	1379	U
2	1	1383	A
2	1	1395	A
2	1	1414	C
2	1	1416	G
2	1	1419	A
2	1	1420	A
2	1	1421	G
2	1	1427	A
2	1	1428	C
2	1	1434	A
2	1	1437	C
2	1	1452	G
2	1	1454	C
2	1	1458	U
2	1	1461	C
2	1	1478	G
2	1	1482	G
2	1	1490	A
2	1	1491	G
2	1	1504	A
2	1	1508	A
2	1	1515	A
2	1	1522	A
2	1	1524	G
2	1	1532	A
2	1	1533	C
2	1	1535	A
2	1	1536	C
2	1	1537	G
2	1	1554	U
2	1	1555	G
2	1	1558	C
2	1	1559	U
2	1	1560	G
2	1	1566	A

Continued on next page...

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Mol	Chain	Res	Type
2	1	1569	A
2	1	1578	U
2	1	1584	U
2	1	1608	A
2	1	1627	G
2	1	1634	A
2	1	1639	C
2	1	1647	U
2	1	1648	U
2	1	1649	G
2	1	1654	A
2	1	1669	A
2	1	1672	A
2	1	1674	G
2	1	1675	C
2	1	1694	C
2	1	1698	A
2	1	1715	G
2	1	1716	U
2	1	1729	U
2	1	1730	C
2	1	1738	G
2	1	1744	A
2	1	1757	A
2	1	1758	U
2	1	1764	C
2	1	1773	A
2	1	1776	G
2	1	1780	A
2	1	1781	U
2	1	1786	A
2	1	1800	C
2	1	1801	A
2	1	1808	A
2	1	1816	C
2	1	1819	A
2	1	1829	A
2	1	1848	A
2	1	1857	G
2	1	1870	C
2	1	1873	G
2	1	1884	G

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Mol	Chain	Res	Type
2	1	1901	A
2	1	1903	G
2	1	1906	G
2	1	1913	A
2	1	1914	C
2	1	1915	U
2	1	1927	A
2	1	1929	G
2	1	1930	G
2	1	1936	A
2	1	1937	A
2	1	1938	A
2	1	1939	U
2	1	1943	U
2	1	1944	U
2	1	1955	U
2	1	1966	A
2	1	1967	C
2	1	1970	A
2	1	1971	U
2	1	1972	G
2	1	1980	G
2	1	1981	A
2	1	1991	U
2	1	1992	G
2	1	1993	U
2	1	1996	C
2	1	1997	C
2	1	2020	A
2	1	2022	U
2	1	2023	C
2	1	2030	A
2	1	2031	A
2	1	2033	A
2	1	2043	C
2	1	2049	G
2	1	2052	A
2	1	2055	C
2	1	2056	G
2	1	2060	A
2	1	2061	G
2	1	2062	A

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Mol	Chain	Res	Type
2	1	2069	G
2	1	2076	U
2	1	2093	G
2	1	2096	C
2	1	2100	G
2	1	2110	G
2	1	2111	U
2	1	2115	G
2	1	2116	G
2	1	2118	U
2	1	2119	A
2	1	2123	G
2	1	2128	G
2	1	2129	C
2	1	2131	U
2	1	2132	U
2	1	2133	G
2	1	2134	A
2	1	2137	U
2	1	2141	G
2	1	2145	C
2	1	2146	C
2	1	2147	A
2	1	2149	U
2	1	2154	A
2	1	2157	G
2	1	2160	C
2	1	2162	G
2	1	2164	C
2	1	2166	U
2	1	2172	U
2	1	2173	A
2	1	2174	C
2	1	2189	U
2	1	2192	U
2	1	2198	A
2	1	2203	U
2	1	2204	G
2	1	2211	A
2	1	2225	A
2	1	2226	C
2	1	2238	G

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Mol	Chain	Res	Type
2	1	2239	G
2	1	2243	U
2	1	2250	G
2	1	2279	G
2	1	2283	C
2	1	2287	A
2	1	2288	A
2	1	2297	A
2	1	2305	U
2	1	2309	A
2	1	2325	G
2	1	2327	A
2	1	2331	G
2	1	2333	A
2	1	2334	U
2	1	2336	A
2	1	2345	G
2	1	2350	C
2	1	2361	G
2	1	2383	G
2	1	2385	C
2	1	2402	U
2	1	2403	C
2	1	2406	A
2	1	2407	A
2	1	2423	U
2	1	2429	G
2	1	2430	A
2	1	2441	U
2	1	2445	G
2	1	2448	A
2	1	2470	G
2	1	2474	U
2	1	2476	A
2	1	2480	C
2	1	2492	U
2	1	2502	G
2	1	2503	A
2	1	2505	G
2	1	2518	A
2	1	2520	C
2	1	2529	G

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Mol	Chain	Res	Type
2	1	2547	A
2	1	2554	U
2	1	2564	A
2	1	2565	A
2	1	2566	A
2	1	2567	G
2	1	2572	A
2	1	2573	C
2	1	2586	U
2	1	2602	A
2	1	2609	U
2	1	2613	U
2	1	2615	U
2	1	2629	U
2	1	2630	G
2	1	2646	C
2	1	2661	G
2	1	2689	U
2	1	2690	U
2	1	2714	G
2	1	2716	C
2	1	2726	A
2	1	2732	G
2	1	2733	A
2	1	2744	G
2	1	2748	A
2	1	2764	A
2	1	2765	A
2	1	2766	A
2	1	2778	A
2	1	2791	G
2	1	2794	C
2	1	2797	U
2	1	2798	U
2	1	2799	A
2	1	2800	A
2	1	2808	G
2	1	2809	A
2	1	2818	U
2	1	2820	A
2	1	2823	A
2	1	2833	U

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Mol	Chain	Res	Type
2	1	2835	A
2	1	2859	G
2	1	2861	U
2	1	2867	G
2	1	2868	A
2	1	2872	A
2	1	2873	A
2	1	2880	C
2	1	2884	U
2	1	2887	A
2	1	2891	U
2	1	2902	C
3	2	4	C
3	2	12	C
3	2	13	G
3	2	15	A
3	2	24	G
3	2	26	C
3	2	31	C
3	2	35	C
3	2	40	U
3	2	44	G
3	2	67	G
3	2	87	U
3	2	88	C
3	2	89	U
3	2	90	C
3	2	108	A
3	2	109	A
4	6	4	G
4	6	8	U
4	6	9	G
4	6	14	A
4	6	16	C
4	6	17	C
4	6	17(A)	U
4	6	18	G
4	6	19	G
4	6	20	U
4	6	21	A
4	6	22	G
4	6	28	C

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Mol	Chain	Res	Type
4	6	35	A
4	6	46	G
4	6	47	U
4	6	52	G
4	6	63	G
4	6	64	G
4	6	69	C
4	6	72	A
4	6	75	C
4	6	76	A
37	4	9	G
37	4	10	G
37	4	11	U
37	4	12	A
37	4	13	A
37	4	14	A
37	4	15	A
37	4	16	A
38	5	3	G
38	5	4	C
38	5	5	G
38	5	10	G
38	5	17	U
38	5	19	G
38	5	20	U
38	5	21	A
38	5	22	G
38	5	41	A
38	5	42	G
38	5	46	G
38	5	47	U
38	5	48	C
38	5	49	G
38	5	62	C
38	5	65	U
38	5	73	A
38	5	76	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3	1256	A

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Mol	Chain	Res	Type
2	1	464	U
2	1	490	C
2	1	784	G
2	1	858	G
2	1	1020	A
2	1	1715	G
2	1	1847	A
2	1	2326	C
2	1	2406	A
2	1	2572	A
2	1	2808	G
3	2	3	C
3	2	66	A
3	2	88	C
37	4	12	A
37	4	13	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

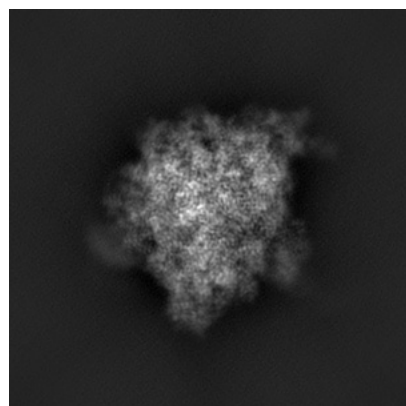
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25418. These allow visual inspection of the internal detail of the map and identification of artifacts.

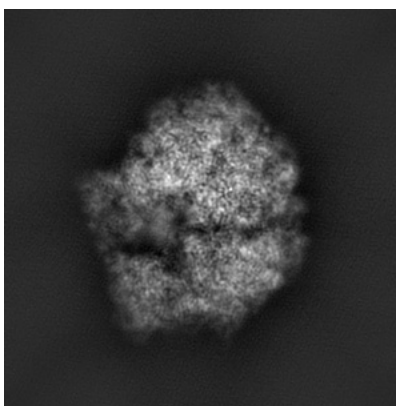
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

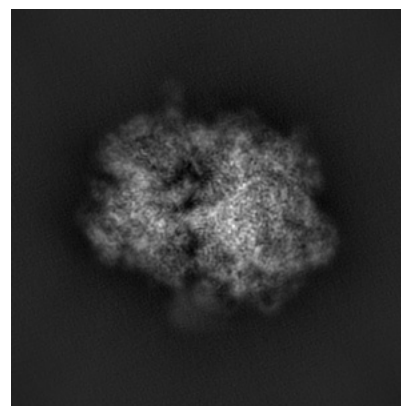
6.1.1 Primary map



X

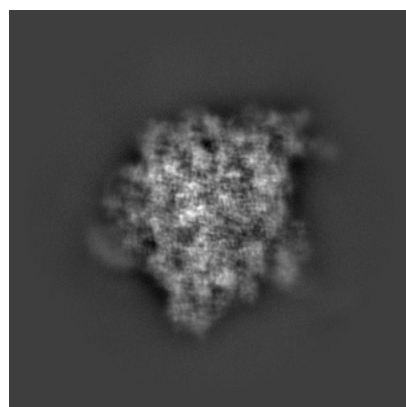


Y

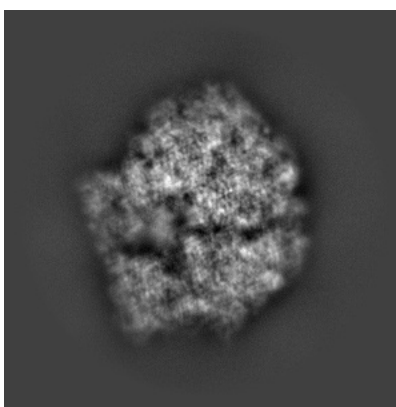


Z

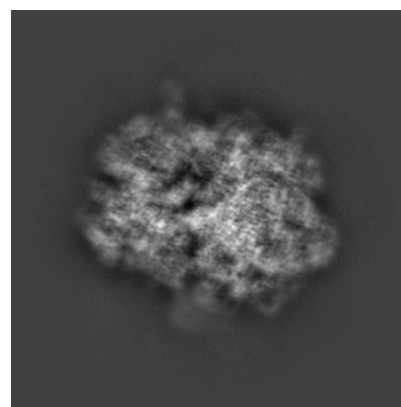
6.1.2 Raw map



X



Y

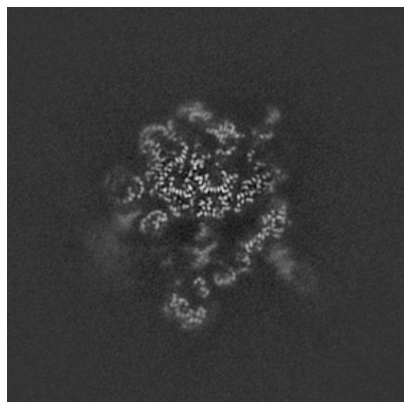


Z

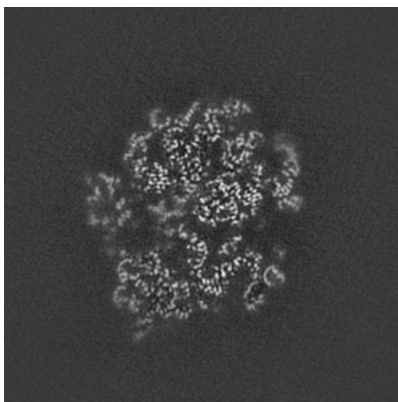
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

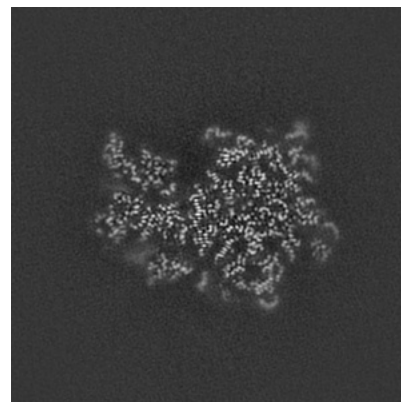
6.2.1 Primary map



X Index: 224

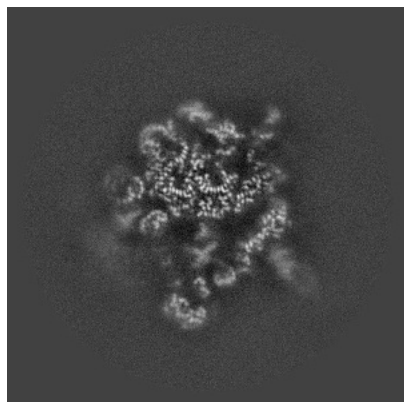


Y Index: 224

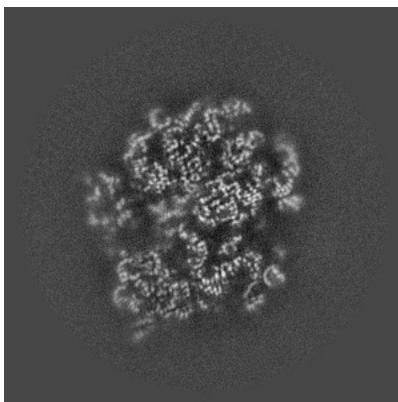


Z Index: 224

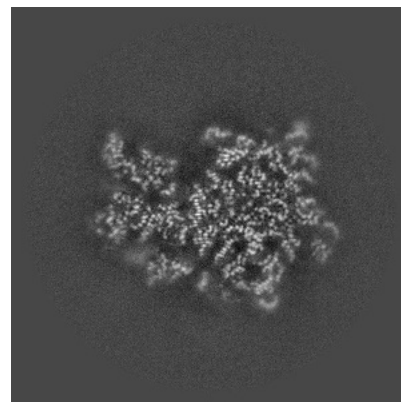
6.2.2 Raw map



X Index: 224



Y Index: 224

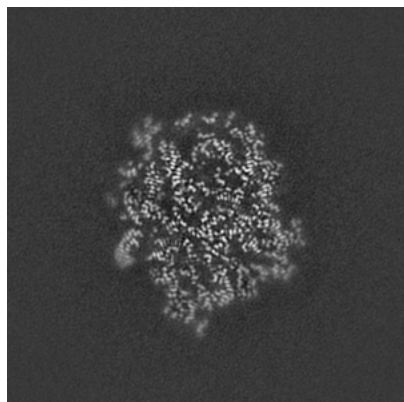


Z Index: 224

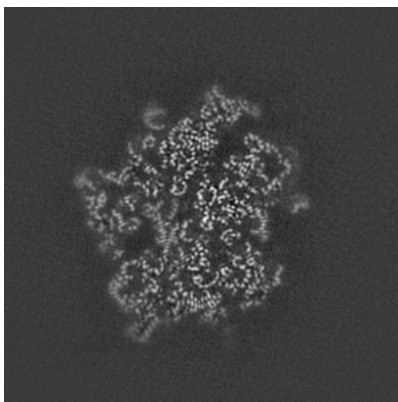
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

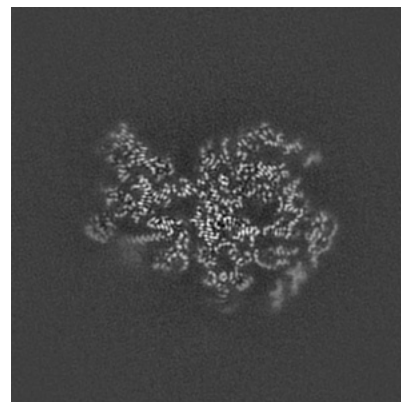
6.3.1 Primary map



X Index: 254

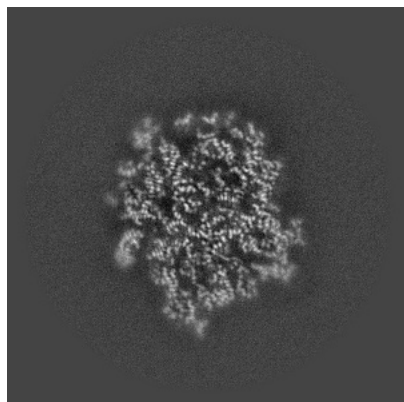


Y Index: 215

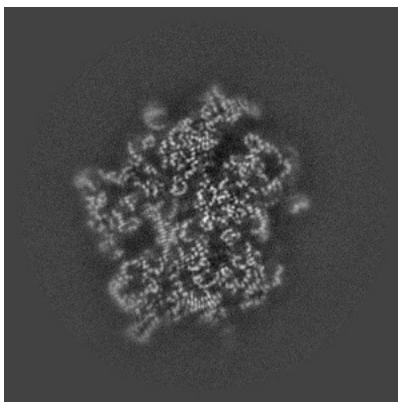


Z Index: 240

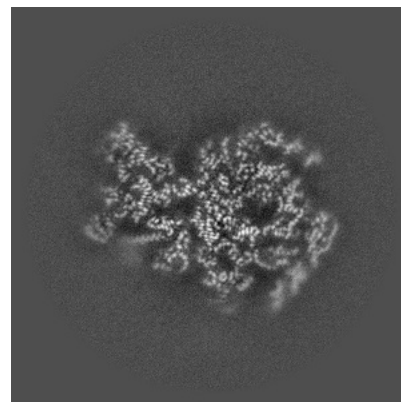
6.3.2 Raw map



X Index: 253



Y Index: 215

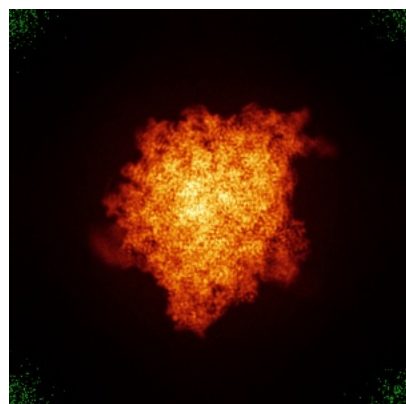


Z Index: 240

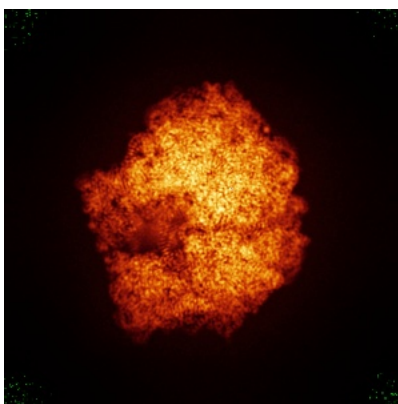
The images above show the largest variance slices of the map in three orthogonal directions.

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

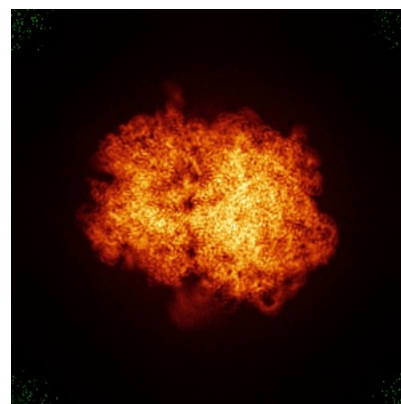
6.4.1 Primary map



X

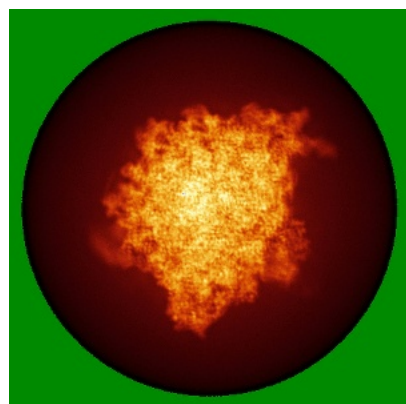


Y

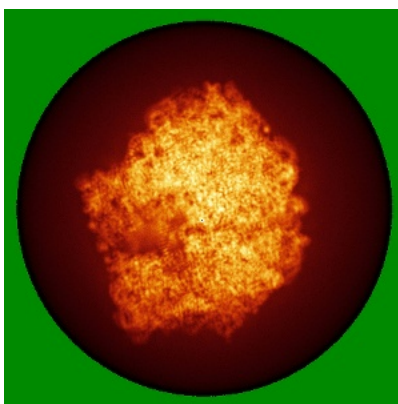


Z

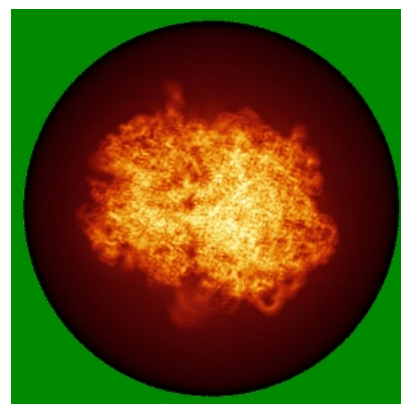
6.4.2 Raw map



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 1.35. 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.

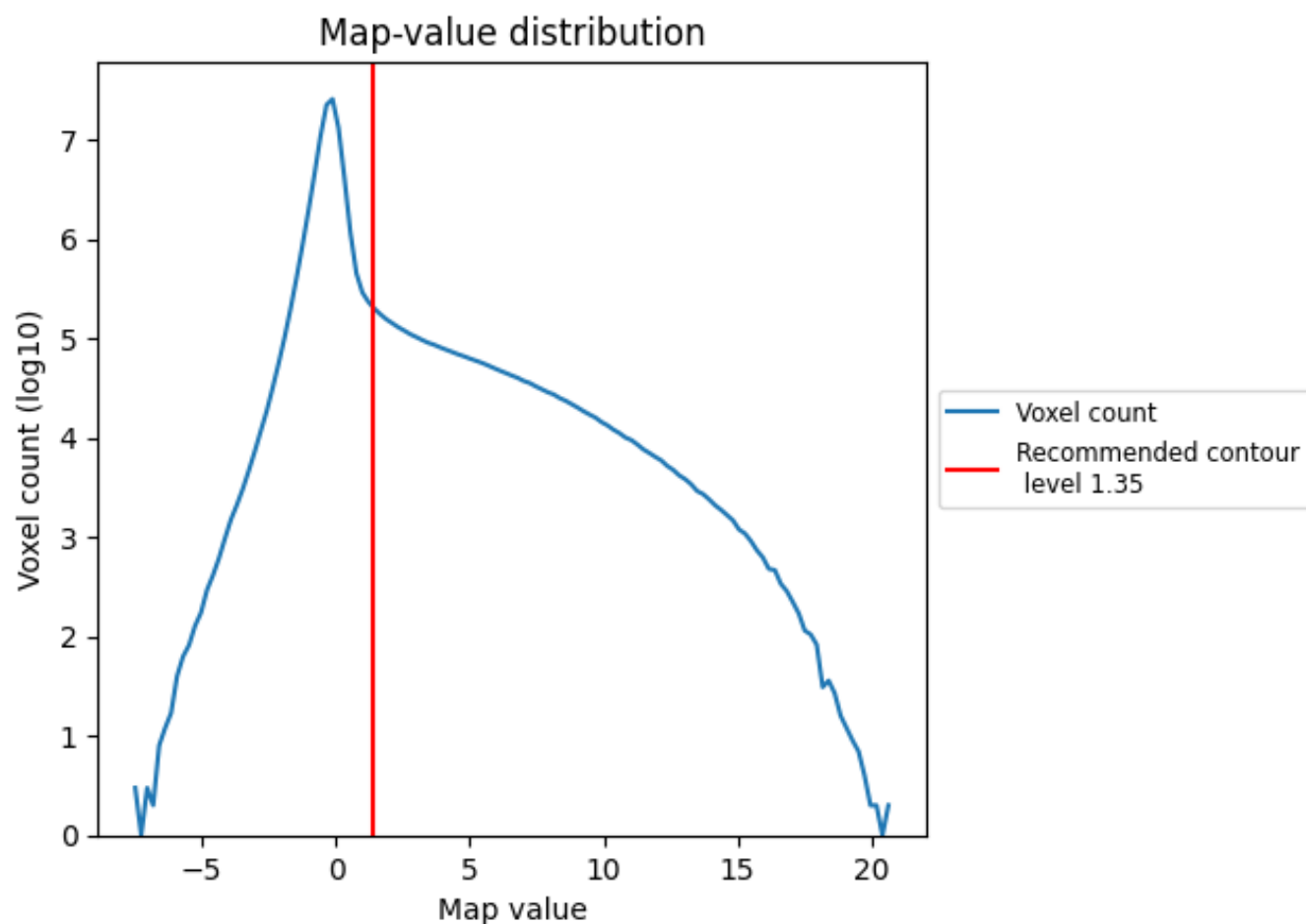
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

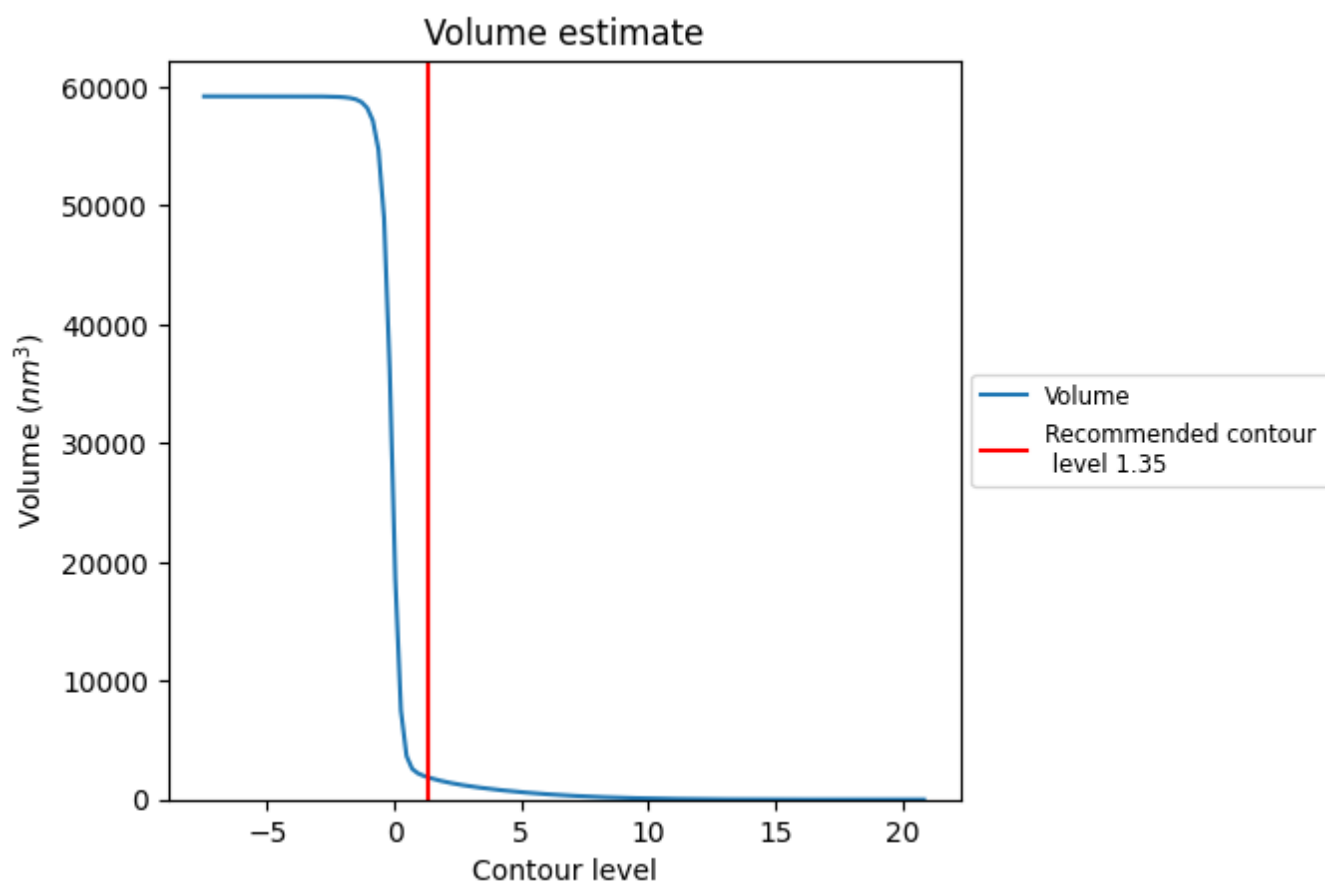
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

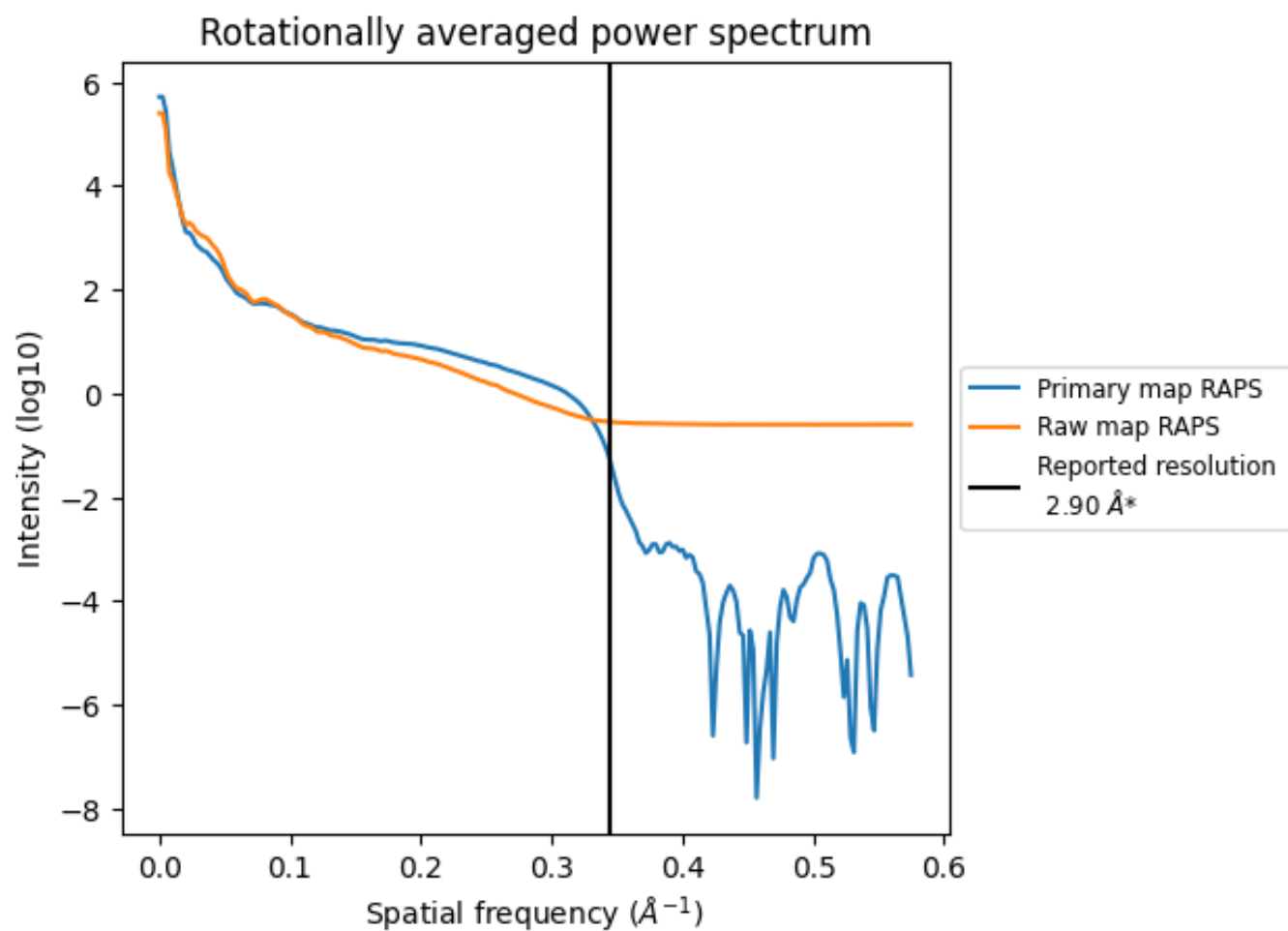
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1857 nm³; this corresponds to an approximate mass of 1677 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 ⓘ

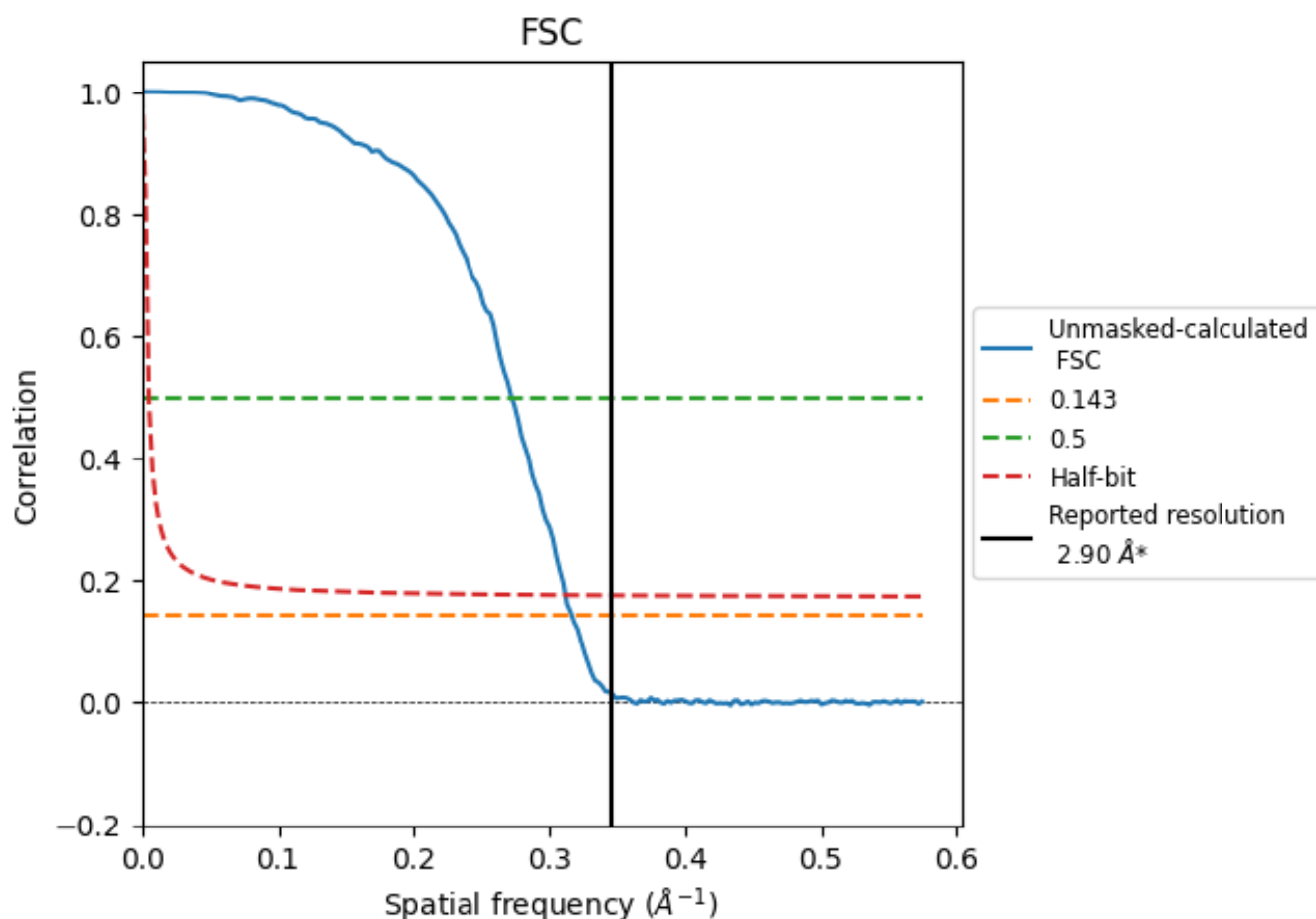


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

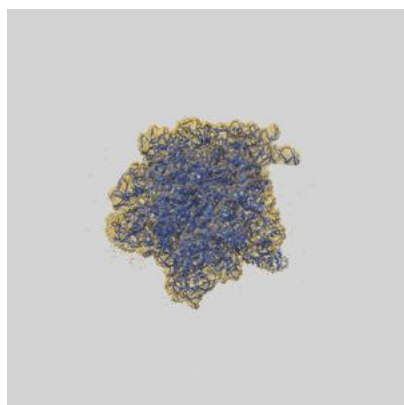
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	3.67	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

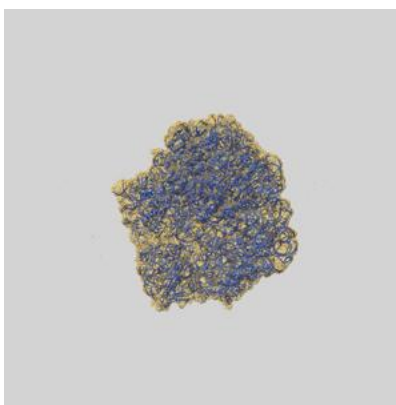
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25418 and PDB model 7ST2. Per-residue inclusion information can be found in section [3](#) on page [15](#).

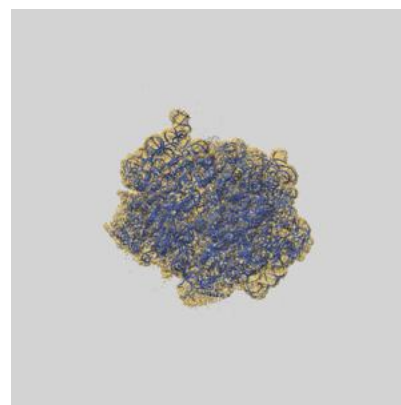
9.1 Map-model overlay [i](#)



X



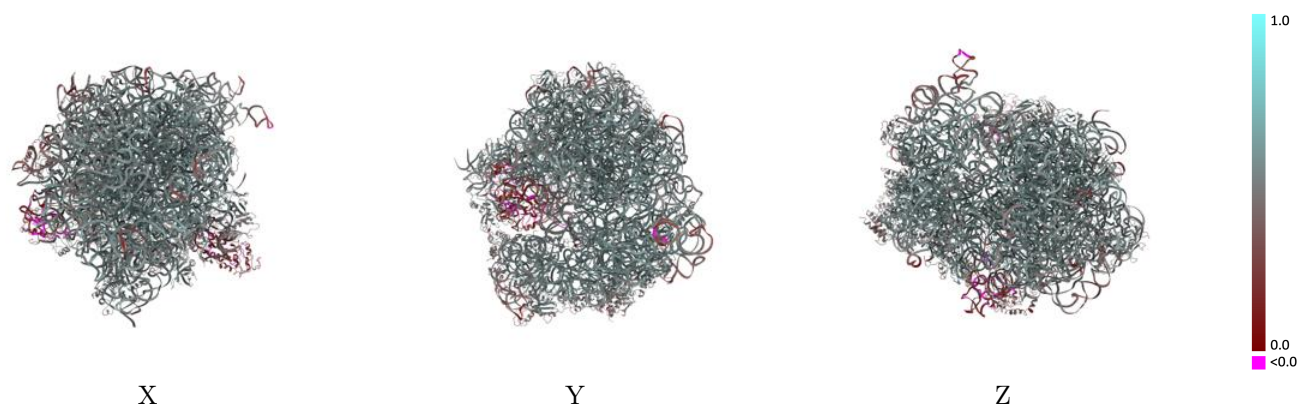
Y



Z

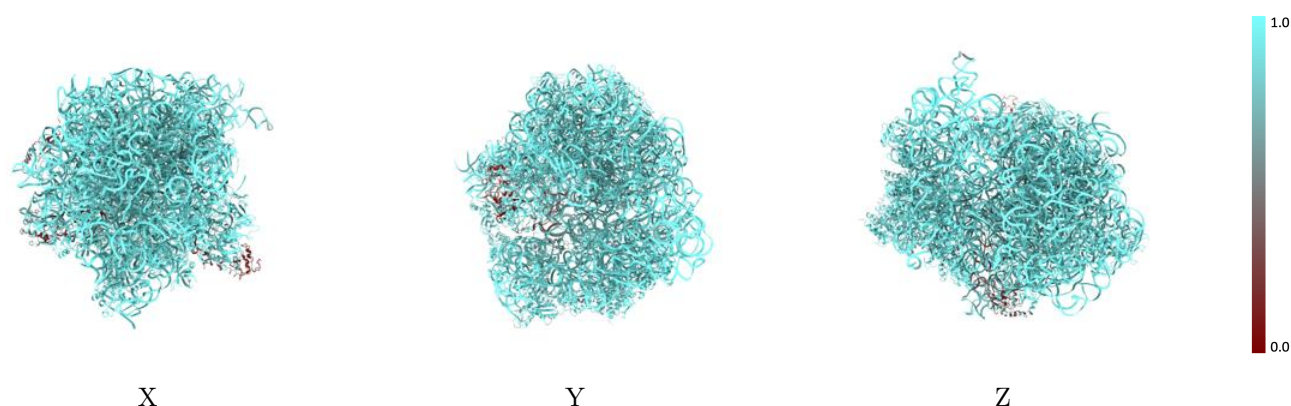
The images above show the 3D surface view of the map at the recommended contour level 1.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



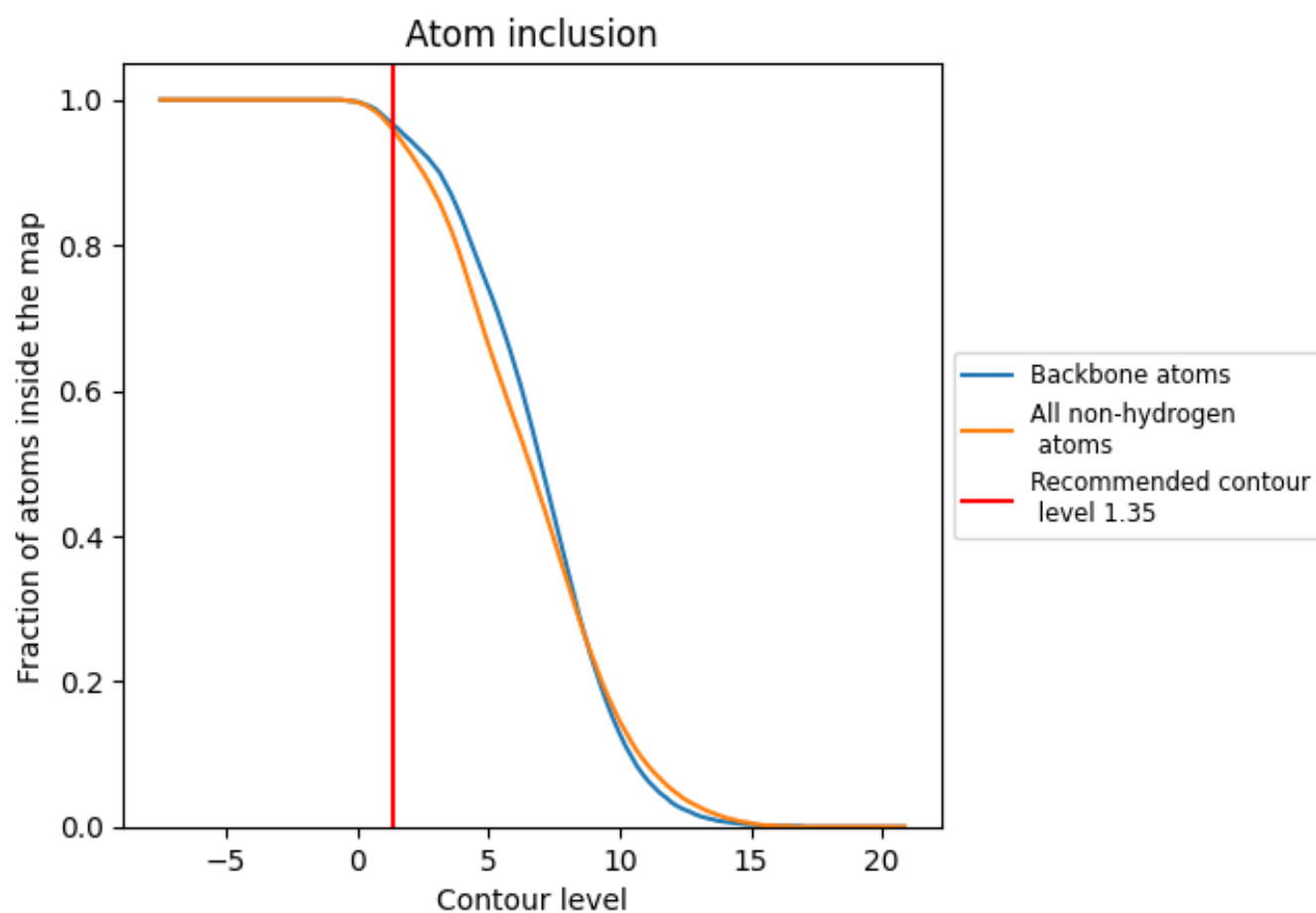
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.35).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.5090
1	 0.9890	 0.5190
2	 0.9980	 0.5200
3	 0.9960	 0.5350
4	 0.9180	 0.3070
5	 0.9950	 0.5100
6	 0.2760	 0.3070
A	 0.9350	 0.4240
B	 0.9720	 0.5370
C	 0.8460	 0.5230
D	 0.9660	 0.5560
E	 0.9780	 0.5670
F	 0.9760	 0.5480
G	 0.9060	 0.4560
H	 0.9510	 0.5190
I	 0.9400	 0.4730
J	 0.9630	 0.5320
K	 0.9670	 0.4820
L	 0.9350	 0.4770
M	 0.9570	 0.5330
N	 0.9510	 0.4870
O	 0.8960	 0.4650
P	 0.9700	 0.5140
Q	 0.9610	 0.5400
R	 0.9450	 0.4810
S	 0.9610	 0.5030
T	 0.9780	 0.5110
U	 0.9590	 0.5080
V	 0.9510	 0.5190
W	 0.9710	 0.4950
X	 0.9610	 0.4840
Y	 0.9460	 0.4990
Z	 0.8570	 0.3510
a	 0.4660	 0.1910
b	 0.9780	 0.5630



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Chain	Atom inclusion	Q-score
c	 0.9810	 0.5460
d	 0.9460	 0.5040
e	 0.9630	 0.4860
f	 0.9750	 0.4860
g	 0.5350	 0.3510
h	 0.3520	 0.1820
i	 0.6260	 0.1690
j	 0.9660	 0.5350
k	 0.9640	 0.5480
l	 0.9660	 0.5270
m	 0.9760	 0.5510
n	 0.9740	 0.5410
o	 0.9770	 0.5040
p	 0.9640	 0.5470
q	 0.9790	 0.5390
r	 0.9650	 0.5250
s	 0.9590	 0.5240
t	 0.9520	 0.5040
u	 0.9670	 0.4890
v	 0.9590	 0.5190
w	 0.9710	 0.5540
x	 0.9670	 0.5340
y	 0.9480	 0.4370
z	 0.9540	 0.5270